



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 29, 2016 – 04:11 PM EDT

PDB ID : 5JQV
Title : Crystal structure of Cytochrome P450 BM3 heme domain T269V/L272W/L322I/A406S (WIVS) variant with iron(III) deuteroporphyrin IX bound
Authors : Reynolds, E.W.; McHenry, M.W.; Cannac, F.; Gober, J.G.; Snow, C.D.; Brustad, E.M.
Deposited on : 2016-05-05
Resolution : 2.34 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
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) : rb-20027939

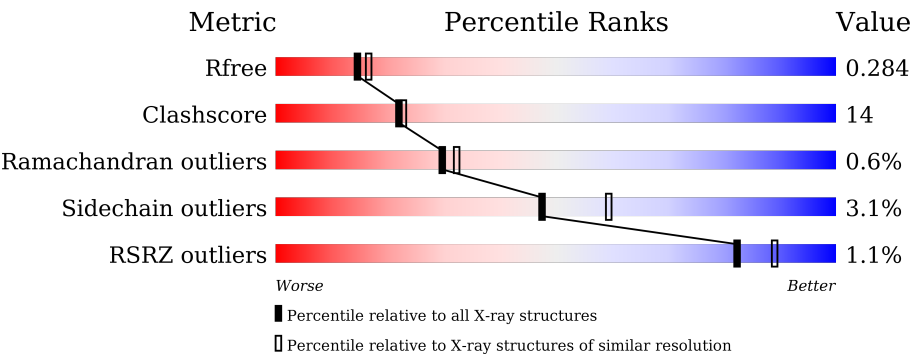
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	471	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>65%31%..</div></div>
1	B	471	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>67%29%..</div></div>
1	C	471	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>68%26%..</div></div>
1	D	471	<div><div>2%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>70%26%. </div></div>
1	E	471	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>67%28%. </div></div>
1	F	471	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>69%27%..</div></div>

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Mol	Chain	Length	Quality of chain
1	G	471	<div><div></div><div>70%</div><div>24%</div><div></div><div></div></div>
1	H	471	<div>%<div><div></div><div>66%</div><div>28%</div><div></div><div></div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30012 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 Bifunctional cytochrome P450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	0	0
			3579	2300	609	653	17			
1	B	453	Total	C	N	O	S	0	0	0
			3597	2307	611	662	17			
1	C	452	Total	C	N	O	S	0	0	0
			3551	2284	602	648	17			
1	D	454	Total	C	N	O	S	0	0	0
			3493	2250	590	636	17			
1	E	451	Total	C	N	O	S	0	1	0
			3589	2302	608	662	17			
1	F	455	Total	C	N	O	S	0	0	0
			3565	2292	602	654	17			
1	G	451	Total	C	N	O	S	0	3	0
			3585	2300	607	661	17			
1	H	450	Total	C	N	O	S	0	0	0
			3578	2300	608	653	17			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	269	VAL	THR	engineered mutation	UNP P14779
A	272	TRP	LEU	engineered mutation	UNP P14779
A	322	ILE	LEU	engineered mutation	UNP P14779
A	406	SER	ALA	engineered mutation	UNP P14779
A	464	LEU	-	expression tag	UNP P14779
A	465	GLU	-	expression tag	UNP P14779
A	466	HIS	-	expression tag	UNP P14779
A	467	HIS	-	expression tag	UNP P14779
A	468	HIS	-	expression tag	UNP P14779
A	469	HIS	-	expression tag	UNP P14779
A	470	HIS	-	expression tag	UNP P14779
A	471	HIS	-	expression tag	UNP P14779
B	269	VAL	THR	engineered mutation	UNP P14779

