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Supporting information for article:

**Conformational heterogeneity in apo and drug-bound structures of
Toxoplasma gondii prolyl-tRNA synthetase**

**Siddhartha Mishra, Nipun Malhotra, Shreya Kumari, Mizuki Sato, Haruhisa
Kikuchi, Manickam Yogavel and Amit Sharma**

331 **397**
Apo1 GAMVTAKKDENFSEWYTQAIVRSEMIEYYDISGCIYIMRPWAFHIWEKVQRFDDDEIKKMGVENSFYFP
Apo2 GAMVTAKKDENFSEWYTQAIVRSEMIEYYDISGCIYIMRPWAFHIWEKVQRFDDDEIKKMGVENSFYFP
Hol1 GAMVTAKKDENFSEWYTQAIVRSEMIEYYDISGCIYIMRPWAFHIWEKVQRFDDDEIKKMGVENSFYFP
Hol2 GAMVTAKKDENFSEWYTQAIVRSEMIEYYDISGCIYIMRPWAFHIWEKVQRFDDDEIKKMGVENSFYFP

398 **464**
Apo1 MFVSRHKLEKEKDHVEGFSPPEVAWVTHYGDSPLPEKIAIRPTSETIMYPAYAKWIRSHRDLPLKLNQ
Apo2 MFVSRHKLEKEKDHVEGFSPPEVAWVTHYGDSPLPEKIAIRPTSETIMYPAYAKWIRSHRDLPLKLNQ
Hol1 MFVSRHKLEKEKDHVEGFSPPEVAWVTHYGDSPLPEKIAIRPTSETIMYPAYAKWIRSHRDLPLKLNQ
Hol2 MFVSRHKLEKEKDHVEGFSPPEVAWVTHYGDSPLPEKIAIRPTSETIMYPAYAKWIRSHRDLPLKLNQ

465 **531**
Apo1 WCSVVRWEFKOPTPFLRTREFLWQEGHTAHATEEEAWELVLDILELYRRWYEECLAVPVIKGEKSEG
Apo2 WCSVVRWEFKOPTPFLRTREFLWQEGHTAHATEEEAWELVLDILELYRRWYEECLAVPVIKGEKSEG
Hol1 WCSVVRWEFKOPTPFLRTREFLWQEGHTAHATEEEAWELVLDILELYRRWYEECLAVPVIKGEKSEG
Hol2 WCSVVRWEFKOPTPFLRTREFLWQEGHTAHATEEEAWELVLDILELYRRWYEECLAVPVIKGEKSEG

532 **598**
Apo1 EKFAAGGKTTTVEAFI PENGRGIQAATSHLLGTNFAKMFIEIEFEDEEGHKRLVHQTSWGCTTRSLGV
Apo2 EKFAAGGKTTTVEAFI PENGRGIQAATSHLLGTNFAKMFIEIEFEDEEGHKRLVHQTSWGCTTRSLGV
Hol1 EKFAAGGKTTTVEAFI PENGRGIQAATSHLLGTNFAKMFIEIEFEDEEGHKRLVHQTSWGCTTRSLGV
Hol2 EKFAAGGKTTTVEAFI PENGRGIQAATSHLLGTNFAKMFIEIEFEDEEGHKRLVHQTSWGCTTRSLGV

599 **665**
Apo1 MIMTHGDDKGLVIPPVAVSVQVVIIPILFKDENTGEILGKCRELKTMLEKADIRVRIDDRSNYTPGW
Apo2 MIMTHGDDKGLVIPPVAVSVQVVIIPILFKDENTGEILGKCRELKTMLEKADIRVRIDDRSNYTPGW
Hol1 MIMTHGDDKGLVIPPVAVSVQVVIIPILFKDENTGEILGKCRELKTMLEKADIRVRIDDRSNYTPGW
Hol2 MIMTHGDDKGLVIPPVAVSVQVVIIPILFKDENTGEILGKCRELKTMLEKADIRVRIDDRSNYTPGW

666 **732**
Apo1 KYNHWEVKGVPRLRLELGPKDLAKGTARVVRRTGEAYQISWADLAPKLELMEGIQRSLFEKAKARL
Apo2 KYNHWEVKGVPRLRLELGPKDLAKGTARVVRRTGEAYQISWADLAPKLELMEGIQRSLFEKAKARL
Hol1 KYNHWEVKGVPRLRLELGPKDLAKGTARVVRRTGEAYQISWADLAPKLELMEGIQRSLFEKAKARL
Hol2 KYNHWEVKGVPRLRLELGPKDLAKGTARVVRRTGEAYQISWADLAPKLELMEGIQRSLFEKAKARL

