



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:20 PM GMT

PDB ID : 1T87  
Title : Crystal Structure of the Ferrous CO-bound Cytochrome P450cam (C334A)  
Authors : Nagano, S.; Tosha, T.; Ishimori, K.; Morishima, I.; Poulos, T.L.  
Deposited on : 2004-05-11  
Resolution : 1.80 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](mailto: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.

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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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CAM	A	1422	-	-	-	X
5	CAM	B	2422	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7174 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	407	Total	C	N	O	S	0	2	0
			3235	2048	565	605	17			
1	B	405	Total	C	N	O	S	0	0	0
			3207	2033	560	597	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	334	ALA	CYS	ENGINEERED	UNP P00183
B	334	ALA	CYS	ENGINEERED	UNP P00183

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

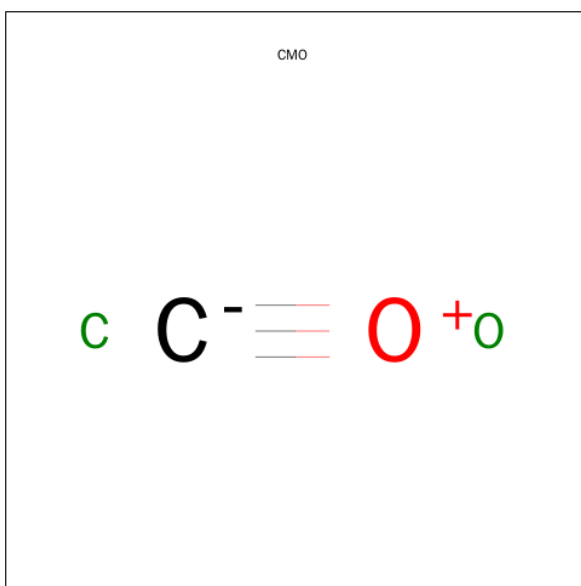
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	K	0	0
			1	1		
2	A	2	Total	K	0	0
			2	2		

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



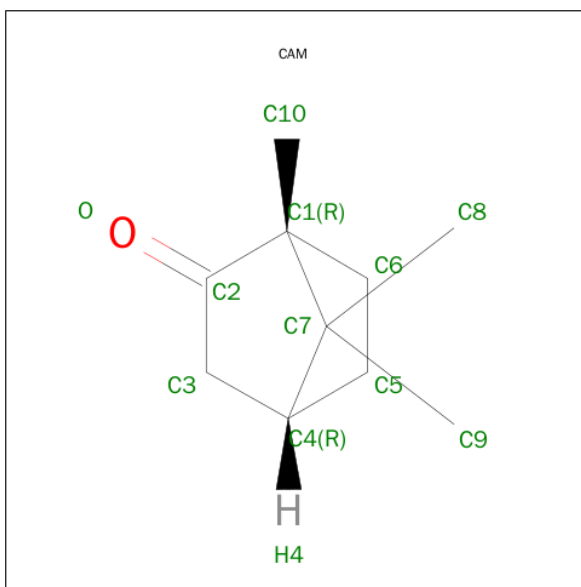
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



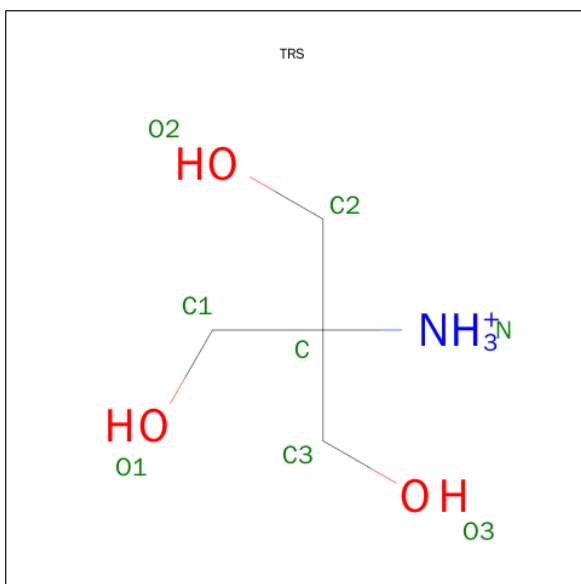
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			2	1	1		

- Molecule 5 is CAMPHOR (three-letter code: CAM) (formula: C<sub>10</sub>H<sub>16</sub>O).



