wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:18 PM GMT

PDB ID	:	3TK3
Title	:	Cytochrome P450 2B4 mutant L437A in complex with 4-(4-chlorophenyl)imidazole
Authors	:	Gay, S.C.; Jang, H.H.; Wilderman, P.R.; Zhang, Q.; Stout, C.D.; Halpert, J.R.
Deposited on	:	2011-08-25
Resolution	:	2.80 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

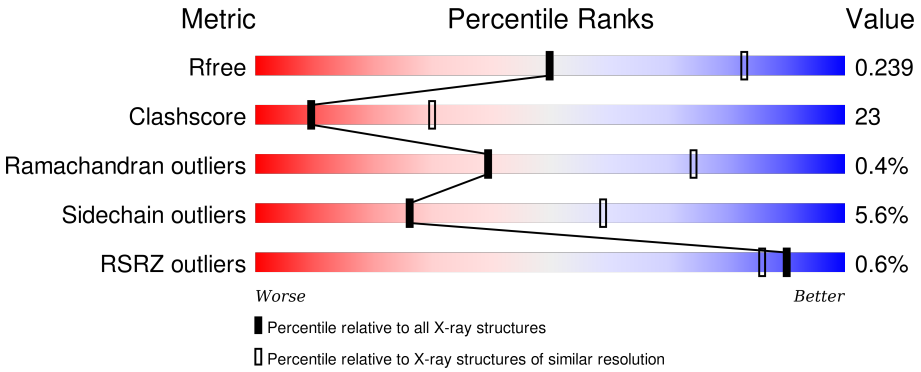
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 <=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	476	% 63% 30%
1	B	476	63% 30%
1	C	476	% 64% 31%
1	D	476	% 68% 26%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15257 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 2B4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	2	2	0
			3688	2377	631	669	11			
1	B	465	Total	C	N	O	S	1	2	0
			3685	2371	634	669	11			
1	C	465	Total	C	N	O	S	3	2	0
			3688	2377	636	664	11			
1	D	465	Total	C	N	O	S	4	3	0
			3686	2377	630	668	11			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ALA	GLU	ENGINEERED MUTATION	UNP P00178
A	?	-	PHE	DELETION	UNP P00178
A	?	-	SER	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	ALA	DELETION	UNP P00178
A	?	-	PHE	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	ALA	DELETION	UNP P00178
A	?	-	GLY	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	PHE	DELETION	UNP P00178
A	?	-	ARG	DELETION	UNP P00178
A	22	LYS	GLY	ENGINEERED MUTATION	UNP P00178

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Chain	Residue	Modelled	Actual	Comment	Reference
A	23	LYS	HIS	ENGINEERED MUTATION	UNP P00178
A	24	THR	PRO	ENGINEERED MUTATION	UNP P00178
A	25	SER	LYS	ENGINEERED MUTATION	UNP P00178
A	26	SER	ALA	ENGINEERED MUTATION	UNP P00178
A	27	LYS	HIS	ENGINEERED MUTATION	UNP P00178
A	29	LYS	ARG	ENGINEERED MUTATION	UNP P00178
A	221	SER	PRO	SEE REMARK 999	UNP P00178
A	226	TYR	HIS	ENGINEERED MUTATION	UNP P00178
A	437	ALA	LEU	ENGINEERED MUTATION	UNP P00178
A	492	HIS	-	EXPRESSION TAG	UNP P00178
A	493	HIS	-	EXPRESSION TAG	UNP P00178
A	494	HIS	-	EXPRESSION TAG	UNP P00178
A	495	HIS	-	EXPRESSION TAG	UNP P00178
B	21	ALA	GLU	ENGINEERED MUTATION	UNP P00178
B	?	-	PHE	DELETION	UNP P00178
B	?	-	SER	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	ALA	DELETION	UNP P00178
B	?	-	PHE	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	ALA	DELETION	UNP P00178
B	?	-	GLY	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	PHE	DELETION	UNP P00178
B	?	-	ARG	DELETION	UNP P00178
B	22	LYS	GLY	ENGINEERED MUTATION	UNP P00178
B	23	LYS	HIS	ENGINEERED MUTATION	UNP P00178
B	24	THR	PRO	ENGINEERED MUTATION	UNP P00178
B	25	SER	LYS	ENGINEERED MUTATION	UNP P00178
B	26	SER	ALA	ENGINEERED MUTATION	UNP P00178
B	27	LYS	HIS	ENGINEERED MUTATION	UNP P00178
B	29	LYS	ARG	ENGINEERED MUTATION	UNP P00178
B	221	SER	PRO	SEE REMARK 999	UNP P00178
B	226	TYR	HIS	ENGINEERED MUTATION	UNP P00178