733 **799**
Apo1 HEGIEKISTFDEVMPALNRKHLVLPAPWCEPSEEQIKKETQKLSEIQAEAGDSEQVMTGAMKTLC
Apo2 HEGIEKISTFDEVMPALNRKHLVLPAPWCEPSEEQIKKETQKLSEIQAEAGDSEQVMTGAMKTLC
Hol1 HEGIEKISTFDEVMPALNRKHLVLPAPWCEPSEEQIKKETQKLSEIQAEAGDSEQVMTGAMKTLC
Hol2 HEGIEKISTFDEVMPALNRKHLVLPAPWCEPSEEQIKKETQKLSEIQAEAGDSEQVMTGAMKTLC

800 **830**
Apo1 IPFDQPPMPEGTKCFYTGKPAKRWTWGRSY
Apo2 IPFDQPPMPEGTKCFYTGKPAKRWTWGRSY
Hol1 IPFDQPPMPEGTKCFYTGKPAKRWTWGRSY
Hol2 IPFDQPPMPEGTKCFYTGKPAKRWTWGRSY

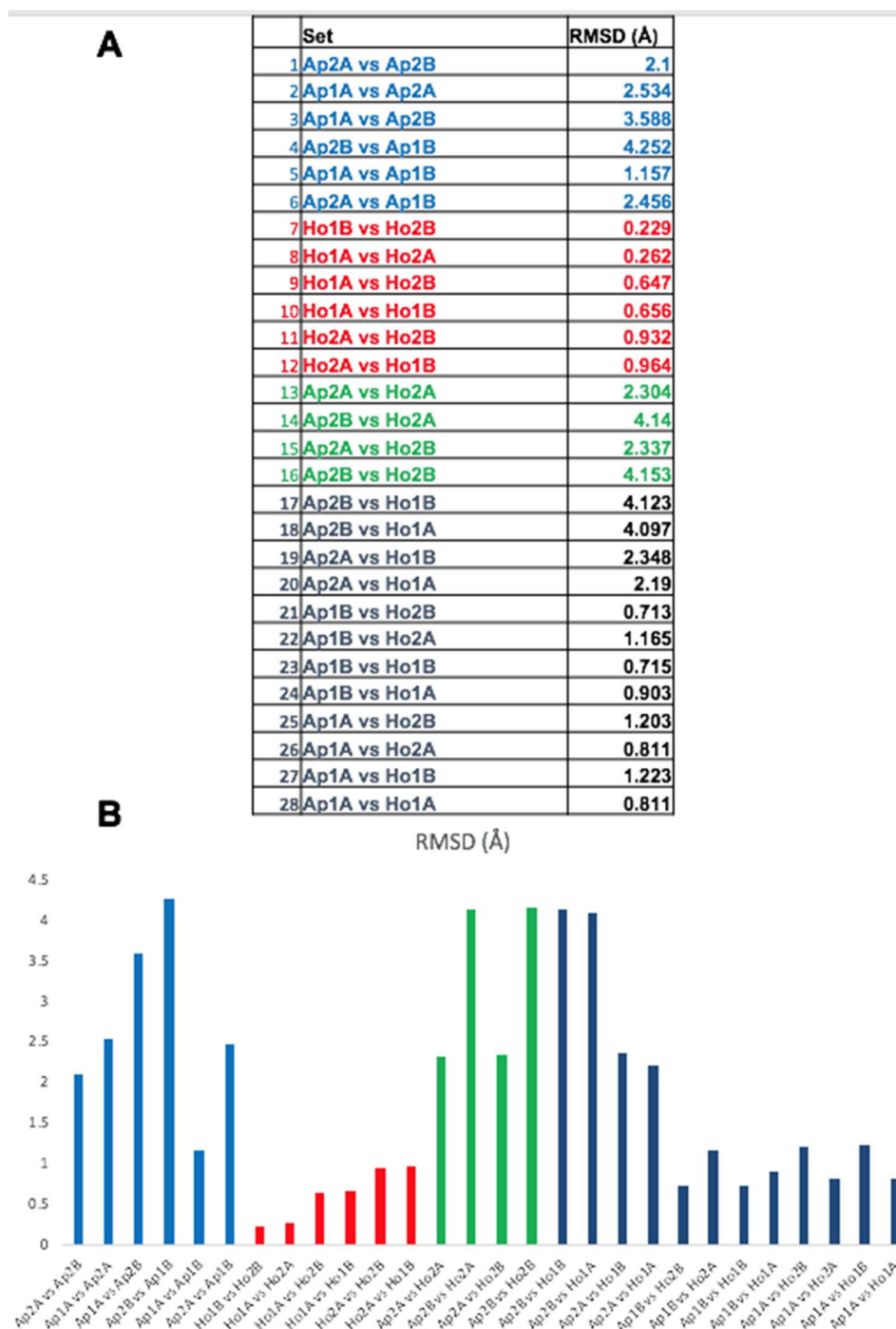


Figure S3 RMSD analyses of TgPRS Apo-Holo comparisons – related to Fig 6. RMSDs computed using GESAMT between A and B chains of Apo1, Apo2, Holo1 and Holo2 are shown color-coded in