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

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			8	4	1	3		

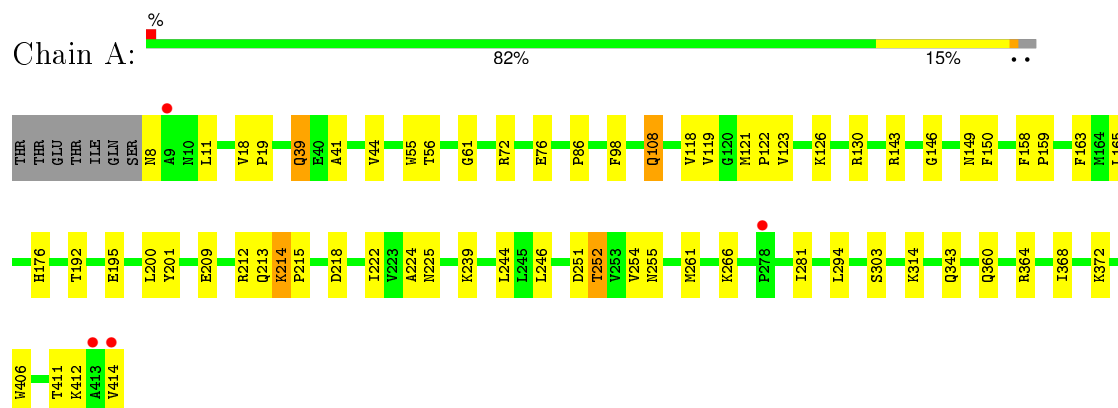
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	350	Total 350	O 350	0	2
7	B	261	Total 261	O 261	0	0

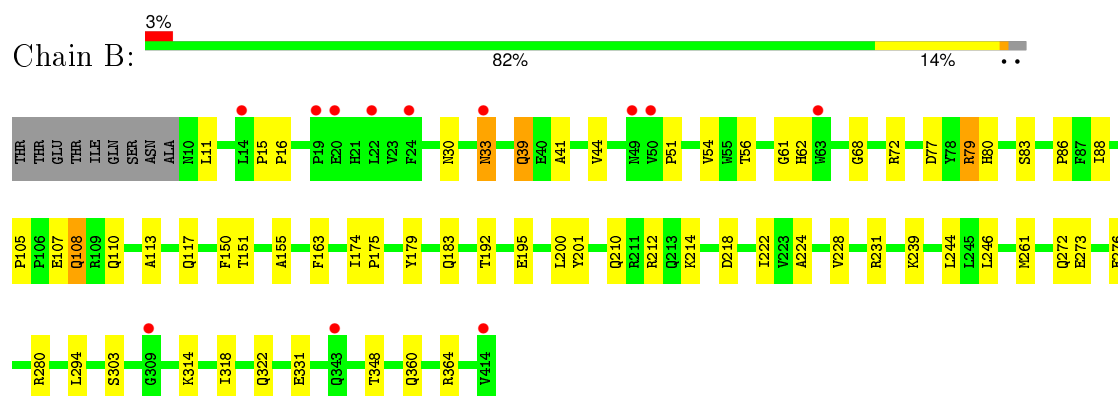
### 3 Residue-property plots

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.

#### • Molecule 1: Cytochrome P450-cam



#### • Molecule 1: Cytochrome P450-cam





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.03Å 62.23Å 94.92Å 90.00° 90.48° 90.00°	Depositor
Resolution (Å)	45.60 – 1.80 45.61 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.60-1.80) 99.1 (45.61-1.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.15 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.185 , 0.207 0.183 , 0.205	Depositor DCC
$R_{free}$ test set	3672 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 48.7	EDS
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 72430 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7174	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: CMO, HEM, K, TRS, 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	0.30	0/3314	0.60	1/4503 (0.0%)
1	B	0.29	0/3286	0.56	0/4464
All	All	0.29	0/6600	0.58	1/8967 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	ASN	N-CA-C	-5.11	97.19	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	3235	0	3177	45	0
1	B	3207	0	3156	47	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	43	0	30	2	0
3	B	43	0	30	0	0
4	B	2	0	0	1	0
5	A	11	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	11	0	16	2	0
6	B	8	0	12	0	0
7	A	350	0	0	5	0
7	B	261	0	0	0	0
All	All	7174	0	6437	94	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 7.

