

## Supplementary material

# The molecular structure of Rv2074, a probable pyridoxine 5'-phosphate oxidase from *Mycobacterium tuberculosis*, at 1.6 Å resolution

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**Table 1. Hydrogen bonds in Rv2074**

Main chain – Main chain		Main chain- Side chain And Side chain – Main chain		Side chain – Side chain	
Donor	Acceptor	Donor	Acceptor	Donor	Acceptor
LEU15 N	SER11 O	ALA14 N	SER11 OG	THR28 OG1	ASN64 OD1
ALA16 N	ASP12 O	SER34 N	ASP32 OD1	ARG30 NH1	SER34 OG
PHE17 N	ASP13 O	PHE42 N	TYR108 OH	SER34 OG	ASP32 OD1
LEU18 N	ALA14 O	LYS47 N	ASP45 OD2	THR55 OG1	SER59 OG
SER19 N	ALA16 O	THR48 N	ASP45 OD2	SER59 OG	THR55 OG1
GLU20 N	ALA16 O	ILE50 N	THR48 OG1	ARG67 NH1	SER68 OG
GLU20 N	PHE17 O	ALA62 N	SER59 OG	SER74 OG	SER83 OG
HIS22 N	GLU20 O	TRP81 N	SER130 OG	ARG80 NH1	GLU20 OE1
ALA24 N	VAL40 O	ASP93 N	ASN91 OD1	ARG80 NH2	GLU20 OE2
MSE25 N	SER74 O	ASP95 N	ASP93 OD2	ARG80 NH2	ASP77 OD2
LEU26 N	VAL38 O	ALA96 N	ASP93 OD2	SER83 OG	SER74 OG
THR27 N	VAL72 O	ARG116 N	ASN114 OD1	ASN91 ND2	GLU121 OE1
THR28 N	HIS36 O	SER11 OG	LEU133 O	ARG103 NH2	ASP45 OD1
ARG30 N	SER34 O	SER19 OG	LEU15 O	ARG103 NE	ASP99 OD2
ASN33 N	ARG30 O	ARG67 NH1	LEU29 O	ASN114 ND2	THR56 OG1
HIS36 N	THR28 O	SER83 OG	LEU128 O	ARG117 NH1	GLU101 OE2
VAL38 N	LEU26 O	ARG107 NE	GLU20 O	SER130 OG	ASP132 OD1
VAL40 N	ALA24 O	ARG107 NH1	GLU20 O		
THR43 N	ARG52 O	ARG107 NH2	PHE42 O		
ASP45 N	ILE50 O	TYR108 OH	HIS22 O		
HIS49 N	ASP45 O	ARG117 NH1	ARG112 O		
ALA51 N	VAL122 O	ARG117 NH2	ARG112 O		
ARG52 N	THR43 O	GLN123 NE2	THR48 O		
VAL53 N	ILE120 O	SER130 OG	TRP81 O		
THR55 N	VAL118 O				
GLY57 N	ARG116 O				

SER59	N	THR56	O		
VAL63	N	SER59	O		
ASN64	N	GLN60	O		
ALA65	N	LYS61	O		
ASP66	N	ALA62	O		
ARG67	N	VAL63	O		
SER68	N	ASN64	O		
GLY69	N	ALA65	O		
ALA71	N	GLY86	O		
VAL72	N	THR27	O		
LEU73	N	LEU84	O		
SER74	N	MSE25	O		
GLN75	N	LEU82	O		
ASP77	N	ARG80	O		
ARG80	N	ASP77	O		
LEU82	N	GLN75	O		
SER83	N	LEU128	O		
LEU84	N	LEU73	O		
GLU85	N	ARG126	O		
GLY86	N	ALA71	O		
ARG87	N	GLN123	O		
ALA88	N	GLY69	O		
ALA89	N	GLU121	O		
ASN91	N	VAL119	O		
VAL97	N	ASP93	O		
ARG98	N	ILE94	O		
ASP99	N	ASP95	O		
ALA100	N	ALA96	O		
GLU101	N	VAL97	O		
LEU102	N	ARG98	O		
ARG103	N	ASP99	O		
TYR104	N	ALA100	O		
ALA105	N	GLU101	O		
GLN106	N	LEU102	O		
ARG107	N	TYR104	O		
TYR108	N	TYR104	O		
ARG117	N	ASN114	O		
VAL118	N	THR55	O		
VAL119	N	ASN91	O		
ILE120	N	VAL53	O		
GLU121	N	ALA89	O		
VAL122	N	ALA51	O		
GLN123	N	ARG87	O		
ILE124	N	HIS49	O		
GLU125	N	GLU85	O		
ARG126	N	GLU85	O		
LEU128	N	SER83	O		
SER130	N	TRP81	O		
LEU133	N	SER130	O		