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Chain	Residue	Modelled	Actual	Comment	Reference
B	437	ALA	LEU	ENGINEERED MUTATION	UNP P00178
B	492	HIS	-	EXPRESSION TAG	UNP P00178
B	493	HIS	-	EXPRESSION TAG	UNP P00178
B	494	HIS	-	EXPRESSION TAG	UNP P00178
B	495	HIS	-	EXPRESSION TAG	UNP P00178
C	21	ALA	GLU	ENGINEERED MUTATION	UNP P00178
C	?	-	PHE	DELETION	UNP P00178
C	?	-	SER	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	ALA	DELETION	UNP P00178
C	?	-	PHE	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	ALA	DELETION	UNP P00178
C	?	-	GLY	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	PHE	DELETION	UNP P00178
C	?	-	ARG	DELETION	UNP P00178
C	22	LYS	GLY	ENGINEERED MUTATION	UNP P00178
C	23	LYS	HIS	ENGINEERED MUTATION	UNP P00178
C	24	THR	PRO	ENGINEERED MUTATION	UNP P00178
C	25	SER	LYS	ENGINEERED MUTATION	UNP P00178
C	26	SER	ALA	ENGINEERED MUTATION	UNP P00178
C	27	LYS	HIS	ENGINEERED MUTATION	UNP P00178
C	29	LYS	ARG	ENGINEERED MUTATION	UNP P00178
C	221	SER	PRO	SEE REMARK 999	UNP P00178
C	226	TYR	HIS	ENGINEERED MUTATION	UNP P00178
C	437	ALA	LEU	ENGINEERED MUTATION	UNP P00178
C	492	HIS	-	EXPRESSION TAG	UNP P00178
C	493	HIS	-	EXPRESSION TAG	UNP P00178
C	494	HIS	-	EXPRESSION TAG	UNP P00178
C	495	HIS	-	EXPRESSION TAG	UNP P00178
D	21	ALA	GLU	ENGINEERED MUTATION	UNP P00178
D	?	-	PHE	DELETION	UNP P00178
D	?	-	SER	DELETION	UNP P00178