All (94) 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:130:ARG:HD2	1:A:165:LEU:HD21	1.56	0.87
1:A:360:GLN:HE21	1:A:364:ARG:HH22	1.26	0.84
1:A:368:ILE:HG22	1:A:372:LYS:HE2	1.61	0.81
1:B:360:GLN:HE21	1:B:364:ARG:HH22	1.29	0.79
1:A:163:PHE:HE2	1:A:246:LEU:HD23	1.51	0.74
1:B:200:LEU:HD11	1:B:246:LEU:HD13	1.69	0.72
1:A:123:VAL:O	1:A:126:LYS:HG2	1.89	0.72
1:B:113:ALA:O	1:B:117:GLN:HG3	1.94	0.67
1:B:51:PRO:HG2	1:B:54:VAL:HG12	1.78	0.66
1:B:68:GLY:HA3	1:B:331:GLU:OE2	1.95	0.66
1:A:163:PHE:CE2	1:A:246:LEU:HD23	2.33	0.63
1:B:105:PRO:HG3	1:B:108:GLN:NE2	2.14	0.62
1:B:72:ARG:HH12	1:B:331:GLU:CD	2.02	0.62
1:A:213:GLN:HB2	1:A:214:LYS:HD3	1.82	0.62
1:A:201:TYR:HB3	1:A:239:LYS:HD2	1.83	0.61
1:B:163:PHE:HE2	1:B:246:LEU:HD23	1.65	0.60
1:A:150:PHE:CZ	1:A:261:MET:HG3	2.35	0.60
1:A:123:VAL:HG13	1:A:126:LYS:HE2	1.84	0.59
1:B:294:LEU:H	1:B:294:LEU:HD23	1.69	0.58
1:A:294:LEU:H	1:A:294:LEU:HD23	1.69	0.57
1:A:281:ILE:HD12	1:A:372:LYS:HG2	1.86	0.56
1:B:210:GLN:HE22	1:B:214:LYS:HD2	1.71	0.56
1:A:411:THR:O	1:A:412:LYS:HD3	2.06	0.55
1:A:251[B]:ASP:O	1:A:255:ASN:ND2	2.39	0.55
1:A:212:ARG:HG3	1:A:224:ALA:HB1	1.89	0.55
1:A:218:ASP:O	1:A:222:ILE:HG12	2.07	0.54
1:B:41:ALA:O	1:B:44:VAL:HG22	2.08	0.54
1:B:79:ARG:HG3	1:B:79:ARG:HH11	1.73	0.54
1:B:83:SER:O	1:B:86:PRO:HD3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1417:HEM:HBB2	3:A:1417:HEM:HMB1	1.90	0.54
1:B:244:LEU:HD11	5:B:2422:CAM:H51	1.91	0.53
1:B:303:SER:HA	1:B:314:LYS:HB2	1.90	0.53
1:B:360:GLN:NE2	1:B:364:ARG:HH22	2.05	0.52
1:A:200:LEU:HD11	1:A:246:LEU:HD13	1.90	0.52
1:B:62:HIS:CD2	1:B:88:ILE:HD13	2.44	0.52
1:B:77:ASP:OD2	1:B:80:HIS:HD2	1.92	0.52
1:B:294:LEU:N	1:B:294:LEU:HD23	2.24	0.51
1:B:56:THR:O	1:B:61:GLY:HA2	2.10	0.51
1:B:201:TYR:HB3	1:B:239:LYS:HD2	1.92	0.51
1:B:192:THR:OG1	1:B:195:GLU:HG3	2.09	0.51
1:A:212:ARG:HA	1:A:225:ASN:HD21	1.76	0.51
1:A:72:ARG:O	1:A:76:GLU:HG3	2.11	0.50
1:A:294:LEU:N	1:A:294:LEU:HD23	2.25	0.50
1:A:254:VAL:HG23	7:A:1833:HOH:O	2.11	0.50
1:B:212:ARG:HG3	1:B:224:ALA:HB1	1.92	0.50
1:B:62:HIS:CG	1:B:88:ILE:HD13	2.46	0.50
1:A:266:LYS:HD2	7:A:1879:HOH:O	2.11	0.50
1:B:11:LEU:N	1:B:11:LEU:HD22	2.26	0.49
1:A:252[B]:THR:HG23	7:A:1717[B]:HOH:O	2.12	0.49
1:B:150:PHE:CZ	1:B:261:MET:HG3	2.47	0.49
