



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:35 PM GMT

PDB ID : 4YDQ
Title : Crystal Structure of Prolyl-tRNA Synthetase (PRS) from Plasmodium falciparum in complex with Halofuginone and AMPPNP
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Deposited on : 2015-02-23
Resolution : 2.30 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 (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

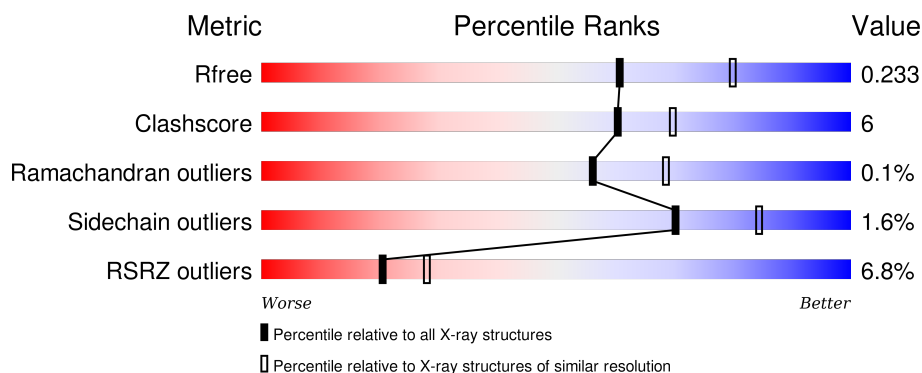
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	497	<div> <div>5%</div> <div>87%</div> <div>10% ..</div> </div>
1	B	497	<div> <div>8%</div> <div>83%</div> <div>13% .</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8230 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.

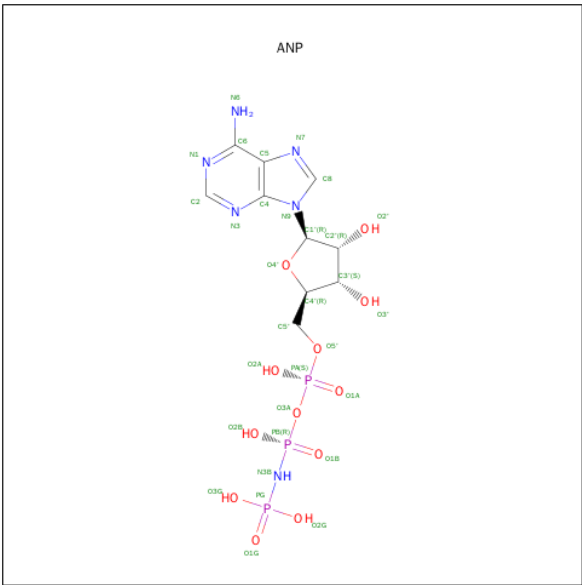
- Molecule 1 is a protein called Proline–tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	6	0
			3942	2548	652	719	23			
1	B	478	Total	C	N	O	S	0	5	0
			3843	2486	634	700	23			

There are 8 discrepancies between the modelled and reference sequences:

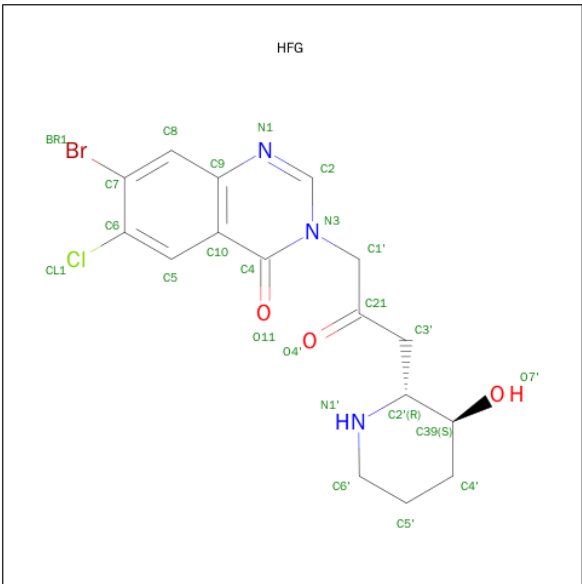
Chain	Residue	Modelled	Actual	Comment	Reference
A	250	GLY	-	expression tag	UNP Q8I5R7
A	251	ALA	-	expression tag	UNP Q8I5R7
A	252	MET	-	expression tag	UNP Q8I5R7
A	253	ALA	-	expression tag	UNP Q8I5R7
B	250	GLY	-	expression tag	UNP Q8I5R7
B	251	ALA	-	expression tag	UNP Q8I5R7
B	252	MET	-	expression tag	UNP Q8I5R7
B	253	ALA	-	expression tag	UNP Q8I5R7