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Chain	Residue	Modelled	Actual	Comment	Reference
B	272	TRP	LEU	engineered mutation	UNP P14779
B	322	ILE	LEU	engineered mutation	UNP P14779
B	406	SER	ALA	engineered mutation	UNP P14779
B	464	LEU	-	expression tag	UNP P14779
B	465	GLU	-	expression tag	UNP P14779
B	466	HIS	-	expression tag	UNP P14779
B	467	HIS	-	expression tag	UNP P14779
B	468	HIS	-	expression tag	UNP P14779
B	469	HIS	-	expression tag	UNP P14779
B	470	HIS	-	expression tag	UNP P14779
B	471	HIS	-	expression tag	UNP P14779
C	269	VAL	THR	engineered mutation	UNP P14779
C	272	TRP	LEU	engineered mutation	UNP P14779
C	322	ILE	LEU	engineered mutation	UNP P14779
C	406	SER	ALA	engineered mutation	UNP P14779
C	464	LEU	-	expression tag	UNP P14779
C	465	GLU	-	expression tag	UNP P14779
C	466	HIS	-	expression tag	UNP P14779
C	467	HIS	-	expression tag	UNP P14779
C	468	HIS	-	expression tag	UNP P14779
C	469	HIS	-	expression tag	UNP P14779
C	470	HIS	-	expression tag	UNP P14779
C	471	HIS	-	expression tag	UNP P14779
D	269	VAL	THR	engineered mutation	UNP P14779
D	272	TRP	LEU	engineered mutation	UNP P14779
D	322	ILE	LEU	engineered mutation	UNP P14779
D	406	SER	ALA	engineered mutation	UNP P14779
D	464	LEU	-	expression tag	UNP P14779
D	465	GLU	-	expression tag	UNP P14779
D	466	HIS	-	expression tag	UNP P14779
D	467	HIS	-	expression tag	UNP P14779
D	468	HIS	-	expression tag	UNP P14779
D	469	HIS	-	expression tag	UNP P14779
D	470	HIS	-	expression tag	UNP P14779
D	471	HIS	-	expression tag	UNP P14779
E	269	VAL	THR	engineered mutation	UNP P14779
E	272	TRP	LEU	engineered mutation	UNP P14779
E	322	ILE	LEU	engineered mutation	UNP P14779
E	406	SER	ALA	engineered mutation	UNP P14779
E	464	LEU	-	expression tag	UNP P14779
E	465	GLU	-	expression tag	UNP P14779
E	466	HIS	-	expression tag	UNP P14779

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Chain	Residue	Modelled	Actual	Comment	Reference
E	467	HIS	-	expression tag	UNP P14779
E	468	HIS	-	expression tag	UNP P14779
E	469	HIS	-	expression tag	UNP P14779
E	470	HIS	-	expression tag	UNP P14779
E	471	HIS	-	expression tag	UNP P14779
F	269	VAL	THR	engineered mutation	UNP P14779
F	272	TRP	LEU	engineered mutation	UNP P14779
F	322	ILE	LEU	engineered mutation	UNP P14779
F	406	SER	ALA	engineered mutation	UNP P14779
F	464	LEU	-	expression tag	UNP P14779
F	465	GLU	-	expression tag	UNP P14779
F	466	HIS	-	expression tag	UNP P14779
F	467	HIS	-	expression tag	UNP P14779
F	468	HIS	-	expression tag	UNP P14779
F	469	HIS	-	expression tag	UNP P14779
F	470	HIS	-	expression tag	UNP P14779
F	471	HIS	-	expression tag	UNP P14779
G	269	VAL	THR	engineered mutation	UNP P14779
G	272	TRP	LEU	engineered mutation	UNP P14779
G	322	ILE	LEU	engineered mutation	UNP P14779
G	406	SER	ALA	engineered mutation	UNP P14779
G	464	LEU	-	expression tag	UNP P14779
G	465	GLU	-	expression tag	UNP P14779
G	466	HIS	-	expression tag	UNP P14779
G	467	HIS	-	expression tag	UNP P14779
G	468	HIS	-	expression tag	UNP P14779
G	469	HIS	-	expression tag	UNP P14779
G	470	HIS	-	expression tag	UNP P14779
G	471	HIS	-	expression tag	UNP P14779
H	269	VAL	THR	engineered mutation	UNP P14779
H	272	TRP	LEU	engineered mutation	UNP P14779
H	322	ILE	LEU	engineered mutation	UNP P14779
H	406	SER	ALA	engineered mutation	UNP P14779
H	464	LEU	-	expression tag	UNP P14779
H	465	GLU	-	expression tag	UNP P14779
H	466	HIS	-	expression tag	UNP P14779
H	467	HIS	-	expression tag	UNP P14779
H	468	HIS	-	expression tag	UNP P14779
H	469	HIS	-	expression tag	UNP P14779
H	470	HIS	-	expression tag	UNP P14779
H	471	HIS	-	expression tag	UNP P14779

- Molecule 2 is FE(III) DEUTEROPORPHYRIN IX (three-letter code: FDE) (formula: C₃₀H₂₈FeN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 39	C 30	Fe 1	N 4	O 4	0	0
2	B	1	Total 39	C 30	Fe 1	N 4	O 4	0	0
2	C	1	Total 39	C 30	Fe 1	N 4	O 4	0	0
2	D	1	Total 39	C 30	Fe 1	N 4	O 4	0	0
2	E	1	Total 39	C 30	Fe 1	N 4	O 4	0	0
2	F	1	Total 39	C 30	Fe 1	N 4	O 4	0	0
2	G	1	Total 39	C 30	Fe 1	N 4	O 4	0	0
2	H	1	Total 39	C 30	Fe 1	N 4	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	159	Total O 159 159	0	0
3	B	154	Total O 154 154	0	0
3	C	132	Total O 132 132	0	0
3	D	89	Total O 89 89	0	0