1:A:158:PHE:HB3	1:A:159:PRO:CD	2.43	0.48
1:B:272:GLN:O	1:B:276:GLU:HG3	2.13	0.48
1:B:163:PHE:CE2	1:B:246:LEU:HD23	2.48	0.48
1:B:33:ASN:HB3	1:B:41:ALA:HA	1.96	0.47
1:B:51:PRO:HG2	1:B:54:VAL:CG1	2.43	0.47
1:A:98:PHE:HB3	1:A:244:LEU:HB2	1.97	0.47
1:A:118:VAL:HG23	1:A:119:VAL:HG13	1.95	0.47
1:A:121:MET:HB3	1:A:122:PRO:HD3	1.97	0.47
1:A:176:HIS:HE1	7:A:1753:HOH:O	1.98	0.47
1:B:179:TYR:O	1:B:183:GLN:HG2	2.15	0.47
4:B:2420:CMO:C	5:B:2422:CAM:H52	2.45	0.46
1:A:192:THR:OG1	1:A:195:GLU:HG3	2.15	0.46
1:A:214:LYS:HD3	1:A:214:LYS:N	2.31	0.46
1:A:303:SER:HA	1:A:314:LYS:HB2	1.97	0.46
1:A:159:PRO:HG2	1:A:254:VAL:HG22	1.97	0.46
1:A:19:PRO:HD3	7:A:1767:HOH:O	2.15	0.46
1:B:108:GLN:HB3	1:B:108:GLN:HE21	1.54	0.45
1:A:56:THR:O	1:A:61:GLY:HA2	2.16	0.45
1:A:39:GLN:NE2	1:A:39:GLN:H	2.15	0.45
1:A:18:VAL:HG11	1:A:55:TRP:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:GLU:OE1	1:B:280:ARG:NH2	2.49	0.44
1:B:228:VAL:O	1:B:228:VAL:HG23	2.17	0.43
1:A:41:ALA:O	1:A:44:VAL:HG22	2.18	0.43
1:A:146:GLY:HA2	1:A:406:TRP:CD1	2.53	0.43
1:B:39:GLN:NE2	1:B:39:GLN:H	2.16	0.43
1:A:8:ASN:HB3	1:A:11:LEU:HG	2.00	0.43
1:A:108:GLN:HE21	1:A:108:GLN:HB3	1.66	0.43
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.83	0.43
1:A:209:GLU:O	1:A:213:GLN:HG2	2.19	0.42
1:A:215:PRO:HB3	1:A:225:ASN:OD1	2.19	0.42
1:B:218:ASP:O	1:B:222:ILE:HG12	2.19	0.42
1:B:318:ILE:HG23	1:B:318:ILE:O	2.20	0.42
1:B:151:THR:HA	1:B:155:ALA:HB3	2.02	0.41
1:B:174:ILE:HB	1:B:175:PRO:HD3	2.02	0.41
1:B:79:ARG:NH1	1:B:79:ARG:HG3	2.35	0.41
1:B:107:GLU:O	1:B:110:GLN:HG2	2.20	0.41
1:B:294:LEU:N	1:B:294:LEU:CD2	2.82	0.41
1:B:228:VAL:HG21	1:B:231:ARG:CZ	2.50	0.41
1:A:414:VAL:O	1:A:414:VAL:HG12	2.21	0.41
1:B:239:LYS:HE2	1:B:239:LYS:HB3	1.95	0.40
1:B:15:PRO:HA	1:B:16:PRO:HD3	1.93	0.40
1:A:244:LEU:HD21	3:A:1417:HEM:HAD1	2.03	0.40
1:B:273:GLU:OE1	1:B:280:ARG:CZ	2.70	0.40
1:B:322:GLN:HB3	1:B:348:THR:O	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	407/414 (98%)	391 (96%)	14 (3%)	2 (0%)	34 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	403/414 (97%)	391 (97%)	12 (3%)	0	100	100
All	All	810/828 (98%)	782 (96%)	26 (3%)	2 (0%)	56	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252[A]	THR
1	A	252[B]	THR

