



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 7, 2017 – 01:16 AM EST

PDB ID : 4JX1  
Title : Crystal structure of reduced Cytochrome P450cam-putidaredoxin complex  
bound to camphor and 5-exo-hydroxycamphor  
Authors : Tripathi, S.M.; Li, H.; Poulos, T.L.  
Deposited on : unknown  
Resolution : 2.09 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

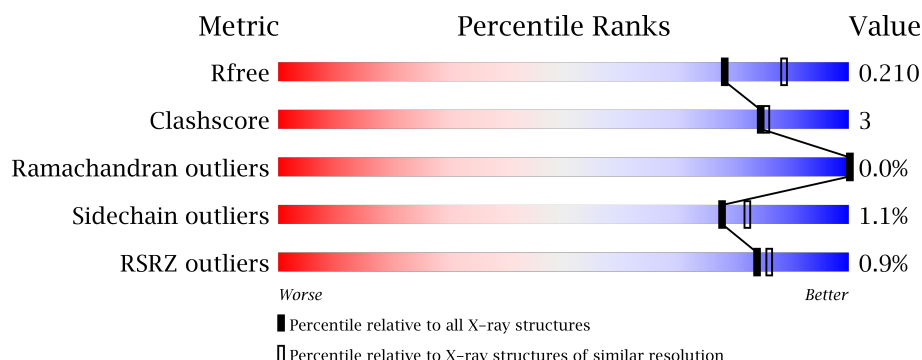
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.09 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))
$R_{free}$	100719	4955 (2.10-2.06)
Clashscore	112137	5537 (2.10-2.06)
Ramachandran outliers	110173	5483 (2.10-2.06)
Sidechain outliers	110143	5484 (2.10-2.06)
RSRZ outliers	101464	4991 (2.10-2.06)

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	415	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>1%</span> <span>93%</span> <span>2%</span> </div> </div>
1	B	415	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 1%, green 95%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>2%</span> <span>92%</span> <span>5%</span> </div> </div>
1	E	415	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>1%</span> <span>91%</span> <span>6%</span> </div> </div>
1	F	415	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>1%</span> <span>90%</span> <span>7%</span> </div> </div>
2	C	113	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>1%</span> <span>88%</span> <span>5%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
2	D	113	
2	G	113	
2	H	113	

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
4	CAM	A	502	-	-	-	X
4	CAM	B	502	-	-	-	X
4	CAM	E	502	-	-	-	X
4	CAM	F	502	-	-	-	X
5	CAH	A	503	-	-	-	X
5	CAH	E	503	-	-	-	X
5	CAH	F	503	-	-	-	X
8	1N0	E	504	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 34135 atoms, of which 15911 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	405	Total	C	H	N	O	S	0	0	0
			6354	2030	3150	559	601	14			
1	B	405	Total	C	H	N	O	S	0	1	0
			6357	2030	3153	557	603	14			
1	E	405	Total	C	H	N	O	S	0	0	0
			6364	2030	3160	559	601	14			
1	F	405	Total	C	H	N	O	S	0	1	0
			6357	2030	3153	557	603	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	58	SER	CYS	ENGINEERED MUTATION	UNP P00183
A	85	SER	CYS	ENGINEERED MUTATION	UNP P00183
A	136	SER	CYS	ENGINEERED MUTATION	UNP P00183
A	285	SER	CYS	ENGINEERED MUTATION	UNP P00183
A	334	ALA	CYS	ENGINEERED MUTATION	UNP P00183
A	344	CYS	LYS	ENGINEERED MUTATION	UNP P00183
B	58	SER	CYS	ENGINEERED MUTATION	UNP P00183
B	85	SER	CYS	ENGINEERED MUTATION	UNP P00183
B	136	SER	CYS	ENGINEERED MUTATION	UNP P00183
B	285	SER	CYS	ENGINEERED MUTATION	UNP P00183
B	334	ALA	CYS	ENGINEERED MUTATION	UNP P00183
B	344	CYS	LYS	ENGINEERED MUTATION	UNP P00183
E	58	SER	CYS	ENGINEERED MUTATION	UNP P00183
E	85	SER	CYS	ENGINEERED MUTATION	UNP P00183
E	136	SER	CYS	ENGINEERED MUTATION	UNP P00183
E	285	SER	CYS	ENGINEERED MUTATION	UNP P00183
E	334	ALA	CYS	ENGINEERED MUTATION	UNP P00183
E	344	CYS	LYS	ENGINEERED MUTATION	UNP P00183
F	58	SER	CYS	ENGINEERED MUTATION	UNP P00183
F	85	SER	CYS	ENGINEERED MUTATION	UNP P00183
F	136	SER	CYS	ENGINEERED MUTATION	UNP P00183