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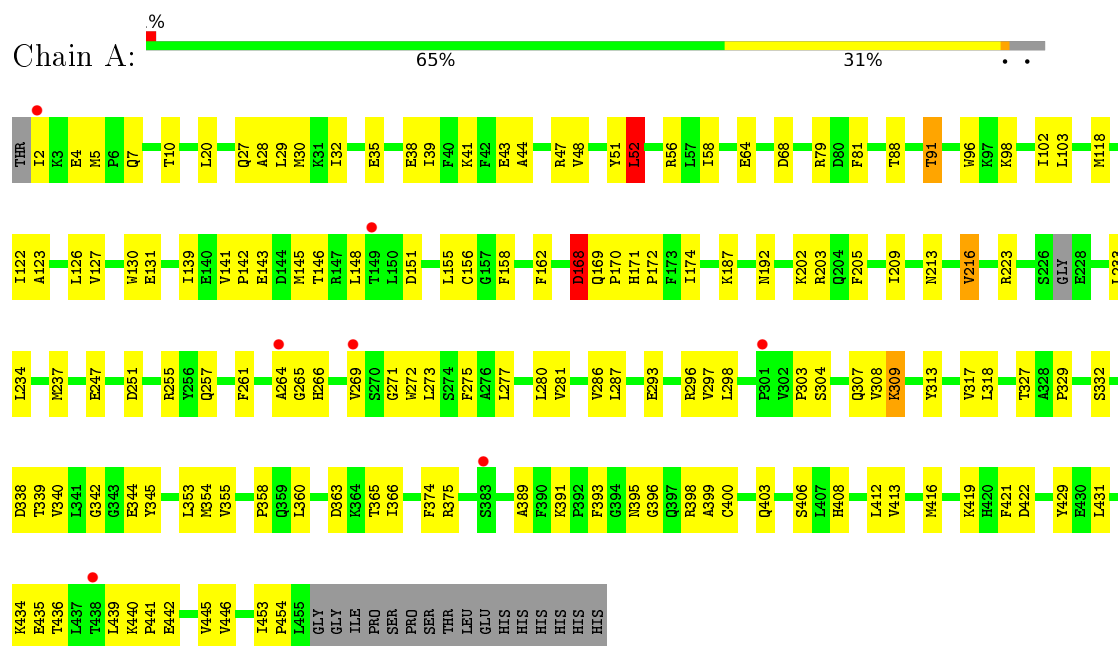
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	164	Total 164	O 164	0	0
3	F	130	Total 130	O 130	0	0
3	G	156	Total 156	O 156	0	0
3	H	179	Total 179	O 179	0	0

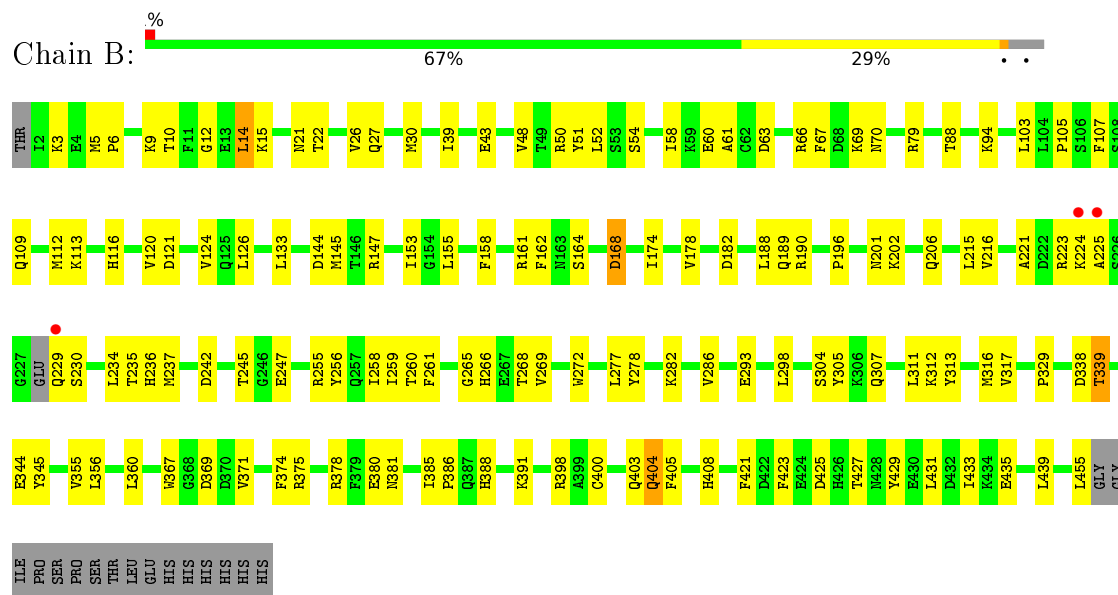
3 Residue-property plots

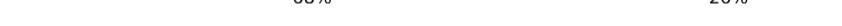
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Bifunctional cytochrome P450/NADPH-P450 reductase

