



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:17 PM GMT

PDB ID : 3WRK  
Title : Crystal structure of P450cam  
Authors : Kishimoto, A.; Takagi, K.; Amano, A.; Sakurai, K.; Mizushima, T.; Shimada, H.  
Deposited on : 2014-02-25  
Resolution : 2.61 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

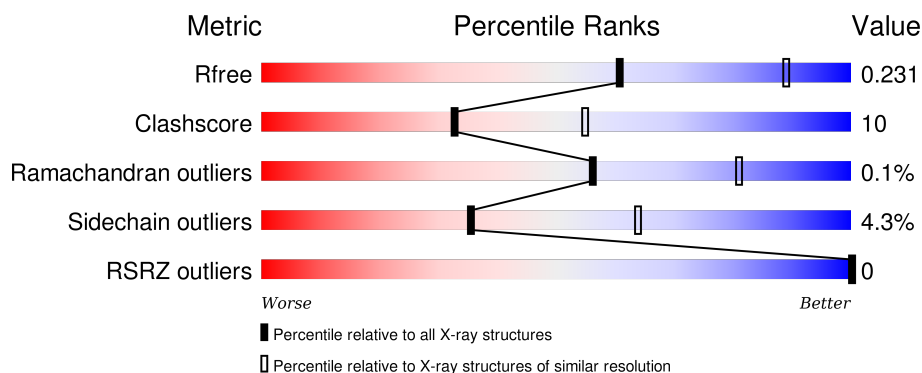
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.61 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))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	421	 74% 16% • 7%
1	D	421	 72% 19% • 7%

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
3	CAM	A	502	-	-	-	X
3	CAM	D	502	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6519 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 Camphor 5-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	2	0
			3120	1976	553	574	17			
1	D	392	Total	C	N	O	S	0	2	0
			3121	1978	552	573	18			

There are 12 discrepancies between the modelled and reference sequences:

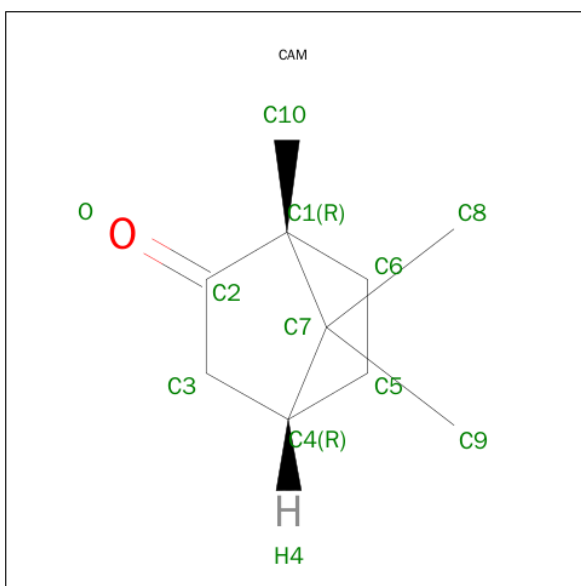
Chain	Residue	Modelled	Actual	Comment	Reference
A	415	HIS	-	EXPRESSION TAG	UNP P00183
A	416	HIS	-	EXPRESSION TAG	UNP P00183
A	417	HIS	-	EXPRESSION TAG	UNP P00183
A	418	HIS	-	EXPRESSION TAG	UNP P00183
A	419	HIS	-	EXPRESSION TAG	UNP P00183
A	420	HIS	-	EXPRESSION TAG	UNP P00183
D	415	HIS	-	EXPRESSION TAG	UNP P00183
D	416	HIS	-	EXPRESSION TAG	UNP P00183
D	417	HIS	-	EXPRESSION TAG	UNP P00183
D	418	HIS	-	EXPRESSION TAG	UNP P00183
D	419	HIS	-	EXPRESSION TAG	UNP P00183
D	420	HIS	-	EXPRESSION TAG	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
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is CAMPHOR (three-letter code: CAM) (formula: C<sub>10</sub>H<sub>16</sub>O).