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Chain	Residue	Modelled	Actual	Comment	Reference
F	285	SER	CYS	ENGINEERED MUTATION	UNP P00183
F	334	ALA	CYS	ENGINEERED MUTATION	UNP P00183
F	344	CYS	LYS	ENGINEERED MUTATION	UNP P00183

- Molecule 2 is a protein called Putidaredoxin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	106	Total	C	H	N	O	S	0	0	0
			1563	487	771	136	160	9			
2	D	106	Total	C	H	N	O	S	0	0	0
			1563	487	771	136	160	9			
2	G	106	Total	C	H	N	O	S	0	0	0
			1562	487	770	136	160	9			
2	H	106	Total	C	H	N	O	S	0	0	0
			1563	487	771	136	160	9			

There are 32 discrepancies between the modelled and reference sequences:

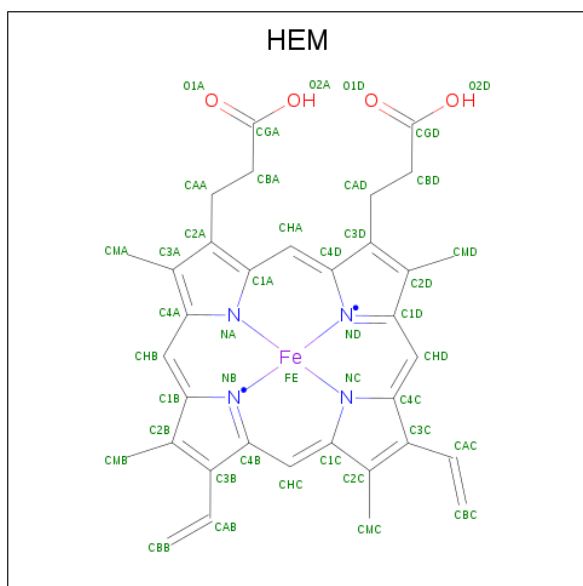
Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	HIS	-	EXPRESSION TAG	UNP P00259
C	-5	HIS	-	EXPRESSION TAG	UNP P00259
C	-4	HIS	-	EXPRESSION TAG	UNP P00259
C	-3	HIS	-	EXPRESSION TAG	UNP P00259
C	-2	HIS	-	EXPRESSION TAG	UNP P00259
C	-1	HIS	-	EXPRESSION TAG	UNP P00259
C	19	CYS	ASP	ENGINEERED MUTATION	UNP P00259
C	73	SER	CYS	ENGINEERED MUTATION	UNP P00259
D	-6	HIS	-	EXPRESSION TAG	UNP P00259
D	-5	HIS	-	EXPRESSION TAG	UNP P00259
D	-4	HIS	-	EXPRESSION TAG	UNP P00259
D	-3	HIS	-	EXPRESSION TAG	UNP P00259
D	-2	HIS	-	EXPRESSION TAG	UNP P00259
D	-1	HIS	-	EXPRESSION TAG	UNP P00259
D	19	CYS	ASP	ENGINEERED MUTATION	UNP P00259
D	73	SER	CYS	ENGINEERED MUTATION	UNP P00259
G	-6	HIS	-	EXPRESSION TAG	UNP P00259
G	-5	HIS	-	EXPRESSION TAG	UNP P00259
G	-4	HIS	-	EXPRESSION TAG	UNP P00259
G	-3	HIS	-	EXPRESSION TAG	UNP P00259
G	-2	HIS	-	EXPRESSION TAG	UNP P00259
G	-1	HIS	-	EXPRESSION TAG	UNP P00259
G	19	CYS	ASP	ENGINEERED MUTATION	UNP P00259