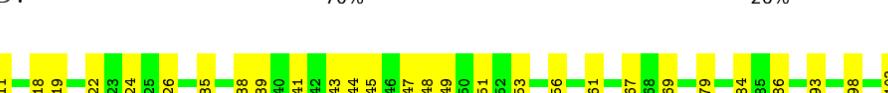


- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

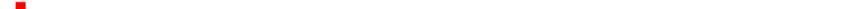


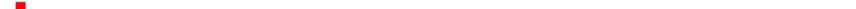
Chain C: 

Label	Value	Color
GLY	T1	Green
ILE	I2	Green
PRO	K3	Green
SER	E4	Green
PRO	W5	Green
SER	P6	Green
THR	T10	Green
LEU	K15	Green
GLU	L20	Green
HIS	M21	Green
HIS	D23	Green
HIS	K24	Green
HIS	P25	Green
	M30	Green
	I39	Green
	P45	Green
	G46	Green
	R47	Red
	V48	Green
	T49	Green
	R50	Green
	Y51	Green
	L52	Green
	S53	Green
	L57	Green
	D68	Green
	K69	Green
	M70	Green
	G83	Green
	D84	Green
	G85	Green
	S89	Green
	L103	Green
	S108	Green
	M112	Green
	Y115	Green
	M118	Green
	M119	Green
	V120	Green
	A123	Green
	V124	Green
	V127	Green
	R132	Green
	V141	Red
	V142	Green
	T146	Green
	R147	Green
	D151	Green
	T152	Green
	I153	Green
	M159	Green
	F162	Green
	M163	Green
	S164	Green
	D168	Green
	I174	Green
	M177	Green
	E183	Green
	M186	Green
	K187	Green
	R190	Green
	A191	Green
	M192	Green
	P193	Green
	D194	Green
	Y198	Green
	N201	Green
	P205	Green
	Q206	Green
	E207	Green
	V211	Red
	V216	Green
	R223	Red
	K224	Green
	A225	Green
	S226	Green
	GLY	Grey
	GLU	Grey
	GLN	Grey
	S230	Green
	L233	Green
	L234	Red
	T235	Green
	E236	Green
	M237	Green
	D242	Green
	T245	Green
	G246	Green
	E247	Green
	Y256	Green
	Q257	Green
	I258	Green
	I259	Green
	T260	Red
	D261	Green
	L262	Green
	L263	Green
	R266	Green
	E267	Green
	G271	Red
	L280	Green
	V286	Green
	L287	Green
	Q288	Green
	E292	Green
	E293	Green
	G294	Green
	N295	Green
	L298	Green
	P303	Green
	S304	Green
	Y305	Green
	K309	Green
	Q310	Green
	L311	Green
	K312	Green
	Y313	Green
	V317	Green
	R323	Green
	A328	Red
	K329	Green
	A330	Green
	E337	Green
	L341	Green
	G342	Green
	G343	Green
	E344	Green
	L455	Grey
	GLY	Grey

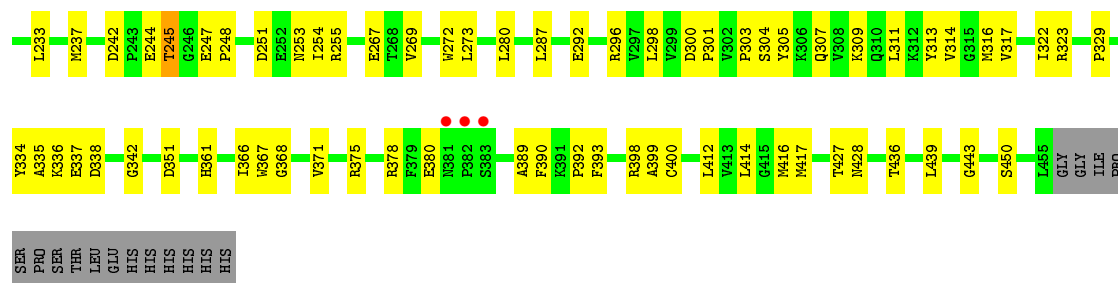
Chain D: 