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

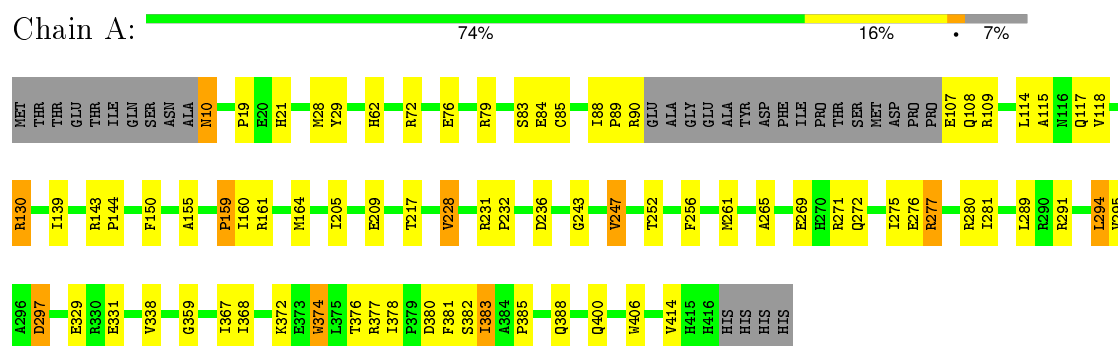
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	86	Total 86	O 86	0	0
4	D	84	Total 84	O 84	0	0

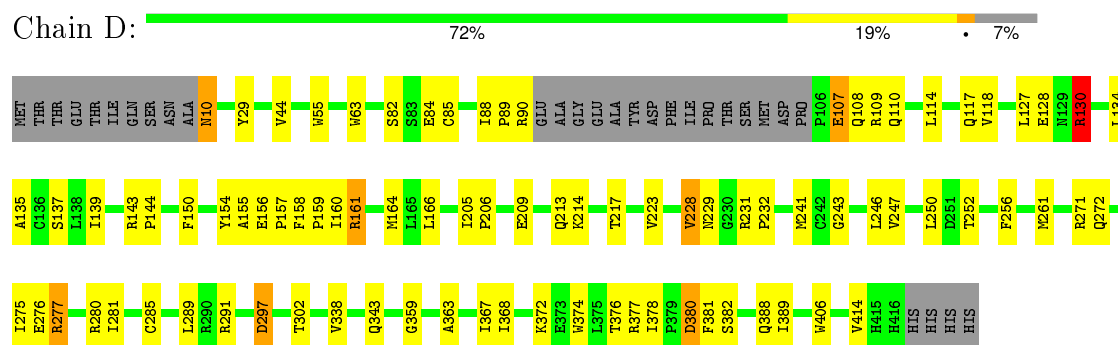
### 3 Residue-property plots

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: Camphor 5-monooxygenase



#### • Molecule 1: Camphor 5-monooxygenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.34Å 93.19Å 73.83Å 90.00° 89.92° 90.00°	Depositor
Resolution (Å)	39.40 – 2.61 46.75 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.40-2.61) 99.2 (46.75-2.61)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.61 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.174 , 0.235 0.167 , 0.231	Depositor DCC
$R_{free}$ test set	1261 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.5	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 12.1	EDS
Estimated twinning fraction	0.470 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 24852 reflections (0.008%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6519	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% 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: 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	0.63	2/3195 (0.1%)	0.71	3/4338 (0.1%)
1	D	0.64	4/3200 (0.1%)	0.71	4/4345 (0.1%)
All	All	0.63	6/6395 (0.1%)	0.71	7/8683 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	406	TRP	CD2-CE2	5.58	1.48	1.41
1	D	374	TRP	CD2-CE2	5.50	1.48	1.41
1	D	406	TRP	CD2-CE2	5.34	1.47	1.41
1	A	374	TRP	CD2-CE2	5.33	1.47	1.41
1	D	63	TRP	CD2-CE2	5.30	1.47	1.41
1	D	55	TRP	CD2-CE2	5.23	1.47	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	D	130	ARG	NE-CZ-NH2	7.06	123.83	120.30
1	A	130	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	D	130	ARG	NE-CZ-NH1	-6.79	116.90	120.30
1	D	109	ARG	NE-CZ-NH2	5.91	123.25	120.30
1	A	383	ILE	CG1-CB-CG2	-5.70	98.86	111.40
1	D	109	ARG	NE-CZ-NH1	-5.47	117.57	120.30

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	3120	0	3074	63	0
1	D	3121	0	3080	65	0
2	A	43	0	30	4	0
2	D	43	0	30	5	0
3	A	11	0	16	1	0
3	D	11	0	16	2	0
4	A	86	0	0	10	0
4	D	84	0	0	5	0
All	All	6519	0	6246	131	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 10.