accordance with clusters of Apo-apo (blue), holo-holo (red) and apo-holo (green) comparisons. A1A – Apo1A, A1B – Apo1B, A2A – Apo2A, A2B – Apo2B, H1A – Holo1A, H1B – Holo1B, H2A – Holo2A, H2B – Holo2B. A shows the tabular data whilst B shows a graphical representation of the same.

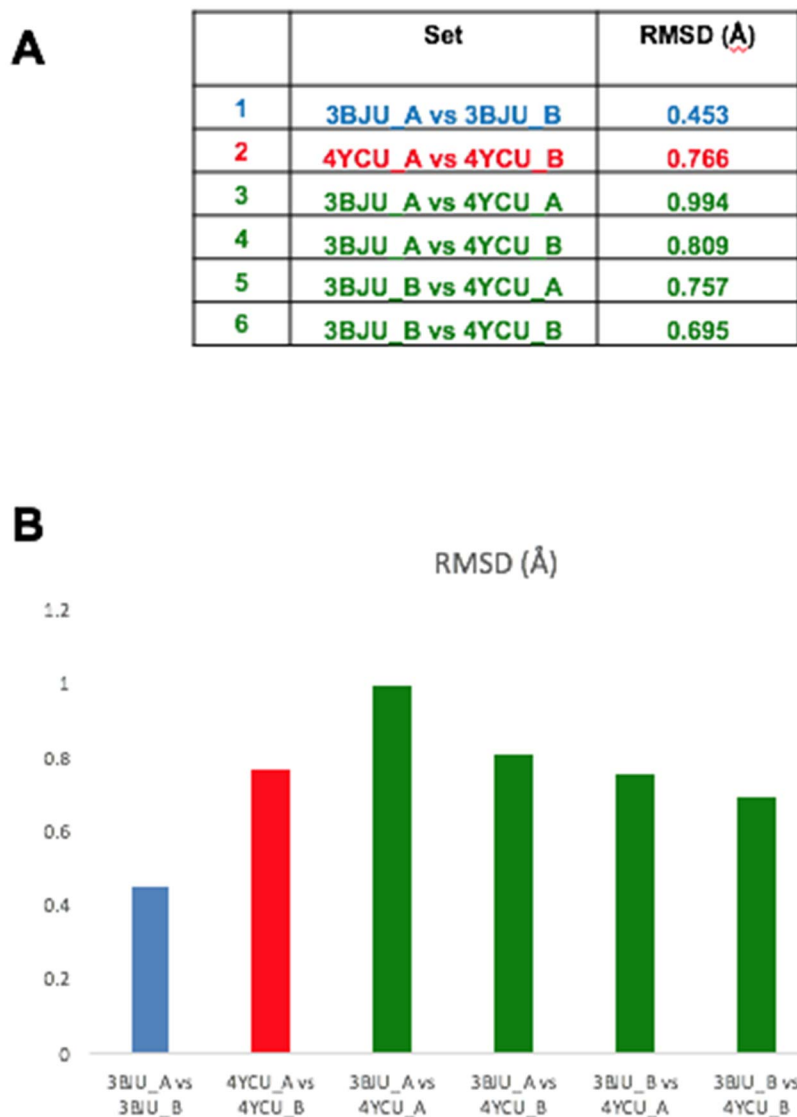


Figure S4 RMSD analyses of HsKRS ATP-Cladosporin bound comparisons – Related to Fig 7. RMSDs computed using GESAMT between A and B chains of 3BJU and 4YCU are shown color-coded in accordance with clusters of ATP-ATP (blue), CLD-CLD (red) and ATP-CLD (green) comparisons. A shows the tabular data whilst B shows a graphical representation of the same.