Amino Acid	Value
T1	1
I2	1
Q7	1
F11	1
P18	1
L19	1
T22	1
I23	1
K24	1
P25	1
V26	1
E35	1
E38	1
I39	1
K41	1
F42	1
E43	1
A44	1
P45	1
G46	1
R47	1
V48	1
T49	1
R50	1
Y51	1
L52	1
S53	1
R56	1
A61	1
F67	1
D68	1
K69	1
R79	1
D84	1
G85	1
L86	1
E93	1
K98	1
L103	1
M118	1
D121	1
T122	1
K123	1
V124	1
R147	1
L150	1
D151	1
T152	1
L155	1
R161	1
F162	1
R163	1
S164	1
H171	1
P172	1
F173	1
I174	1
V178	1
E183	1
M192	1
E200	1
R203	1
Q204	1
F205	1
L215	1
V216	1
R223	1
G227	1
GLU	1
Q229	1
D232	1
L233	1
L234	1
M237	1
L238	1
M239	1
E244	1
T245	1
G246	1
E247	1
P248	1
L249	1
D250	1
M253	1
T254	1
P255	1
Y256	1
Q257	1
L258	1
H266	1
V269	1
S270	1
G271	1
L280	1
V281	1
R282	1
N283	1
V286	1
L287	1
E293	1
V297	1
S304	1
V308	1
Y313	1
V314	1
V317	1
E320	1
R323	1
T327	1
A328	1
P329	1
A330	1
F331	1
S332	1
L333	1
T334	1
A335	1
E344	1
M354	1
V355	1
L356	1
I357	1
P358	1
Q359	1
L360	1
H361	1
R362	1
I366	1
V371	1
R375	1
P376	1
E377	1
R378	1
F379	1
E380	1
P386	1
Q387	1
H388	1
A389	1
F390	1
K391	1
P392	1
F393	1
R398	1
A399	1
C400	1
L414	1
M417	1
F423	1
E424	1
D425	1
H426	1
Y429	1
E430	1
L431	1
D432	1
E435	1
T436	1
L437	1
T438	1
L439	1
K440	1
P441	1
E442	1
G443	1
V446	1
K447	1
L455	1
GLY	1
GLY	1
I45	1
P40	1
SER	1
P40	1
THR	1
LEU	1
GLU	1
VAL	1

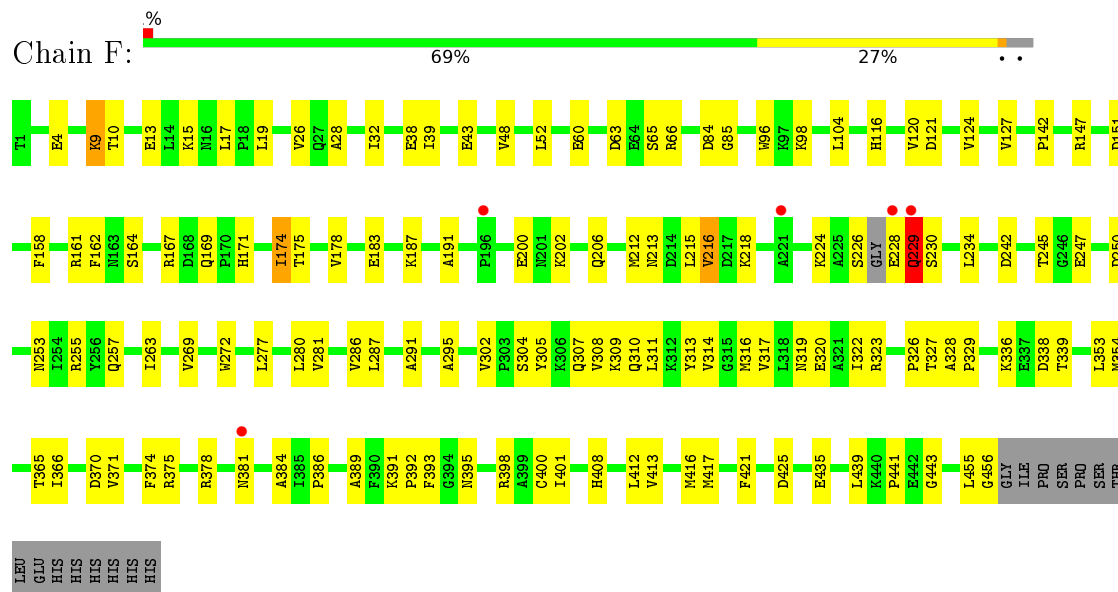
Chain E: 