All (131) 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:D:377:ARG:HH21	1:D:414:VAL:HG13	1.29	0.96
1:A:400:GLN:HE21	1:D:110:GLN:HE21	1.14	0.94
1:A:400:GLN:NE2	1:D:110:GLN:HE21	1.70	0.87
1:A:28:MET:HE3	1:A:29:TYR:CZ	2.10	0.86
1:D:363:ALA:O	1:D:367:ILE:HG12	1.77	0.84
1:D:377:ARG:HH21	1:D:414:VAL:CG1	1.92	0.83
1:D:130:ARG:HG2	1:D:130:ARG:HH21	1.46	0.81
1:A:83:SER:HB2	4:A:670:HOH:O	1.81	0.80
1:A:236:ASP:HB2	4:A:651:HOH:O	1.80	0.80
1:A:277:ARG:HG2	1:A:277:ARG:HH21	1.50	0.76
1:D:231:ARG:HB2	1:D:232:PRO:HD2	1.70	0.74
1:A:109:ARG:HD3	4:A:642:HOH:O	1.87	0.73
1:A:378:ILE:HG22	1:A:378:ILE:O	1.90	0.72
1:A:400:GLN:HE21	1:D:110:GLN:NE2	1.86	0.72
1:D:277:ARG:HH21	1:D:277:ARG:HG2	1.55	0.72
1:A:28:MET:CE	1:A:29:TYR:CZ	2.73	0.71
1:D:291:ARG:HG2	1:D:338:VAL:HG22	1.71	0.70
1:A:277:ARG:HG2	1:A:277:ARG:NH2	2.07	0.70
1:A:272[A]:GLN:HG3	1:A:276:GLU:OE1	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:PHE:CD2	1:D:367:ILE:HD12	2.27	0.69
1:D:277:ARG:NH2	1:D:277:ARG:HG2	2.09	0.68
1:A:377:ARG:HH21	1:A:414:VAL:HG12	1.57	0.68
1:A:297:ASP:OD2	2:A:501:HEM:O1A	2.11	0.67
1:A:130:ARG:HG3	4:A:646:HOH:O	1.93	0.67
1:D:377:ARG:NH2	1:D:414:VAL:HG13	2.05	0.67
1:D:272:GLN:HG3	1:D:276:GLU:OE1	1.93	0.67
1:D:377:ARG:NH2	1:D:414:VAL:CG1	2.57	0.67
1:A:231:ARG:HB2	1:A:232:PRO:HD2	1.78	0.66
1:A:85[B]:CYS:SG	1:A:90:ARG:HB2	2.36	0.66
1:D:271:ARG:HD2	1:D:381:PHE:CE1	2.32	0.65
1:A:291:ARG:HG2	1:A:338:VAL:HG22	1.77	0.65
1:D:107:GLU:CG	1:D:107:GLU:O	2.46	0.63
1:D:29:TYR:OH	1:D:88:ILE:O	2.11	0.62
2:A:501:HEM:HBC2	2:A:501:HEM:HMC2	1.80	0.62
1:D:143:ARG:N	1:D:144:PRO:CD	2.63	0.61
1:D:256:PHE:CE2	1:D:367:ILE:HD12	2.36	0.61
1:D:291:ARG:HG2	1:D:338:VAL:CG2	2.31	0.61
1:D:271:ARG:O	1:D:275:ILE:HG12	2.01	0.61
1:A:271:ARG:HD2	1:A:381:PHE:CE1	2.35	0.61
1:D:380:ASP:HA	4:D:634:HOH:O	2.00	0.60
1:A:205:ILE:O	1:A:209:GLU:HG3	2.02	0.60
1:D:378:ILE:HG22	1:D:378:ILE:O	2.02	0.60
1:A:85[A]:CYS:SG	1:A:90:ARG:HD3	2.43	0.58
1:A:265:ALA:HB3	1:A:383:ILE:CD1	2.34	0.57
1:D:297:ASP:OD2	2:D:501:HEM:O1A	2.22	0.57
1:A:291:ARG:HG2	1:A:338:VAL:CG2	2.33	0.57
1:A:10:ASN:N	1:A:10:ASN:HD22	2.02	0.56
1:D:252:THR:HG23	4:D:675:HOH:O	2.05	0.56
1:A:271:ARG:O	1:A:275:ILE:HG12	2.05	0.56
1:D:382:SER:HB2	4:D:631:HOH:O	2.05	0.56
2:D:501:HEM:C4D	3:D:502:CAM:H103	2.42	0.55
1:D:85[B]:CYS:SG	1:D:90:ARG:HB2	2.46	0.54
1:D:377:ARG:HE	1:D:414:VAL:HG12	1.72	0.54
1:A:29:TYR:OH	1:A:88:ILE:O	2.13	0.53
1:D:228:VAL:O	1:D:231:ARG:HD2	2.08	0.53
1:D:372:LYS:O	1:D:376:THR:HG23	2.09	0.53
1:A:243:GLY:O	1:A:247:VAL:HG13	2.09	0.53
1:D:277:ARG:HD3	1:D:280:ARG:NE	2.24	0.53
1:A:107:GLU:O	1:A:107:GLU:HG3	2.07	0.53
1:D:114:LEU:O	1:D:117:GLN:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85[A]:CYS:SG	1:D:90:ARG:HD3	2.48	0.53
1:D:107:GLU:HG3	1:D:107:GLU:O	2.08	0.52
1:D:205:ILE:O	1:D:209:GLU:HG3	2.09	0.52
1:A:377:ARG:NH2	1:A:414:VAL:HG12	2.21	0.52