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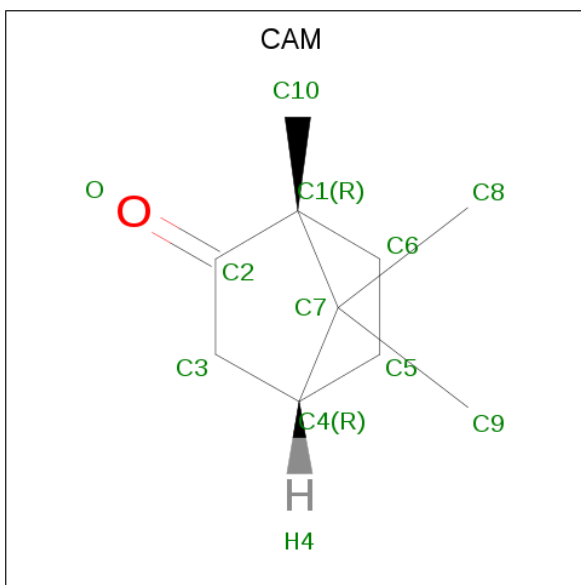
Chain	Residue	Modelled	Actual	Comment	Reference
G	73	SER	CYS	ENGINEERED MUTATION	UNP P00259
H	-6	HIS	-	EXPRESSION TAG	UNP P00259
H	-5	HIS	-	EXPRESSION TAG	UNP P00259
H	-4	HIS	-	EXPRESSION TAG	UNP P00259
H	-3	HIS	-	EXPRESSION TAG	UNP P00259
H	-2	HIS	-	EXPRESSION TAG	UNP P00259
H	-1	HIS	-	EXPRESSION TAG	UNP P00259
H	19	CYS	ASP	ENGINEERED MUTATION	UNP P00259
H	73	SER	CYS	ENGINEERED MUTATION	UNP P00259

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



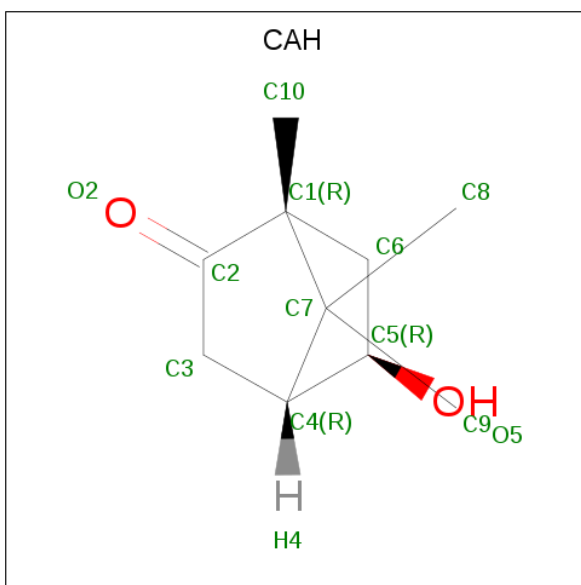
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
3	B	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
3	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
3	F	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 4 is CAMPHOR (three-letter code: CAM) (formula:  $C_{10}H_{16}O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			11	10	1			
4	B	1	Total	C	H	O	0	0
			27	10	16	1		
4	E	1	Total	C	H	O	0	0
			27	10	16	1		
4	F	1	Total	C	O		0	0
			11	10	1			

- Molecule 5 is 5-EXO-HYDROXYCAMPHOR (three-letter code: CAH) (formula:  $C_{10}H_{16}O_2$ ).