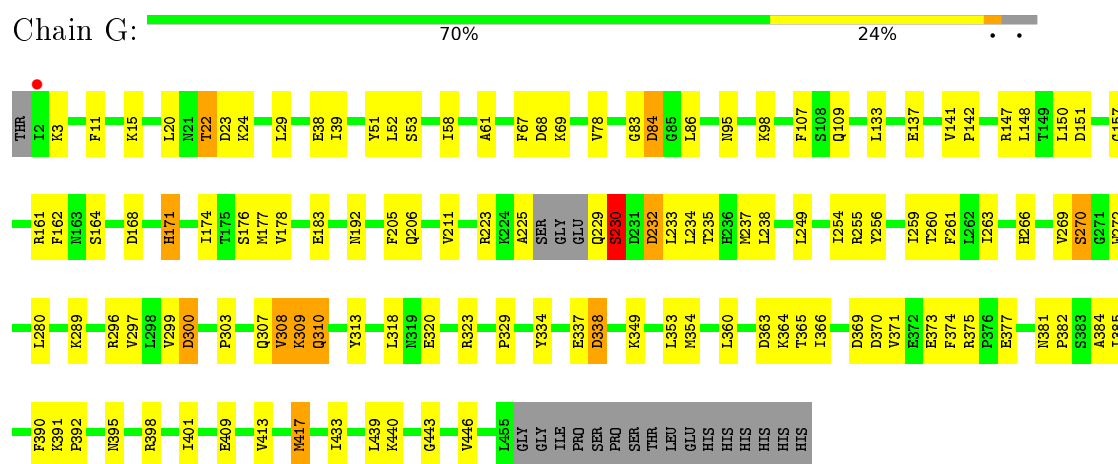
THR	12	35	39	G12	E13	L14	L17	P18	L19	Q27	E38	I39	F40	K41	F42	E43	G46	R47	V48	T49	R50	Y51	L52	S53	S54	A55	R56	L57	I58	K59	D60	K69	L75	K76	F77	R78	R79	D80	F81	D84	R87	T88	S89	N90	E93	N96
K97	K98	A99	H100	L103	L104	S108	Q109	Q110	V120	V124	W130	E131	I139	E143	R147	L148	D151	T152	I153	F162	M163	S164	A173	I174	V178	R179	K180	Q189	R190	A191	D195	P196	K202	R203	L215	V216	D217	S226	GLY	GLU	GLN	GLN				



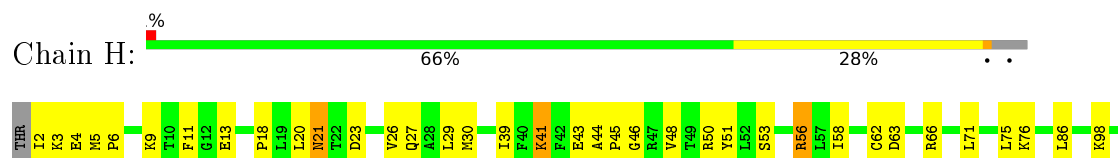
- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