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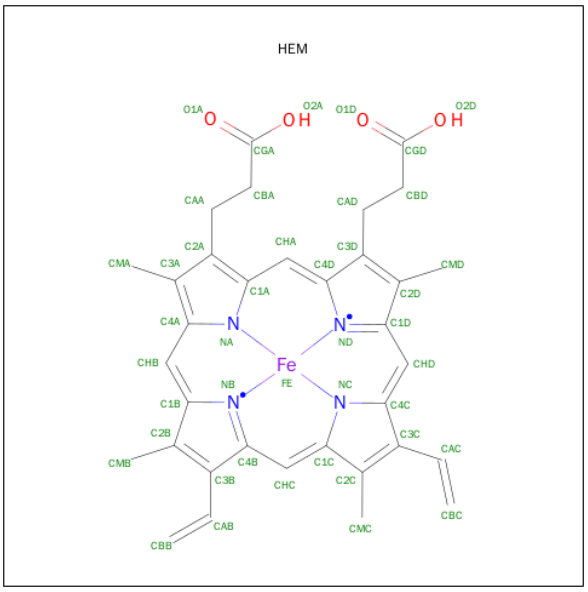
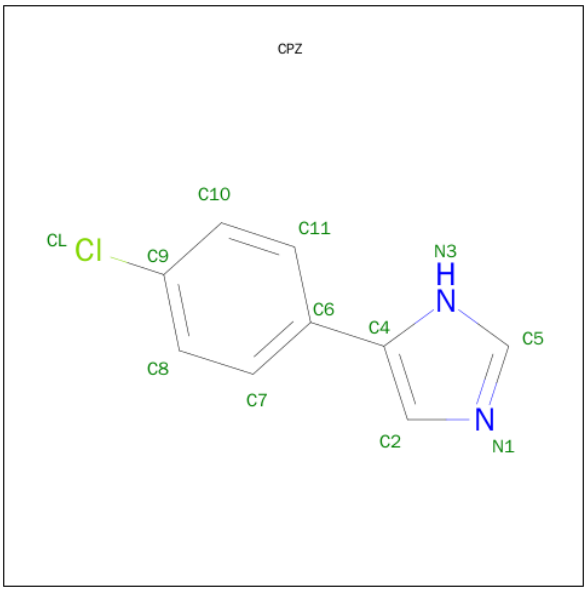
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	ALA	DELETION	UNP P00178
D	?	-	PHE	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	ALA	DELETION	UNP P00178
D	?	-	GLY	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	PHE	DELETION	UNP P00178
D	?	-	ARG	DELETION	UNP P00178
D	22	LYS	GLY	ENGINEERED MUTATION	UNP P00178
D	23	LYS	HIS	ENGINEERED MUTATION	UNP P00178
D	24	THR	PRO	ENGINEERED MUTATION	UNP P00178
D	25	SER	LYS	ENGINEERED MUTATION	UNP P00178
D	26	SER	ALA	ENGINEERED MUTATION	UNP P00178
D	27	LYS	HIS	ENGINEERED MUTATION	UNP P00178
D	29	LYS	ARG	ENGINEERED MUTATION	UNP P00178
D	221	SER	PRO	SEE REMARK 999	UNP P00178
D	226	TYR	HIS	ENGINEERED MUTATION	UNP P00178
D	437	ALA	LEU	ENGINEERED MUTATION	UNP P00178
D	492	HIS	-	EXPRESSION TAG	UNP P00178
D	493	HIS	-	EXPRESSION TAG	UNP P00178
D	494	HIS	-	EXPRESSION TAG	UNP P00178
D	495	HIS	-	EXPRESSION TAG	UNP P00178

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

- Molecule 3 is 4-(4-CHLOROPHENYL)IMIDAZOLE (three-letter code: CPZ) (formula: $C_9H_7ClN_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	0	0
			12	9	1	2		
3	B	1	Total	C	Cl	N	0	0
			12	9	1	2		
3	C	1	Total	C	Cl	N	0	0
			12	9	1	2		
3	D	1	Total	C	Cl	N	0	0
			12	9	1	2		

- Molecule 4 is water.

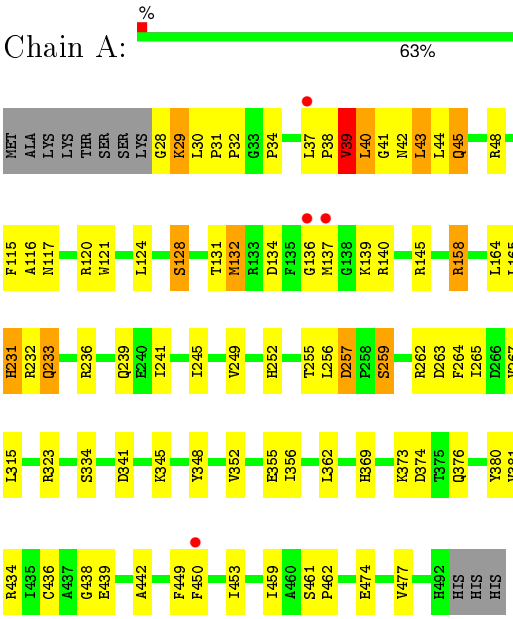
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	64	Total	O	0	0
			64	64		
4	B	82	Total	O	0	0
			82	82		
4	C	73	Total	O	0	0
			73	73		
4	D	71	Total	O	0	0
			71	71		