1:A:265:ALA:CB	1:A:383:ILE:CD1	2.87	0.52
1:A:143:ARG:N	1:A:144:PRO:CD	2.71	0.52
1:D:10:ASN:HD22	1:D:10:ASN:N	2.06	0.52
1:A:256:PHE:CE2	1:A:367:ILE:HD13	2.46	0.51
1:A:62:HIS:CG	1:A:88:ILE:HD13	2.45	0.51
1:D:359:GLY:HA3	2:D:501:HEM:C3C	2.46	0.51
1:A:331:GLU:HG2	4:A:631:HOH:O	2.09	0.50
1:D:243:GLY:O	1:D:247:VAL:HG13	2.12	0.50
1:D:231:ARG:HB2	1:D:232:PRO:CD	2.41	0.50
1:A:277:ARG:HD3	1:A:280:ARG:NE	2.27	0.50
1:A:139:ILE:HD13	1:A:374:TRP:HA	1.93	0.49
1:A:79:ARG:CD	4:A:662:HOH:O	2.59	0.49
1:A:281:ILE:HG22	1:A:368:ILE:HG23	1.95	0.49
2:D:501:HEM:HBC2	2:D:501:HEM:HMC1	1.94	0.49
2:D:501:HEM:ND	3:D:502:CAM:H103	2.27	0.49
1:A:28:MET:CE	1:A:29:TYR:OH	2.62	0.48
1:D:213:GLN:C	1:D:214:LYS:HG2	2.34	0.48
1:A:150:PHE:CZ	1:A:261:MET:HG3	2.49	0.47
1:D:377:ARG:NE	1:D:414:VAL:HG12	2.30	0.47
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.44	0.47
1:A:114:LEU:O	1:A:117:GLN:HB2	2.14	0.47
1:A:79:ARG:HD3	4:A:662:HOH:O	2.14	0.47
1:D:134:LEU:HD21	1:D:161:ARG:HB3	1.97	0.47
1:A:372:LYS:O	1:A:376:THR:HG23	2.15	0.47
1:A:231:ARG:HB2	1:A:232:PRO:CD	2.45	0.46
1:D:143:ARG:N	1:D:144:PRO:HD3	2.29	0.46
1:A:72:ARG:O	1:A:76:GLU:HG3	2.15	0.46
1:A:143:ARG:HB3	1:A:144:PRO:HD3	1.97	0.45
1:A:160:ILE:O	1:A:164:MET:HG2	2.16	0.45
1:D:256:PHE:CE1	1:D:289:LEU:HA	2.51	0.45
1:A:88:ILE:HA	1:A:89:PRO:HA	1.85	0.45
1:D:155:ALA:O	1:D:159:PRO:HD3	2.16	0.45
1:D:246:LEU:O	1:D:250:LEU:HG	2.17	0.45
1:D:110:GLN:NE2	4:D:664:HOH:O	2.49	0.45
1:A:359:GLY:HA3	2:A:501:HEM:C3C	2.52	0.44
1:D:135:ALA:O	1:D:139:ILE:HG13	2.18	0.44
1:D:277:ARG:HH21	1:D:277:ARG:CG	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285[B]:CYS:SG	1:D:368:ILE:HG12	2.58	0.43
1:A:385:PRO:HD2	4:A:647:HOH:O	2.18	0.43
1:D:82:SER:HB2	1:D:302:THR:CG2	2.48	0.43
1:D:158:PHE:HB3	1:D:159:PRO:HD3	2.00	0.42
1:D:150:PHE:CZ	1:D:261:MET:HG3	2.55	0.42
1:A:265:ALA:CB	1:A:383:ILE:HD12	2.49	0.42
1:A:378:ILE:CG2	1:A:378:ILE:O	2.61	0.42
1:D:281:ILE:HG22	1:D:368:ILE:HG23	2.01	0.42
1:A:155:ALA:O	1:A:159:PRO:HD3	2.19	0.42
1:D:388:GLN:HB3	1:D:388:GLN:HE21	1.60	0.42
1:A:265:ALA:HB1	1:A:383:ILE:HD12	2.02	0.42
1:D:223:VAL:HG13	1:D:241:MET:HE1	2.01	0.42
1:A:388:GLN:HB3	1:A:388:GLN:HE21	1.60	0.42
1:A:294:LEU:HD12	1:A:295:VAL:HG23	2.02	0.41
1:D:205:ILE:HB	1:D:206:PRO:HD3	2.02	0.41
1:D:156:GLU:N	1:D:157:PRO:HD2	2.36	0.41
1:A:228:VAL:O	1:A:231:ARG:HD2	2.20	0.41
1:A:28:MET:HE2	1:A:29:TYR:CE2	2.55	0.41
1:D:88:ILE:HA	1:D:89:PRO:HA	1.86	0.41
1:D:160:ILE:O	1:D:164:MET:HG2	2.21	0.41
1:D:229:ASN:HA	4:D:664:HOH:O	2.20	0.41
1:A:252:THR:HG23	4:A:643:HOH:O	2.19	0.41
1:A:269:GLU:HG2	4:A:619:HOH:O	2.20	0.41
1:A:115:ALA:O	1:A:118:VAL:HG22	2.20	0.41
1:D:118:VAL:HG11	1:D:223:VAL:HG23	2.01	0.41
1:A:256:PHE:CE1	1:A:289:LEU:HA	2.56	0.41
1:D:127:LEU:O	1:D:128:GLU:C	2.59	0.40
1:A:19:PRO:HB2	1:A:21:HIS:CE1	2.57	0.40
3:A:502:CAM:H82	3:A:502:CAM:H32	1.93	0.40
1:D:154:TYR:CD1	1:D:154:TYR:C	2.95	0.40