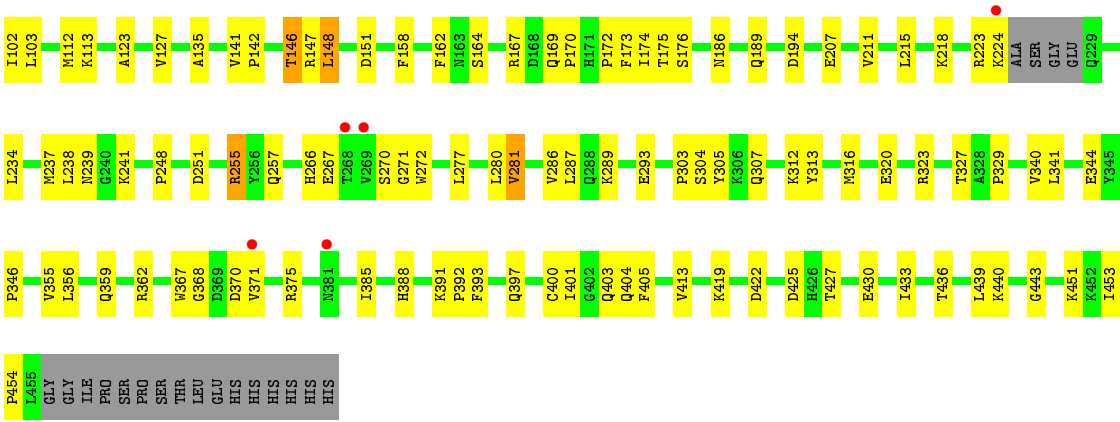


- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.71Å 167.41Å 228.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.97 – 2.34 32.97 – 2.34	Depositor EDS
% Data completeness (in resolution range)	100.0 (32.97-2.34) 100.0 (32.97-2.34)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.17 (at 2.34Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.215 , 0.284 0.214 , 0.284	Depositor DCC
R_{free} test set	1620 reflections (0.94%)	DCC
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.25$, $\langle L^2 \rangle = 0.11$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	30012	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.46	0/3665	0.66	3/4969 (0.1%)
1	B	0.46	0/3683	0.67	0/4990
1	C	0.45	0/3637	0.65	1/4935 (0.0%)
1	D	0.42	0/3579	0.62	0/4868
1	E	0.49	0/3678	0.67	0/4986
1	F	0.47	0/3651	0.66	1/4957 (0.0%)
1	G	0.46	0/3681	0.67	0/4992
1	H	0.45	0/3664	0.65	0/4963
All	All	0.46	0/29238	0.66	5/39660 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	310	GLN	CA-CB-CG	-7.88	96.06	113.40
1	A	168	ASP	C-N-CA	6.33	137.53	121.70
1	A	4	GLU	C-N-CA	-5.92	106.91	121.70
1	A	52	LEU	CA-CB-CG	5.16	127.16	115.30
1	C	234	LEU	CA-CB-CG	5.16	127.16	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	230	SER	Peptide

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	3579	0	3486	119	0
1	B	3597	0	3507	103	0
1	C	3551	0	3453	94	0
1	D	3493	0	3302	84	0
1	E	3589	0	3498	92	0
1	F	3565	0	3440	94	0
1	G	3585	0	3465	92	0
1	H	3578	0	3503	109	0
2	A	39	0	26	1	0
2	B	39	0	26	2	0
2	C	39	0	26	1	0
2	D	39	0	26	1	0
2	E	39	0	26	1	0
2	F	39	0	25	1	0
2	G	39	0	26	2	0
2	H	39	0	26	5	0
3	A	159	0	0	36	0
3	B	154	0	0	19	0
3	C	132	0	0	18	0
3	D	89	0	0	5	0
3	E	164	0	0	23	0
3	F	130	0	0	12	0
3	G	156	0	0	18	0
3	H	179	0	0	28	0
All	All	30012	0	27861	786	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 14.

The worst 5 of 786 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:F:228:GLU:CB	3:F:707:HOH:O	2.19	0.90
1:A:142:PRO:O	3:A:601:HOH:O	1.89	0.89
1:B:145:MET:SD	3:B:728:HOH:O	2.30	0.88
1:E:27:GLN:NE2	3:E:603:HOH:O	2.07	0.87
1:A:168:ASP:CG	1:A:169:GLN:H	1.77	0.87

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	449/471 (95%)	433 (96%)	14 (3%)	2 (0%)	39	45
1	B	449/471 (95%)	434 (97%)	14 (3%)	1 (0%)	52	61
1	C	448/471 (95%)	433 (97%)	12 (3%)	3 (1%)	26	28
1	D	450/471 (96%)	432 (96%)	16 (4%)	2 (0%)	39	45
1	E	448/471 (95%)	433 (97%)	13 (3%)	2 (0%)	39	45
1	F	451/471 (96%)	432 (96%)	15 (3%)	4 (1%)	21	21
1	G	450/471 (96%)	435 (97%)	10 (2%)	5 (1%)	17	16
1	H	446/471 (95%)	433 (97%)	10 (2%)	3 (1%)	26	28
All	All	3591/3768 (95%)	3465 (96%)	104 (3%)	22 (1%)	30	32

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	ASP
1	E	191	ALA
1	G	310	GLN
1	B	224	LYS
1	C	225	ALA

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	373/414 (90%)	360 (96%)	13 (4%)	43	55
1	B	378/414 (91%)	366 (97%)	12 (3%)	46	58
1	C	369/414 (89%)	353 (96%)	16 (4%)	35	45
1	D	345/414 (83%)	340 (99%)	5 (1%)	74	85
1	E	379/414 (92%)	373 (98%)	6 (2%)	70	82
1	F	367/414 (89%)	353 (96%)	14 (4%)	40	51
1	G	373/414 (90%)	356 (95%)	17 (5%)	33	41
1	H	376/414 (91%)	365 (97%)	11 (3%)	50	62
All	All	2960/3312 (89%)	2866 (97%)	94 (3%)	47	58