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 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.

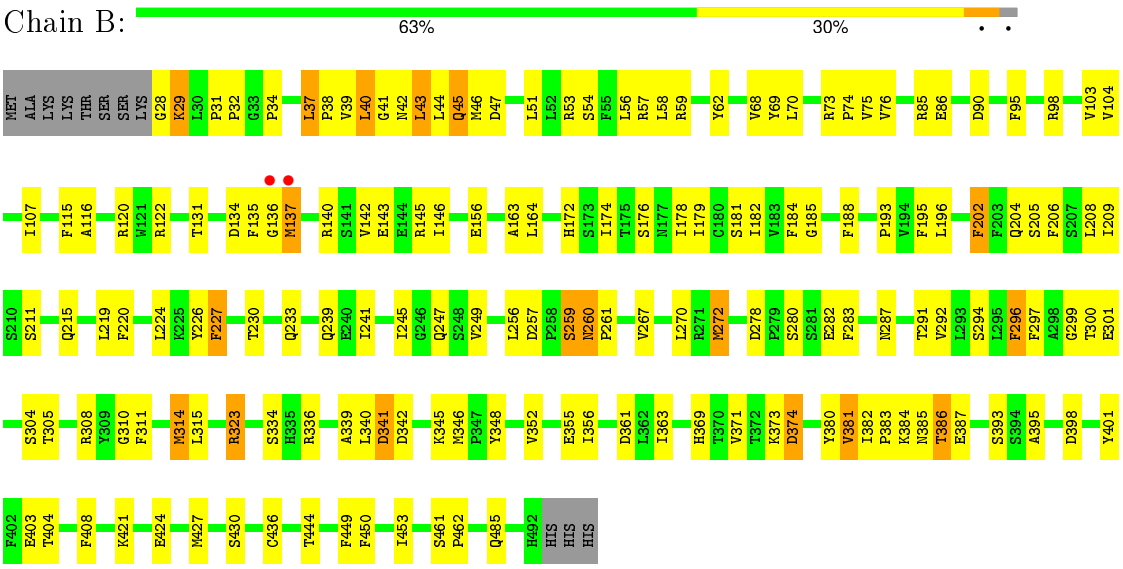
- Molecule 1: Cytochrome P450 2B4

Chain A:



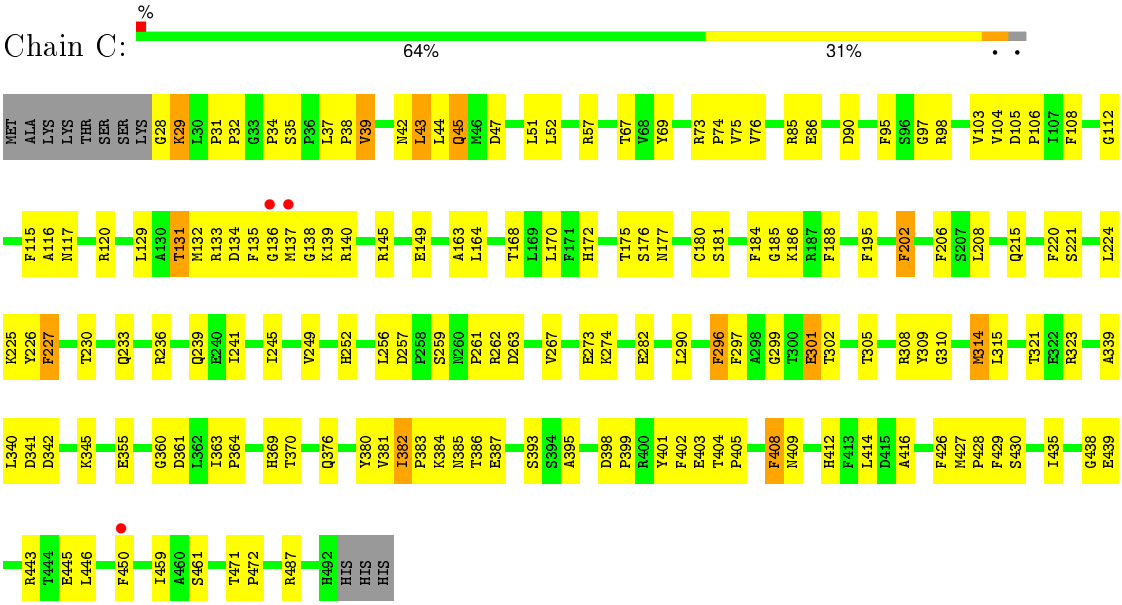
- Molecule 1: Cytochrome P450 2B4

Chain B:



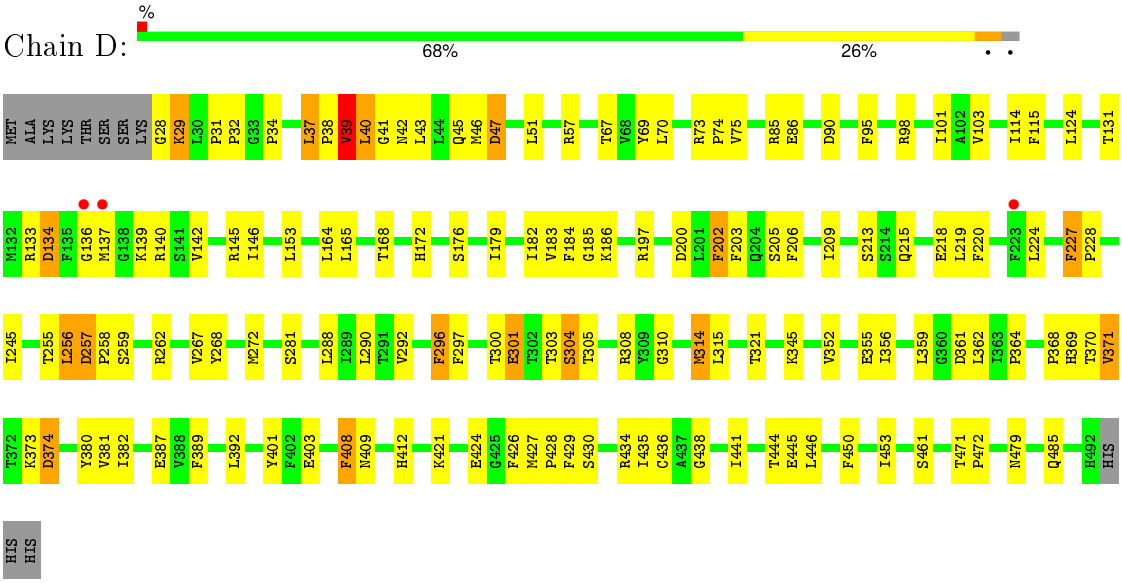
• Molecule 1: Cytochrome P450 2B4

Chain C:



• Molecule 1: Cytochrome P450 2B4

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	232.91Å 232.91Å 56.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.43 – 2.80 76.24 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.43-2.80) 98.8 (76.24-2.80)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.20	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 2.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.193 , 0.241 0.193 , 0.239	Depositor DCC
R_{free} test set	4207 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	54.0	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.4	EDS
Estimated twinning fraction	0.419 for -h,-k,l 0.428 for h,-h-k,-l 0.428 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 84142 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15257	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CPZ