There are no symmetry-related clashes.

## 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	389/421 (92%)	375 (96%)	14 (4%)	0	100	100
1	D	390/421 (93%)	374 (96%)	15 (4%)	1 (0%)	46	72
All	All	779/842 (92%)	749 (96%)	29 (4%)	1 (0%)	56	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	107	GLU

### 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	340/365 (93%)	326 (96%)	14 (4%)	37	66
1	D	341/365 (93%)	326 (96%)	15 (4%)	35	63
All	All	681/730 (93%)	652 (96%)	29 (4%)	35	64

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	84	GLU
1	A	108	GLN
1	A	159	PRO
1	A	161	ARG
1	A	217	THR
1	A	228	VAL
1	A	247	VAL
1	A	277	ARG
1	A	294	LEU
1	A	297	ASP
1	A	329	GLU

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Mol	Chain	Res	Type
1	A	380	ASP
1	A	382	SER
1	D	10	ASN
1	D	44	VAL
1	D	84	GLU
1	D	108	GLN
1	D	130	ARG
1	D	137	SER
1	D	161	ARG
1	D	166	LEU
1	D	217	THR
1	D	228	VAL
1	D	277	ARG
1	D	297	ASP
1	D	343	GLN
1	D	380	ASP
1	D	389	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	69	GLN
1	A	116	ASN
1	A	132	GLN
1	A	255	ASN
1	A	388	GLN
1	A	400	GLN
1	D	30	ASN
1	D	69	GLN
1	D	116	ASN
1	D	132	GLN
1	D	255	ASN
1	D	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 ⓘ

4 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	501	1	30,50,50	3.03	13 (43%)	24,82,82	2.59	8 (33%)
3	CAM	A	502	-	12,12,12	1.02	1 (8%)	21,21,21	0.98	1 (4%)
2	HEM	D	501	1	30,50,50	2.95	12 (40%)	24,82,82	2.62	8 (33%)
3	CAM	D	502	-	12,12,12	0.84	0	21,21,21	1.13	2 (9%)