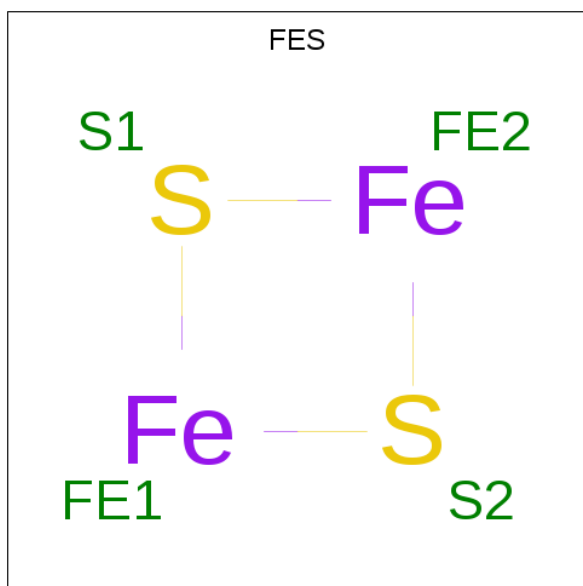


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			28	10	16	2		
5	E	1	Total	C	H	O	0	0
			28	10	16	2		
5	F	1	Total	C	H	O	0	0
			28	10	16	2		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	A	1	Total	Ca	0	0
			1	1		
6	F	1	Total	Ca	0	0
			1	1		
6	E	1	Total	Ca	0	0
			1	1		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	Fe	S	0	0
			4	2	2		
7	D	1	Total	Fe	S	0	0
			4	2	2		
7	G	1	Total	Fe	S	0	0
			4	2	2		

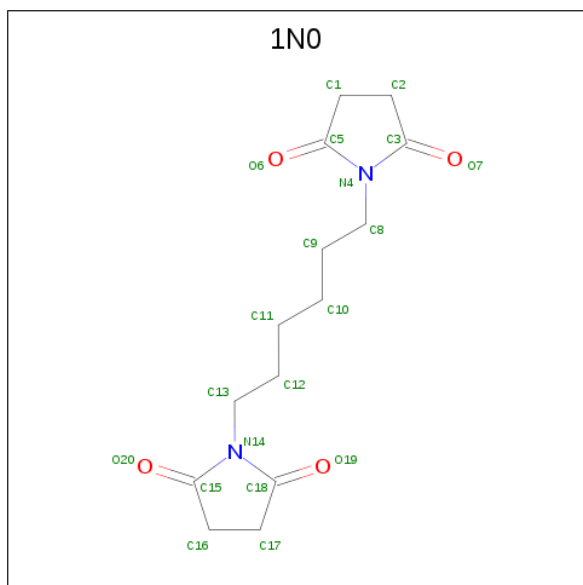
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is 1,1'-hexane-1,6-diylpyrrolidine-2,5-dione (three-letter code: 1N0) (formula:  $C_{14}H_{20}N_2O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	E	1	Total	C	H	N	O	0	0
			32	14	12	2	4		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	376	Total	O	0	0
			376	376		
9	B	342	Total	O	0	0
			342	342		
9	C	111	Total	O	0	0
			111	111		
9	D	82	Total	O	0	0
			82	82		
9	E	422	Total	O	0	0
			422	422		
9	F	418	Total	O	0	0
			418	418		
9	G	116	Total	O	0	0
			116	116		

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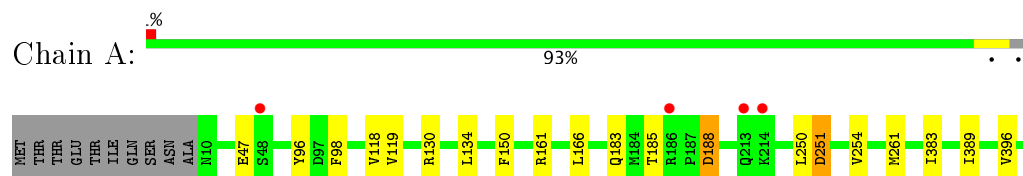
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	81	Total	O	0	0
			81	81		