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	0.71	0/3788	0.65	2/5141 (0.0%)
1	B	0.76	2/3784 (0.1%)	0.65	1/5135 (0.0%)
1	C	0.80	3/3787 (0.1%)	0.67	2/5136 (0.0%)
1	D	0.78	2/3789 (0.1%)	0.67	4/5143 (0.1%)
All	All	0.76	7/15148 (0.0%)	0.66	9/20555 (0.0%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	401	TYR	CD2-CE2	-5.92	1.30	1.39
1	C	301[A]	GLU	N-CA	5.75	1.57	1.46
1	C	301[B]	GLU	N-CA	5.75	1.57	1.46
1	B	143	GLU	CG-CD	-5.44	1.43	1.51
1	C	401	TYR	CD2-CE2	-5.39	1.31	1.39

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	301[A]	GLU	N-CA-C	5.80	126.67	111.00
1	D	301[B]	GLU	N-CA-C	5.80	126.67	111.00
1	D	47	ASP	N-CA-CB	-5.55	100.62	110.60
1	C	408	PHE	CB-CA-C	-5.53	99.34	110.40
1	A	301[A]	GLU	N-CA-C	5.51	125.87	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	3688	0	3626	177	0
1	B	3685	0	3621	166	0
1	C	3688	0	3649	163	0
1	D	3686	0	3622	160	0
2	A	43	0	30	9	0
2	B	43	0	30	12	0
2	C	43	0	30	10	0
2	D	43	0	30	10	0
3	A	12	0	7	0	0
3	B	12	0	7	0	0
3	C	12	0	7	0	0
3	D	12	0	7	0	0
4	A	64	0	0	7	0
4	B	82	0	0	8	0
4	C	73	0	0	5	0
4	D	71	0	0	4	0
All	All	15257	0	14666	670	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 23.

The worst 5 of 670 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:136:GLY:HA3	1:D:145:ARG:CZ	1.51	1.39
1:D:256:LEU:HD12	1:D:257:ASP:N	1.34	1.36
1:C:34:PRO:HG2	1:C:42:ASN:ND2	1.47	1.27
1:B:137:MET:HB2	1:B:185:GLY:O	1.36	1.26
1:B:43:LEU:HD12	1:B:43:LEU:O	1.37	1.24

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	465/476 (98%)	438 (94%)	25 (5%)	2 (0%)	39	74
1	B	465/476 (98%)	447 (96%)	17 (4%)	1 (0%)	52	84
1	C	465/476 (98%)	445 (96%)	18 (4%)	2 (0%)	39	74
1	D	466/476 (98%)	449 (96%)	15 (3%)	2 (0%)	39	74
All	All	1861/1904 (98%)	1779 (96%)	75 (4%)	7 (0%)	39	74

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	VAL
1	C	39	VAL
1	D	39	VAL
1	A	29	LYS
1	D	29	LYS

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	399/420 (95%)	372 (93%)	27 (7%)	20	49
1	B	398/420 (95%)	374 (94%)	24 (6%)	24	56
1	C	399/420 (95%)	381 (96%)	18 (4%)	34	68
1	D	398/420 (95%)	379 (95%)	19 (5%)	31	66
All	All	1594/1680 (95%)	1506 (94%)	88 (6%)	26	59

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	260	ASN
1	B	386	THR
1	D	304	SER
1	B	272	MET
1	B	334	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	172	HIS
1	C	233	GLN
1	D	233	GLN
1	B	247	GLN
1	B	369	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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)