### 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	352/357 (99%)	347 (99%)	5 (1%)	74	65
1	B	349/357 (98%)	344 (99%)	5 (1%)	74	65
All	All	701/714 (98%)	691 (99%)	10 (1%)	74	65

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	86	PRO
1	A	108	GLN
1	A	214	LYS
1	A	343	GLN
1	B	30	ASN
1	B	33	ASN
1	B	39	GLN
1	B	79	ARG
1	B	108	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	46	GLN
1	A	69	GLN
1	A	108	GLN
1	A	110	GLN
1	A	117	GLN
1	A	132	GLN
1	A	145	GLN
1	A	149	ASN
1	A	176	HIS
1	A	210	GLN
1	A	225	ASN
1	A	229	ASN
1	A	272	GLN
1	A	343	GLN
1	A	360	GLN
1	B	30	ASN
1	B	33	ASN
1	B	39	GLN
1	B	46	GLN
1	B	80	HIS
1	B	108	GLN
1	B	110	GLN
1	B	117	GLN
1	B	129	ASN
1	B	132	GLN
1	B	145	GLN
1	B	210	GLN
1	B	343	GLN
1	B	360	GLN
1	B	388	GLN
1	B	390	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

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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$
3	HEM	A	1417	1	30,50,50	2.63	9 (30%)	24,82,82	2.23	8 (33%)
5	CAM	A	1422	-	12,12,12	1.99	4 (33%)	21,21,21	1.84	5 (23%)
3	HEM	B	2417	1,4	30,50,50	2.83	11 (36%)	24,82,82	2.24	9 (37%)
4	CMO	B	2420	3	0,1,1	0.00	-	0,0,0	0.00	-
5	CAM	B	2422	-	12,12,12	1.94	4 (33%)	21,21,21	1.83	5 (23%)
6	TRS	B	2430	-	7,7,7	2.18	4 (57%)	9,9,9	3.12	5 (55%)

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
3	HEM	A	1417	1	-	0/10/54/54	0/0/8/8
5	CAM	A	1422	-	-	0/0/31/31	0/0/2/2
3	HEM	B	2417	1,4	-	0/10/54/54	0/0/8/8
4	CMO	B	2420	3	-	0/0/0/0	0/0/0/0
5	CAM	B	2422	-	-	0/0/31/31	0/0/2/2
6	TRS	B	2430	-	-	0/9/9/9	0/0/0/0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2417	HEM	C3C-CAC	-6.62	1.38	1.51
3	B	2417	HEM	C3B-C4B	-6.56	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1417	HEM	C2D-C3D	-5.96	1.36	1.54
3	A	1417	HEM	C3C-CAC	-5.96	1.40	1.51
3	B	2417	HEM	C2D-C3D	-5.87	1.36	1.54
3	B	2417	HEM	C3B-CAB	-5.77	1.40	1.51
3	A	1417	HEM	C3B-C4B	-5.68	1.46	1.51
3	A	1417	HEM	C3B-CAB	-5.15	1.41	1.51
3	B	2417	HEM	C3D-C4D	-5.12	1.45	1.51
3	A	1417	HEM	C3D-C4D	-4.96	1.45	1.51
3	B	2417	HEM	C2C-C1C	-4.01	1.45	1.52
3	A	1417	HEM	C2C-C1C	-3.50	1.45	1.52
3	A	1417	HEM	C2D-C1D	-2.25	1.44	1.51
3	B	2417	HEM	C2B-C1B	-2.10	1.45	1.51
3	B	2417	HEM	C2D-C1D	-2.06	1.45	1.51
6	B	2430	TRS	C1-C	2.16	1.57	1.53
3	B	2417	HEM	CHD-C4C	2.37	1.42	1.36
3	A	1417	HEM	C4C-NC	2.38	1.38	1.36
5	B	2422	CAM	C8-C7	2.50	1.61	1.53
3	B	2417	HEM	C1C-NC	2.66	1.39	1.36
5	B	2422	CAM	C3-C4	2.66	1.60	1.53
5	A	1422	CAM	C8-C7	2.69	1.61	1.53
5	A	1422	CAM	C3-C4	2.72	1.61	1.53
6	B	2430	TRS	O2-C2	2.75	1.51	1.42
6	B	2430	TRS	O1-C1	2.78	1.51	1.42
5	A	1422	CAM	C1-C2	2.86	1.56	1.53
5	B	2422	CAM	C1-C2	3.14	1.57	1.53
5	B	2422	CAM	C5-C4	3.20	1.62	1.53
6	B	2430	TRS	O3-C3	3.31	1.53	1.42
3	B	2417	HEM	C4C-NC	3.36	1.40	1.36
3	A	1417	HEM	C1C-NC	3.46	1.40	1.36
5	A	1422	CAM	C5-C4	3.54	1.63	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	2430	TRS	C3-C-C2	-4.95	100.06	110.78
5	A	1422	CAM	C4-C3-C2	-4.49	94.15	101.96
5	B	2422	CAM	C4-C3-C2	-4.41	94.28	101.96
6	B	2430	TRS	C2-C-C1	-3.69	102.79	110.78
5	B	2422	CAM	C5-C6-C1	-3.26	97.76	104.72
5	A	1422	CAM	C5-C6-C1	-3.07	98.17	104.72
3	B	2417	HEM	CAA-C2A-C1A	-2.26	124.56	127.01
6	B	2430	TRS	O2-C2-C	-2.24	106.65	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2417	HEM	CMA-C3A-C4A	-2.21	124.71	128.36
3	A	1417	HEM	CAA-C2A-C1A	-2.20	124.62	127.01
5	B	2422	CAM	C9-C7-C1	2.13	118.23	113.01
5	A	1422	CAM	C9-C7-C1	2.20	118.40	113.01
5	A	1422	CAM	C6-C1-C7	2.62	107.59	101.61
5	B	2422	CAM	C6-C1-C7	2.64	107.64	101.61
3	B	2417	HEM	C2D-C3D-C4D	2.89	106.41	101.50
3	B	2417	HEM	CMD-C2D-C3D	2.90	127.18	114.35
5	A	1422	CAM	C3-C4-C7	2.91	109.17	102.73
3	A	1417	HEM	C3B-CAB-CBB	2.97	129.00	124.46
5	B	2422	CAM	C3-C4-C7	3.04	109.45	102.73
3	B	2417	HEM	C3B-CAB-CBB	3.08	129.19	124.46
3	A	1417	HEM	C2D-C3D-C4D	3.13	106.80	101.50
3	A	1417	HEM	CMD-C2D-C3D	3.13	128.19	114.35
6	B	2430	TRS	C3-C-C1	3.26	117.84	110.78
3	A	1417	HEM	CAD-C3D-C4D	3.33	124.23	112.47
3	B	2417	HEM	CAD-C3D-C4D	3.63	125.28	112.47
3	B	2417	HEM	CMC-C2C-C3C	3.84	126.12	116.53
3	A	1417	HEM	CMC-C2C-C3C	4.03	126.58	116.53
3	B	2417	HEM	CMB-C2B-C3B	4.62	128.06	116.53
3	A	1417	HEM	CMB-C2B-C3B	4.72	128.32	116.53
3	B	2417	HEM	CAD-C3D-C2D	5.21	128.19	113.22
3	A	1417	HEM	CAD-C3D-C2D	5.35	128.61	113.22
6	B	2430	TRS	C3-C-N	5.65	118.36	108.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1417	HEM	2	0
4	B	2420	CMO	1	0
5	B	2422	CAM	2	0