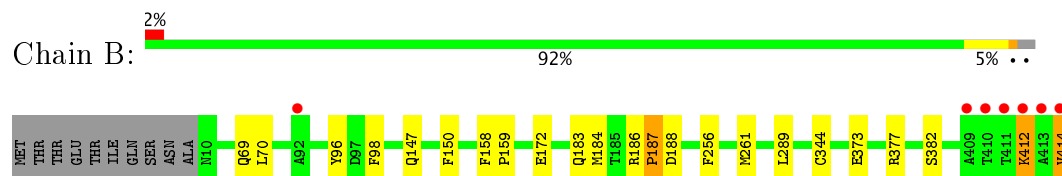
### 3 Residue-property plots [i](#)

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 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.

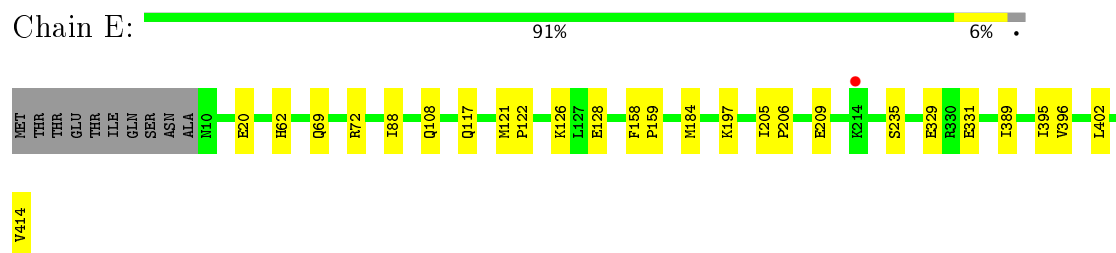
- Molecule 1: Camphor 5-monooxygenase



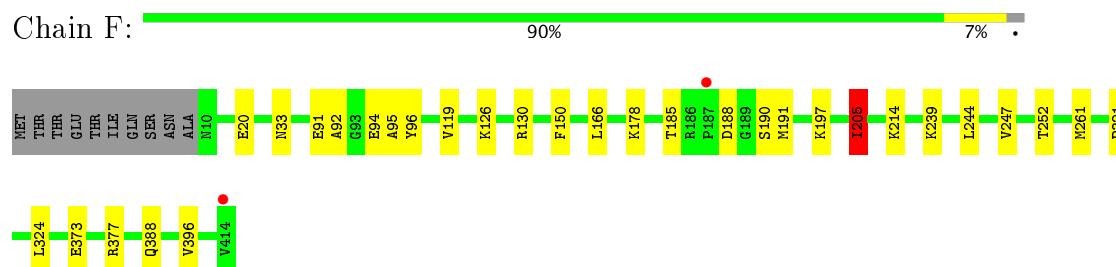
- Molecule 1: Camphor 5-monooxygenase



- Molecule 1: Camphor 5-monooxygenase



- Molecule 1: Camphor 5-monooxygenase

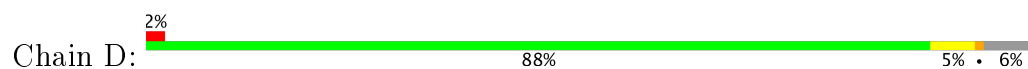


- Molecule 2: Putidaredoxin

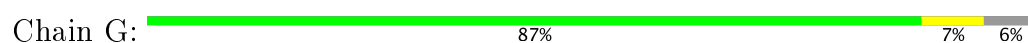




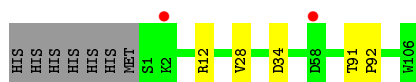
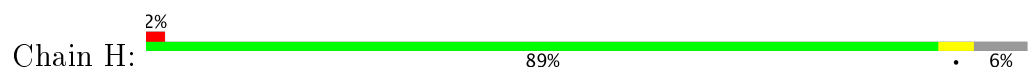
## ● Molecule 2: Putidaredoxin