8 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	500	1,3	30,50,50	2.05	10 (33%)	24,82,82	2.58	12 (50%)
3	CPZ	A	501	2	11,13,13	1.13	1 (9%)	13,17,17	1.50	2 (15%)
2	HEM	B	500	1,3	30,50,50	2.30	8 (26%)	24,82,82	2.51	11 (45%)
3	CPZ	B	501	2	11,13,13	1.23	1 (9%)	13,17,17	1.10	1 (7%)
2	HEM	C	500	1,3	30,50,50	2.32	8 (26%)	24,82,82	2.45	10 (41%)
3	CPZ	C	501	2	11,13,13	1.17	1 (9%)	13,17,17	1.27	1 (7%)
2	HEM	D	500	1,3	30,50,50	2.21	10 (33%)	24,82,82	2.46	13 (54%)
3	CPZ	D	501	2	11,13,13	1.11	2 (18%)	13,17,17	1.19	1 (7%)

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	500	1,3	-	0/10/54/54	0/0/8/8
3	CPZ	A	501	2	-	0/4/4/4	0/2/2/2
2	HEM	B	500	1,3	-	0/10/54/54	0/0/8/8
3	CPZ	B	501	2	-	0/4/4/4	0/2/2/2
2	HEM	C	500	1,3	-	0/10/54/54	0/0/8/8
3	CPZ	C	501	2	-	0/4/4/4	0/2/2/2
2	HEM	D	500	1,3	-	0/10/54/54	0/0/8/8
3	CPZ	D	501	2	-	0/4/4/4	0/2/2/2

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	HEM	C3B-C4B	-8.43	1.44	1.51
2	B	500	HEM	C3B-C4B	-8.07	1.44	1.51
2	D	500	HEM	C3B-C4B	-6.77	1.45	1.51
2	A	500	HEM	C3B-C4B	-5.53	1.46	1.51
2	D	500	HEM	C3D-C4D	-5.07	1.45	1.51

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500	HEM	CAA-CBA-CGA	-3.80	105.78	112.75
3	A	501	CPZ	C2-C4-C6	-3.50	124.56	129.44
2	B	500	HEM	C3C-CAC-CBC	-3.49	119.11	124.46
2	D	500	HEM	CBD-CAD-C3D	-3.45	103.52	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	501	CPZ	C2-C4-C6	-3.21	124.97	129.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	9	0
2	B	500	HEM	12	0
2	C	500	HEM	10	0
2	D	500	HEM	10	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

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^{th} 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^2)	Q<0.9
1	A	465/476 (97%)	-0.12	4 (0%)	85	79	27, 51, 82, 99	9 (1%)
1	B	465/476 (97%)	-0.12	2 (0%)	93	90	26, 51, 82, 99	9 (1%)
1	C	465/476 (97%)	-0.10	3 (0%)	90	86	25, 51, 81, 94	6 (1%)
1	D	465/476 (97%)	-0.10	3 (0%)	90	86	27, 50, 81, 98	8 (1%)
All	All	1860/1904 (97%)	-0.11	12 (0%)	90	86	25, 51, 82, 99	32 (1%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	136	GLY	6.1
1	A	136	GLY	5.1
1	B	136	GLY	4.7
1	D	136	GLY	4.4
1	B	137	MET	3.5

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

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^{th} 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^2)	Q<0.9
3	CPZ	A	501	12/12	0.96	0.26	1.31	39,50,58,81	0
3	CPZ	B	501	12/12	0.96	0.26	1.18	35,46,60,83	0
3	CPZ	C	501	12/12	0.95	0.24	1.06	35,48,57,77	0
2	HEM	A	500	43/43	0.99	0.21	0.78	35,41,46,50	0
3	CPZ	D	501	12/12	0.95	0.23	0.73	36,53,57,82	0
2	HEM	C	500	43/43	0.99	0.20	0.18	33,39,44,46	0
2	HEM	B	500	43/43	0.99	0.19	0.13	35,41,48,50	0
2	HEM	D	500	43/43	0.99	0.20	-0.02	34,42,46,48	0

6.5 Other polymers (i)

There are no such residues in this entry.