## 5.7 Other polymers

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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	407/414 (98%)	-0.13	4 (0%) 84 82	10, 16, 30, 44	0
1	B	405/414 (97%)	0.09	12 (2%) 54 48	12, 21, 35, 43	0
All	All	812/828 (98%)	-0.02	16 (1%) 68 64	10, 19, 34, 44	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	309	GLY	4.2
1	B	414	VAL	4.1
1	A	9	ALA	3.9
1	B	24	PHE	3.6
1	A	414	VAL	3.5
1	B	22	LEU	3.1
1	B	49	ASN	2.8
1	B	20	GLU	2.7
1	B	14	LEU	2.6
1	B	19	PRO	2.5
1	B	50	VAL	2.4
1	A	413	ALA	2.4
1	B	343	GLN	2.3
1	B	33	ASN	2.2
1	A	278	PRO	2.2
1	B	63	TRP	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CAM	B	2422	11/11	0.78	0.21	10.15	27,29,30,30	0
5	CAM	A	1422	11/11	0.85	0.16	2.94	20,22,23,24	0
6	TRS	B	2430	8/8	0.92	0.10	1.03	18,20,22,25	0
3	HEM	A	1417	43/43	0.98	0.09	-0.43	9,11,13,17	0
3	HEM	B	2417	43/43	0.97	0.09	-0.58	11,13,17,21	0
2	K	A	1515	1/1	1.00	0.08	-0.87	12,12,12,12	0
2	K	B	2515	1/1	0.98	0.08	-1.04	21,21,21,21	0
2	K	A	1715	1/1	0.99	0.06	-3.40	17,17,17,17	0
4	CMO	B	2420	2/2	0.93	0.21	-	17,17,17,20	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.