## ● Molecule 2: Putidaredoxin



## ● Molecule 2: Putidaredoxin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.85Å 108.96Å 115.16Å 90.00° 109.03° 90.00°	Depositor
Resolution (Å)	44.87 – 2.09 44.87 – 2.09	Depositor EDS
% Data completeness (in resolution range)	98.6 (44.87-2.09) 98.6 (44.87-2.09)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.26 (at 2.08Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.144 , 0.212 0.142 , 0.210	Depositor DCC
$R_{free}$ test set	5960 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.5	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 55.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	34135	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.22 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.4309e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 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: 1N0, CA, CAH, FES, CAM, HEM

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	0.57	0/3283	0.66	0/4461
1	B	0.53	0/3283	0.63	0/4462
1	E	0.58	0/3283	0.65	0/4461
1	F	0.56	0/3283	0.67	1/4462 (0.0%)
2	C	0.58	1/803 (0.1%)	0.68	0/1090
2	D	0.52	1/803 (0.1%)	0.61	0/1090
2	G	0.53	0/803	0.64	0/1090
2	H	0.51	0/803	0.65	0/1090
All	All	0.56	2/16344 (0.0%)	0.65	1/22206 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	85	CYS	CB-SG	-7.78	1.69	1.82
2	D	85	CYS	CB-SG	-5.19	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	205	ILE	CB-CA-C	-6.14	99.32	111.60

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	3204	3150	3148	14	0
1	B	3204	3153	3141	14	0
1	E	3204	3160	3147	18	0
1	F	3204	3153	3141	20	0
2	C	792	771	771	3	0
2	D	792	771	771	3	0
2	G	792	770	770	4	0
2	H	792	771	771	4	0
3	A	43	30	30	0	0
3	B	43	30	30	1	0
3	E	43	30	30	2	0
3	F	43	30	30	1	0
4	A	11	0	16	4	0
4	B	11	16	16	0	0
4	E	11	16	16	3	0
4	F	11	0	16	5	0
5	A	12	16	15	3	0
5	E	12	16	15	1	0
5	F	12	16	15	3	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	C	4	0	0	1	0
7	D	4	0	0	0	0
7	G	4	0	0	0	0
7	H	4	0	0	0	0
8	E	20	12	18	0	0
9	A	376	0	0	3	0
9	B	342	0	0	3	0
9	C	111	0	0	1	0
9	D	82	0	0	0	0
9	E	422	0	0	6	0
9	F	418	0	0	7	0
9	G	116	0	0	0	0
9	H	81	0	0	2	0
All	All	18224	15911	15907	88	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 3.

The worst 5 of 88 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:E:72:ARG:NH1	1:E:331:GLU:OE2	2.06	0.88
1:F:96:TYR:CZ	4:F:502:CAM:H103	2.10	0.87
2:H:12:ARG:NH1	9:H:377:HOH:O	2.19	0.75
1:F:185:THR:HA	4:F:502:CAM:H81	1.73	0.71
2:H:28:VAL:O	9:H:369:HOH:O	2.09	0.71

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	403/415 (97%)	389 (96%)	14 (4%)	0	100	100
1	B	404/415 (97%)	388 (96%)	15 (4%)	1 (0%)	51	50
1	E	403/415 (97%)	392 (97%)	11 (3%)	0	100	100
1	F	404/415 (97%)	389 (96%)	15 (4%)	0	100	100
2	C	104/113 (92%)	103 (99%)	1 (1%)	0	100	100
2	D	104/113 (92%)	101 (97%)	3 (3%)	0	100	100
2	G	104/113 (92%)	103 (99%)	1 (1%)	0	100	100
2	H	104/113 (92%)	101 (97%)	3 (3%)	0	100	100
All	All	2030/2112 (96%)	1966 (97%)	63 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	187	PRO



