

CORRECTION

Correction: *Brucella melitensis* Methionyl-tRNA-Synthetase (MetRS), a Potential Drug Target for Brucellosis

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There is an error in the third-to-last sentence of the “BmMetRS in complex with inhibitors” section. The correct sentence is: A superposition of 4PY2 Chain B and 4MVW Chain A gives a good illustration of this (Fig 7).

There is an error in the caption for Fig 7. Please see the correct Fig 7 caption here.



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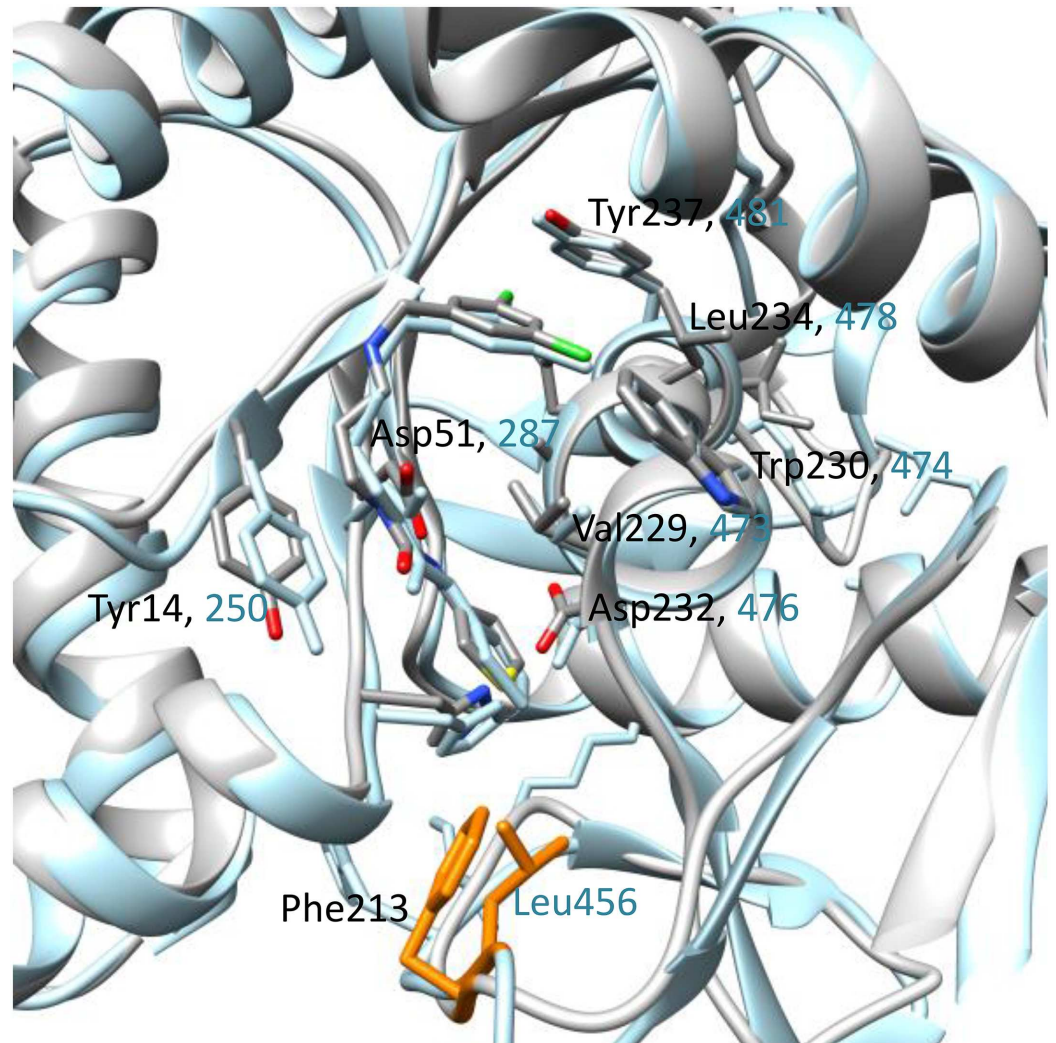


Fig 7. A superposition of *BmMetRS* (PDB ID 4PY2 Chain B) and *TbMetRS* (PDB ID 4MVW Chain) bound to compound 1433. A key difference is the interaction of *BmMetRS* Phe213 which is functionally equivalent to Leu456 in *TbMetRS* but led to different protein geometry. The *TbMetRS* structure is shown in blue and the 2 different residues in orange.

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Additionally, in Table 2, the “PDB code” value for “1433” should read “4PY2”. Please view the corrected [Table 2](#) here.

Table 2. Data collection and model refinement statistics.

| Crystal | SeMet | 1312 | 1415 | 1433 |
|--|------------------------|------------------------|------------------------|------------------------|
| PDB code | 4DLP | 5K0S | 5K0T | 4PY2 |
| Data collection | | | | |
| Space Group | P 1 21 1 | P 1 | P 1 | P 1 |
| Cell dimensions | | | | |
| <i>a</i> , <i>b</i> , <i>c</i> (Å) | 116.25, 77.62, 116.27 | 45.27, 99.74, 104.63 | 45.16, 99.65, 104.30 | 45.01, 99.48, 104.00 |
| α , β , γ (°) | 90, 119.67, 90 | 110.58, 87.63, 99.91 | 110.46, 88.09, 99.72 | 110.47, 87.24, 99.99 |
| Resolution range (Å) | 50.00–2.65 (2.72–2.65) | 50.00–2.40 (2.46–2.40) | 50.00–2.60 (2.67–2.60) | 50.00–2.15 (2.21–2.15) |
| No. of unique reflections | 52379 | 63652 | 49660 | 88924 |
| R_{merge} (%) ^a | 7.1 (48.6) | 6.4 (52.5) | 7.5 (47.0) | 6.6 (53.6) |
| Redundancy ^a | 3.7 (3.7) | 2.4 (2.4) | 2.4 (2.4) | 3.9 (4.0) |
| Completeness (%) ^a | 99.3 (99.5) | 96.3 (85.2) | 96.0 (97.5) | 98.2 (97.3) |
| I/σ ^a | 15.21 (2.63) | 11.43 (2.13) | 10.12 (2.07) | 15.76 (2.73) |
| Refinement | | | | |
| Resolution range | 50.00–2.65 (2.72–2.65) | 50.00–2.40 (2.46–2.40) | 50.00–2.60 (2.67–2.60) | 50.00–2.15 (2.21–2.15) |
| No. of protein atoms | 10934 | 11469 | 11189 | 11480 |
| No. of water molecules | 88 | 219 | 169 | 135 |
| R_{cryst} (%) | 19.7 | 21.0 | 25.6 | 17.8 |
| R_{free} (%) | 23.7 | 25.6 | 28.6 | 21.1 |
| Root-mean-square deviations from ideal stereochemistry | | | | |
| Bond lengths (Å) | 0.012 | 0.003 | 0.008 | 0.011 |
| Bond angles (°) | 1.421 | 0.577 | 1.183 | 1.384 |
| Mean B factor (all atoms) (Å ²) | 48.25 | 43.29 | 49.76 | 35.98 |
| Ramachandran plot | | | | |
| Favored region (%) | 96.87 | 98.77 | 98.67 | 97.43 |
| Allowed regions (%) | 3.13 | 1.23 | 1.33 | 2.57 |
| Outlier regions (%) | 0.00 | 0.00 | 0.00 | 0.00 |
| Clashscore | 2.3 | 2.5 | 0.46 | 0.79 |
| Molprobrity Score | 1.18 | 1.15 | 0.74 | 0.75 |

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Reference

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