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	124	VAL
1	F	9	LYS
1	H	146	THR
1	D	192	ASN
1	E	245	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	388	HIS
1	G	310	GLN
1	E	404	GLN
1	B	116	HIS
1	E	128	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 ⓘ

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	FDE	A	501	1,3	29,46,46	6.18	15 (51%)	20,76,76	3.93	15 (75%)
2	FDE	B	501	1	29,46,46	6.11	16 (55%)	20,76,76	3.57	15 (75%)
2	FDE	C	501	1,3	29,46,46	6.03	15 (51%)	20,76,76	3.70	16 (80%)
2	FDE	D	501	1	29,46,46	5.95	15 (51%)	20,76,76	3.88	14 (70%)
2	FDE	E	501	1,3	29,46,46	5.89	14 (48%)	20,76,76	3.70	13 (65%)
2	FDE	F	501	1	29,46,46	5.98	14 (48%)	20,76,76	3.57	13 (65%)
2	FDE	G	501	1	29,46,46	5.89	15 (51%)	20,76,76	3.77	14 (70%)
2	FDE	H	501	1	29,46,46	5.93	15 (51%)	20,76,76	3.52	12 (60%)

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	FDE	A	501	1,3	-	0/6/86/86	0/0/8/8
2	FDE	B	501	1	-	0/6/86/86	0/0/8/8
2	FDE	C	501	1,3	-	0/6/86/86	0/0/8/8
2	FDE	D	501	1	-	0/6/86/86	0/0/8/8
2	FDE	E	501	1,3	-	0/6/86/86	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FDE	F	501	1	-	0/6/86/86	0/0/8/8
2	FDE	G	501	1	-	0/6/86/86	0/0/8/8
2	FDE	H	501	1	-	0/6/86/86	0/0/8/8

The worst 5 of 119 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FDE	C1C-NC	-12.51	1.32	1.49
2	E	501	FDE	C1C-NC	-12.31	1.32	1.49
2	H	501	FDE	C1C-NC	-12.19	1.32	1.49
2	D	501	FDE	C1C-NC	-11.96	1.32	1.49
2	A	501	FDE	C1C-NC	-11.85	1.32	1.49

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	FDE	CBD-CAD-C3D	-6.44	101.17	112.49
2	G	501	FDE	CBD-CAD-C3D	-6.21	101.58	112.49
2	H	501	FDE	CBD-CAD-C3D	-6.13	101.71	112.49
2	E	501	FDE	CMF-C3C-C2C	-6.03	118.91	128.11
2	D	501	FDE	CBD-CAD-C3D	-5.95	102.03	112.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FDE	1	0
2	B	501	FDE	2	0
2	C	501	FDE	1	0
2	D	501	FDE	1	0
2	E	501	FDE	1	0
2	F	501	FDE	1	0
2	G	501	FDE	2	0
2	H	501	FDE	5	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, 95th 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	453/471 (96%)	-0.07	7 (1%) 76 84	10, 22, 39, 56	0
1	B	453/471 (96%)	-0.22	3 (0%) 89 93	7, 18, 36, 52	0
1	C	452/471 (95%)	-0.21	3 (0%) 89 93	10, 22, 37, 52	0
1	D	454/471 (96%)	0.07	11 (2%) 62 73	14, 30, 46, 59	0
1	E	451/471 (95%)	-0.26	3 (0%) 89 93	6, 17, 34, 54	0
1	F	455/471 (96%)	-0.05	5 (1%) 82 89	10, 23, 44, 66	0
1	G	451/471 (95%)	-0.20	1 (0%) 95 98	7, 21, 38, 60	0
1	H	450/471 (95%)	-0.16	5 (1%) 82 89	7, 19, 37, 49	0
All	All	3619/3768 (96%)	-0.14	38 (1%) 82 89	6, 22, 41, 66	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	196	PRO	4.9
1	D	455	LEU	3.6
1	B	225	ALA	3.4
1	F	381	ASN	3.4
1	D	245	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, 95th 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
2	FDE	B	501	39/39	0.96	0.19	1.17	6,9,16,17	0
2	FDE	E	501	39/39	0.97	0.16	0.94	7,10,14,19	0
2	FDE	D	501	39/39	0.96	0.19	0.85	14,21,29,33	0
2	FDE	H	501	39/39	0.97	0.19	0.78	6,10,14,19	0
2	FDE	A	501	39/39	0.96	0.19	0.72	8,15,20,26	0
2	FDE	G	501	39/39	0.97	0.17	0.64	7,15,21,21	0
2	FDE	C	501	39/39	0.97	0.15	-0.09	4,10,15,17	0
2	FDE	F	501	39/39	0.97	0.14	-0.43	7,13,20,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.