### 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	349/358 (98%)	346 (99%)	3 (1%)	82	86
1	B	349/358 (98%)	346 (99%)	3 (1%)	82	86
1	E	349/358 (98%)	346 (99%)	3 (1%)	82	86
1	F	349/358 (98%)	342 (98%)	7 (2%)	60	65
2	C	89/96 (93%)	88 (99%)	1 (1%)	78	82
2	D	89/96 (93%)	88 (99%)	1 (1%)	78	82
2	G	89/96 (93%)	87 (98%)	2 (2%)	57	61
2	H	89/96 (93%)	89 (100%)	0	100	100
All	All	1752/1816 (96%)	1732 (99%)	20 (1%)	78	82

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	126	LYS
1	E	414	VAL
1	F	214	LYS
2	D	80	PRO
1	E	108	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	501	1,9	28,50,50	2.13	9 (32%)	17,82,82	2.00	7 (41%)
4	CAM	A	502	-	12,12,12	4.06	7 (58%)	20,21,21	4.41	7 (35%)
5	CAH	A	503	-	13,13,13	4.78	6 (46%)	15,23,23	2.61	3 (20%)
3	HEM	B	501	1	28,50,50	2.22	6 (21%)	17,82,82	2.07	4 (23%)
4	CAM	B	502	-	12,12,12	4.35	7 (58%)	20,21,21	3.70	8 (40%)
7	FES	C	201	2	0,4,4	0.00	-	0,4,4	0.00	-
7	FES	D	201	2	0,4,4	0.00	-	0,4,4	0.00	-
3	HEM	E	501	1,9	28,50,50	2.24	6 (21%)	17,82,82	1.79	4 (23%)
4	CAM	E	502	-	12,12,12	4.18	7 (58%)	20,21,21	4.02	6 (30%)
5	CAH	E	503	-	13,13,13	4.82	6 (46%)	15,23,23	2.67	4 (26%)
8	1N0	E	504	1,2	21,21,21	1.26	4 (19%)	28,28,28	2.50	7 (25%)
3	HEM	F	501	1,9	28,50,50	2.09	7 (25%)	17,82,82	1.84	5 (29%)
4	CAM	F	502	-	12,12,12	3.85	7 (58%)	20,21,21	4.71	7 (35%)
5	CAH	F	503	-	13,13,13	4.72	5 (38%)	15,23,23	2.30	3 (20%)
7	FES	G	201	2	0,4,4	0.00	-	0,4,4	0.00	-
7	FES	H	201	2	0,4,4	0.00	-	0,4,4	0.00	-

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	501	1,9	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CAM	A	502	-	-	0/0/31/31	0/0/2/2
5	CAH	A	503	-	-	0/0/34/34	0/0/2/2
3	HEM	B	501	1	-	0/6/54/54	0/0/8/8
4	CAM	B	502	-	-	0/0/31/31	0/0/2/2
7	FES	C	201	2	-	0/0/4/4	0/1/1/1
7	FES	D	201	2	-	0/0/4/4	0/1/1/1
3	HEM	E	501	1,9	-	0/6/54/54	0/0/8/8
4	CAM	E	502	-	-	0/0/31/31	0/0/2/2
5	CAH	E	503	-	-	0/0/34/34	0/0/2/2
8	1N0	E	504	1,2	-	0/9/35/35	0/2/2/2
3	HEM	F	501	1,9	-	0/6/54/54	0/0/8/8
4	CAM	F	502	-	-	0/0/31/31	0/0/2/2
5	CAH	F	503	-	-	0/0/34/34	0/0/2/2
7	FES	G	201	2	-	0/0/4/4	0/1/1/1
7	FES	H	201	2	-	0/0/4/4	0/1/1/1