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	501	1	-	0/10/54/54	0/0/8/8
3	CAM	A	502	-	-	0/0/31/31	0/0/2/2
2	HEM	D	501	1	-	0/10/54/54	0/0/8/8
3	CAM	D	502	-	-	0/0/31/31	0/0/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C3B-C4B	-3.04	1.49	1.51
2	A	501	HEM	C3B-C4B	-2.76	1.49	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C2D-C3D	-2.46	1.47	1.54
2	A	501	HEM	C2D-C3D	-2.46	1.47	1.54
2	D	501	HEM	C3D-C4D	-2.45	1.48	1.51
2	A	501	HEM	C3D-C4D	-2.42	1.48	1.51
3	A	502	CAM	C7-C1	-2.07	1.50	1.56
2	D	501	HEM	FE-NB	2.51	2.10	1.97
2	A	501	HEM	C4A-CHB	2.59	1.47	1.39
2	D	501	HEM	CHD-C1D	2.59	1.46	1.38
2	A	501	HEM	FE-NB	2.61	2.11	1.97
2	D	501	HEM	CHC-C4B	2.64	1.46	1.38
2	A	501	HEM	FE-ND	2.73	2.11	1.97
2	A	501	HEM	CHD-C1D	2.78	1.46	1.38
2	D	501	HEM	FE-ND	2.83	2.12	1.97
2	A	501	HEM	C2A-C3A	2.95	1.46	1.37
2	D	501	HEM	C2A-C3A	3.11	1.46	1.37
2	A	501	HEM	CHC-C4B	3.16	1.47	1.38
2	A	501	HEM	CHD-C4C	3.38	1.44	1.36
2	D	501	HEM	CHD-C4C	3.80	1.45	1.36
2	A	501	HEM	CHC-C1C	4.30	1.46	1.36
2	D	501	HEM	CHC-C1C	4.38	1.46	1.36
2	D	501	HEM	C4C-NC	8.13	1.46	1.36
2	A	501	HEM	C4C-NC	8.33	1.46	1.36
2	D	501	HEM	C1C-NC	9.28	1.47	1.36
2	A	501	HEM	C1C-NC	9.81	1.48	1.36

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C1D-CHD-C4C	-3.16	120.55	125.82
2	D	501	HEM	C1D-CHD-C4C	-2.84	121.08	125.82
3	D	502	CAM	C4-C3-C2	-2.63	97.38	101.96
2	A	501	HEM	C3B-CAB-CBB	-2.12	121.21	124.46
3	D	502	CAM	C10-C1-C2	2.06	117.31	108.51
2	D	501	HEM	C3B-C4B-NB	2.29	116.01	111.63
3	A	502	CAM	C9-C7-C8	2.56	113.44	107.52
2	A	501	HEM	C2C-C1C-NC	3.17	115.55	110.21
2	D	501	HEM	C2C-C1C-NC	3.18	115.56	110.21
2	D	501	HEM	CMD-C2D-C3D	3.46	129.63	114.35
2	A	501	HEM	CMD-C2D-C3D	3.63	130.41	114.35
2	A	501	HEM	CAD-C3D-C4D	4.04	126.70	112.47
2	D	501	HEM	CAD-C3D-C4D	4.71	129.10	112.47
2	A	501	HEM	CMC-C2C-C3C	4.83	128.59	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CMB-C2B-C3B	5.00	129.01	116.53
2	D	501	HEM	CMB-C2B-C3B	5.32	129.80	116.53
2	D	501	HEM	CMC-C2C-C3C	5.47	130.18	116.53
2	D	501	HEM	CAD-C3D-C2D	5.73	129.68	113.22
2	A	501	HEM	CAD-C3D-C2D	6.24	131.15	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	4	0
3	A	502	CAM	1	0
2	D	501	HEM	5	0
3	D	502	CAM	2	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](#)

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	391/421 (92%)	-0.66	0 100 100	14, 26, 47, 83	1 (0%)
1	D	392/421 (93%)	-0.66	0 100 100	13, 26, 48, 78	1 (0%)
All	All	783/842 (92%)	-0.66	0 100 100	13, 26, 48, 83	2 (0%)

There are no RSRZ outliers to report.

### 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(Å <sup>2</sup> )	Q<0.9
3	CAM	A	502	11/11	0.89	0.29	4.28	20,26,35,39	11
3	CAM	D	502	11/11	0.92	0.25	3.69	17,22,33,35	11
2	HEM	D	501	43/43	0.98	0.13	0.52	5,14,19,20	0
2	HEM	A	501	43/43	0.98	0.11	-0.42	6,15,19,23	0

## 6.5 Other polymers

There are no such residues in this entry.