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is 7-bromo-6-chloro-3-{3-[(2R,3S)-3-hydroxypiperidin-2-yl]-2-oxopropyl}quinazol in-4(3H)-one (three-letter code: HFG) (formula: C₁₆H₁₇BrClN₃O₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	Br	C	Cl	N	O	0	0
			24	1	16	1	3	3		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	Br	C	Cl	N	O	0	0
			24	1	16	1	3	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	196	Total	O	0	0
			196	196		
5	B	137	Total	O	0	0
			137	137		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.03Å 88.93Å 86.30Å 90.00° 96.71° 90.00°	Depositor
Resolution (Å)	27.82 – 2.30 27.82 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (27.82-2.30) 99.4 (27.82-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.184 , 0.232 0.193 , 0.233	Depositor DCC
R_{free} test set	2731 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 54064 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8230	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, ANP, HFG

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	0.55	1/4060 (0.0%)	0.62	1/5505 (0.0%)
1	B	0.47	1/3956 (0.0%)	0.60	0/5368
All	All	0.51	2/8016 (0.0%)	0.61	1/10873 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	407	TRP	CB-CG	-7.19	1.37	1.50
1	B	407	TRP	CB-CG	-6.18	1.39	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	434	TRP	CB-CA-C	5.71	121.82	110.40

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	3942	0	3868	45	0
1	B	3843	0	3742	44	0
2	A	31	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	0	13	0	0
3	A	24	0	17	2	0
3	B	24	0	17	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	196	0	0	1	0
5	B	137	0	0	3	0
All	All	8230	0	7670	87	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 6.

The worst 5 of 87 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:A:407:TRP:CZ3	1:A:409:GLU:HB3	2.06	0.90
1:A:434:TRP:HH2	1:A:515:SER:HB3	1.36	0.89
1:B:407:TRP:CZ3	1:B:409:GLU:HB3	2.09	0.87
1:A:434:TRP:CH2	1:A:515:SER:HB3	2.12	0.82
1:A:298:VAL:HB	1:A:434:TRP:CD1	2.15	0.82

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	486/497 (98%)	475 (98%)	11 (2%)	0	100	100
1	B	476/497 (96%)	461 (97%)	14 (3%)	1 (0%)	52	64
All	All	962/994 (97%)	936 (97%)	25 (3%)	1 (0%)	56	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	PRO

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	426/450 (95%)	419 (98%)	7 (2%)	70	84
1	B	410/450 (91%)	403 (98%)	7 (2%)	68	83
All	All	836/900 (93%)	822 (98%)	14 (2%)	70	83

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	698	LEU
1	B	255	THR
1	B	513	THR
1	A	609	ASN
1	B	374	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	408	GLN

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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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$
2	ANP	A	801	4	27,33,33	2.36	5 (18%)	30,52,52	1.35	4 (13%)
3	HFG	A	802	-	25,26,26	2.97	13 (52%)	20,37,37	1.82	3 (15%)
2	ANP	B	801	4	27,33,33	1.48	5 (18%)	30,52,52	1.04	2 (6%)
3	HFG	B	802	-	25,26,26	2.89	13 (52%)	20,37,37	2.17	6 (30%)

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	ANP	A	801	4	-	0/12/38/38	0/3/3/3
3	HFG	A	802	-	-	0/8/19/19	0/3/3/3
2	ANP	B	801	4	-	0/12/38/38	0/3/3/3
3	HFG	B	802	-	-	0/8/19/19	0/3/3/3

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	HFG	C1'-N3	-5.36	1.41	1.47
3	B	802	HFG	C1'-N3	-4.74	1.42	1.47
3	B	802	HFG	C8-C9	-4.40	1.35	1.41
3	A	802	HFG	C8-C9	-3.44	1.36	1.41
3	B	802	HFG	C39-C2'	-3.18	1.49	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	ANP	O3A-PA-O5'	-4.13	91.98	102.94
2	B	801	ANP	O1G-PG-N3B	-2.99	107.32	111.90
2	B	801	ANP	O1B-PB-N3B	-2.73	107.71	111.90
2	A	801	ANP	O5'-C5'-C4'	-2.71	99.14	109.12
3	B	802	HFG	C5-C10-C4	-2.47	119.18	122.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	HFG	2	0
3	B	802	HFG	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	486/497 (97%)	0.12	25 (5%) 32 41	24, 37, 63, 125	0
1	B	478/497 (96%)	0.44	41 (8%) 13 18	26, 45, 83, 110	0
All	All	964/994 (96%)	0.28	66 (6%) 20 28	24, 41, 80, 125	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	335	PHE	9.3
1	A	547	TYR	6.6
1	B	546	PHE	6.5
1	B	581	TYR	5.6
1	A	434	TRP	5.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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(\AA^2)	Q<0.9
2	ANP	B	801	31/31	0.93	0.16	-0.04	31,39,70,76	0
3	HFG	B	802	24/24	0.88	0.18	-0.08	24,34,43,77	24
3	HFG	A	802	24/24	0.96	0.17	-0.17	22,29,38,53	0
2	ANP	A	801	31/31	0.96	0.13	-0.80	26,32,48,113	0
4	MG	A	803	1/1	0.93	0.05	-1.99	45,45,45,45	0
4	MG	B	803	1/1	0.95	0.09	-	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.