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	503	CAH	C7-C4	-12.23	1.36	1.55
5	E	503	CAH	C7-C4	-12.17	1.36	1.55
5	F	503	CAH	C7-C4	-11.48	1.37	1.55
4	B	502	CAM	C1-C2	-10.92	1.39	1.53
4	E	502	CAM	C1-C2	-9.98	1.41	1.53

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	503	CAH	C4-C3-C2	-8.13	90.03	105.03
5	E	503	CAH	C4-C3-C2	-7.83	90.59	105.03
4	F	502	CAM	C8-C7-C1	-7.60	95.33	113.06
5	F	503	CAH	C4-C3-C2	-7.41	91.36	105.03
4	E	502	CAM	C9-C7-C4	-7.40	95.86	113.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	CAM	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	503	CAH	3	0
3	B	501	HEM	1	0
7	C	201	FES	1	0
3	E	501	HEM	2	0
4	E	502	CAM	3	0
5	E	503	CAH	1	0
3	F	501	HEM	1	0
4	F	502	CAM	5	0
5	F	503	CAH	3	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	405/415 (97%)	-0.37	5 (1%) 79 82	11, 19, 39, 61	0
1	B	405/415 (97%)	-0.21	7 (1%) 70 74	13, 24, 46, 84	0
1	E	405/415 (97%)	-0.41	1 (0%) 94 95	11, 19, 37, 58	0
1	F	405/415 (97%)	-0.44	2 (0%) 90 92	11, 20, 39, 65	0
2	C	106/113 (93%)	-0.33	0 100 100	12, 23, 41, 55	0
2	D	106/113 (93%)	-0.15	2 (1%) 67 70	16, 27, 44, 75	0
2	G	106/113 (93%)	-0.42	0 100 100	13, 22, 36, 45	0
2	H	106/113 (93%)	0.09	2 (1%) 67 70	15, 34, 54, 84	0
All	All	2044/2112 (96%)	-0.33	19 (0%) 84 86	11, 22, 44, 84	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	409	ALA	6.5
1	B	414	VAL	5.2
1	B	413	ALA	5.1
1	B	410	THR	4.4
1	B	411	THR	3.2

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

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
4	CAM	E	502	11/11	0.88	0.23	10.02	37,62,75,75	0
5	CAH	A	503	12/12	0.91	0.19	7.79	28,47,66,66	0
5	CAH	E	503	12/12	0.91	0.25	7.78	27,48,62,62	0
5	CAH	F	503	12/12	0.91	0.20	7.01	29,43,59,68	0
4	CAM	F	502	11/11	0.81	0.21	6.71	45,56,63,64	0
4	CAM	B	502	11/11	0.91	0.21	5.87	32,48,89,89	0
8	1N0	E	504	20/20	0.77	0.27	4.89	91,97,117,117	0
4	CAM	A	502	11/11	0.90	0.17	4.29	40,50,55,62	0
3	HEM	B	501	43/43	0.98	0.14	1.21	5,14,21,25	0
3	HEM	E	501	43/43	0.99	0.13	0.91	4,12,25,32	0
3	HEM	A	501	43/43	0.99	0.12	0.87	6,11,18,30	0
3	HEM	F	501	43/43	0.99	0.12	0.65	6,12,21,37	0
7	FES	G	201	4/4	0.99	0.08	-0.83	13,14,17,18	0
6	CA	A	504	1/1	0.98	0.09	-0.83	22,22,22,22	0
6	CA	F	504	1/1	0.99	0.09	-1.01	18,18,18,18	0
7	FES	D	201	4/4	0.99	0.07	-1.27	16,16,17,19	0
6	CA	E	505	1/1	0.99	0.07	-1.81	21,21,21,21	0
7	FES	C	201	4/4	1.00	0.07	-1.98	10,10,11,12	0
7	FES	H	201	4/4	0.99	0.07	-2.03	14,16,17,17	0
6	CA	B	503	1/1	0.99	0.06	-5.82	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.