

In silico structural characterisation of *Plasmodium falciparum*
dihydro-6-hydroxymethylpterin pyrophosphokinase
dihydropteroate synthase (PPPK-DHPS)

by

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List of Abbreviations

Å	Angstrom
ABNR	Adopted Basis Newton-Raphson
ADP	Adenosine Diphosphate
AMP	Adenosine Monophosphate
ATP	Adenosine Triphosphate
Ba	<i>Bacillus anthracis</i>
CHARMM	Chemistry at HARvard Macromolecular Mechanics
CG	Conjugate Gradient
DHFR	Dihydrofolate reductase
DHFS	Dihydrofolate synthase
DHP	6-hydroxymethyl-7,8-dihydropterin pyrophosphate
DHPS	Dihydropteroate synthase
EC	Enzyme Commission
Ec	<i>Escherichia coli</i>
EM	Electron Microscopy
ESFF	Extensible Systematic Forcefield
FPGS	Tetrahydrofolylpolyglutamate synthase
GTP	Guanine triphosphate
Hi	<i>Haemophilus influenzae</i>
HP	6-hydroxymethyl-7,8-dihydropterin
HMM	Hidden Markov Model
K	Kelvin
kb	kilobases
kD	kilo Dalton
MANIC	6-methylamino-5-nitroisocytosine
MMFP	Miscellaneous Mean Field Potential
MSP	Merozoite Surface Protein

List of Abbreviations

Mtb	<i>Mycobacterium tuberculosis</i>
NCBI	National Center for Biotechnology Information
NMA	Normal Mode Analysis
NMR	Nuclear Magnetic Resonance
NOE	Nuclear Overhauser effect
ns	nanosecond
Pb	<i>Plasmodium berghei</i>
Pc	<i>Plasmodium chabaudi</i>
PDB	Protein Data Bank
Pf	<i>Plasmodium falciparum</i>
PPPK	Hydroxymethyl-dihydropteridine pyrophosphokinase
ps	picosecond
Pv	<i>Plasmodium vivax</i>
Py	<i>Plasmodium yoelli yoelli</i>
QM	Quantum mechanics
RESA	Ring-infected erythrocyte surface antigen
Sa	<i>Staphylococcus aureus</i>
SAN	Sulfanilamide
SD	Steepest Descent
TS	Thymidilate synthase

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Typographical Conventions

- Amino acids will be referred to either by their one-letter or three-letter abbreviations. A mutation will be indicated by the amino acid being mutated followed by its number, followed by the new residue e.g. Ala437Gly or A437G indicates Alanine 437 being mutated to Glycine.
- Species will be referred to by a two or three letter abbreviation e.g. *Plasmodium falciparum* will be Pf and *Mycobacterium tuberculosis* will be Mtb.