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Supporting information for article:

**Crystal structure of hemoglobin from mouse (*Mus musculus*)
compared with those from human and from other small animals**

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Table S1 Difference in the amino acids of mouse and human Hbs

| S.No | Residue No | Mouse | Human | Residue No | Mouse | Human |
|------|------------------|-------|-------|-----------------|-------|-------|
| | α – chain | | | β – chain | | |
| 1 | 4 | Gly | Pro | 5 | Asp | Pro |
| 2 | 5 | Glu | Ala | 6 | Ala | Glu |
| 3 | 8 | Ser | Thr | 9 | Ala | Ser |
| 4 | 10 | Ile | Val | 12 | Ser | Thr |
| 5 | 17 | Ile | Val | 13 | Cys | Ala |
| 6 | 19 | Gly | Ala | 20 | Ser | Val |
| 7 | 21 | Gly | Ala | 41 | Tyr | Phe |
| 8 | 22 | Ala | Gly | 43 | Asp | Glu |
| 9 | 34 | Ala | Leu | 50 | Ser | Thr |
| 10 | 48 | Val | Leu | 51 | Ala | Pro |
| 11 | 67 | Ala | Thr | 52 | Ser | Asp |
| 12 | 68 | Ser | Asn | 54 | Ile | Val |
| 13 | 70 | Ala | Val | 58 | Ala | Pro |
| 14 | 71 | Gly | Ala | 68 | Ile | Leu |
| 15 | 73 | Leu | Val | 69 | Thr | Gly |
| 16 | 76 | Leu | Met | 72 | Asn | Ser |
| 17 | 78 | Gly | Asn | 76 | Asn | Ala |
| 18 | 111 | Ser | Ala | 80 | Ser | Asn |
| 19 | 113 | His | Leu | 87 | Ser | Thr |
| 20 | 116 | Asp | Glu | 109 | Met | Val |
| 21 | | | | 110 | Ile | Leu |
| 22 | | | | 112 | Ile | Cys |
| 23 | | | | 115 | Gly | Ala |
| 24 | | | | 118 | Leu | Phe |
| 25 | | | | 121 | Asp | Glu |
| 26 | | | | 125 | Ala | Pro |
| 27 | | | | 126 | Ala | Val |
| 28 | | | | 130 | Phe | Tyr |
| 29 | | | | 139 | Thr | Asn |

Table S2 Percent identity matrix for α and β chains of mouse, human and other small animal Hbs

| | Mouse | | BRat | | DMouse | | GPig | | Mongoose | | APika | | Rabbit | | EHare | | Cat | | Human | |
|-----------------|--------------|---------|-------------|---------|---------------|---------|-------------|---------|-----------------|---------|--------------|---------|---------------|---------|--------------|---------|------------|---------|--------------|---------|
| | α | β | α | β | α | β | α | β | α | β | α | β | α | β | α | β | α | β | α | β |
| Mouse | 100 | | 84.4 | 91.8 | 92.2 | 85.6 | 76.6 | 74.0 | 87.2 | 78.1 | 86.5 | 80.1 | 82.3 | 79.5 | 83.0 | 79.5 | 81.6 | 77.9 | 85.8 | 80.1 |
| BRat | 84.4 | 91.8 | 100 | | 83.7 | 84.3 | 75.9 | 74.7 | 79.4 | 80.1 | 80.1 | 80.8 | 78.0 | 80.8 | 77.3 | 80.8 | 77.3 | 78.6 | 78.0 | 81.5 |
| DMouse | 92.2 | 85.6 | 83.7 | 84.3 | 100 | | 78.7 | 74.0 | 84.4 | 79.5 | 85.8 | 79.5 | 81.6 | 78.1 | 82.3 | 78.1 | 81.6 | 75.9 | 85.1 | 76.7 |
| GPig | 76.6 | 74.0 | 75.9 | 74.7 | 78.7 | 74.0 | 100 | | 73.8 | 74.7 | 76.6 | 74.0 | 73.8 | 77.4 | 73.1 | 76.7 | 75.2 | 76.6 | 75.9 | 74.7 |
| Mongoose | 87.2 | 78.1 | 79.4 | 80.1 | 84.4 | 79.5 | 73.8 | 74.7 | 100 | | 87.2 | 81.5 | 87.2 | 87.0 | 87.9 | 84.3 | 87.2 | 85.5 | 87.9 | 85.6 |
| APika | 86.5 | 80.1 | 80.1 | 80.8 | 85.8 | 79.5 | 76.6 | 74.0 | 87.2 | 81.5 | 100 | | 84.4 | 87.7 | 85.1 | 89.7 | 84.4 | 79.3 | 90.1 | 84.3 |
| Rabbit | 82.3 | 79.5 | 78.0 | 80.8 | 81.6 | 78.1 | 73.8 | 77.4 | 87.2 | 87.0 | 84.4 | 87.7 | 100 | | 99.3 | 96.6 | 78.0 | 82.1 | 82.3 | 90.4 |
| EHare | 83.0 | 79.5 | 77.3 | 80.8 | 82.3 | 78.1 | 73.1 | 76.7 | 87.9 | 84.3 | 85.1 | 89.7 | 99.3 | 96.6 | 100 | | 78.7 | 80.7 | 83.0 | 91.1 |
| Cat | 81.6 | 77.9 | 77.3 | 78.6 | 81.6 | 75.9 | 75.2 | 76.6 | 87.2 | 85.5 | 84.4 | 79.3 | 78.0 | 82.1 | 78.7 | 80.7 | 100 | | 85.1 | 83.5 |
| Human | 85.8 | 80.1 | 78.0 | 81.5 | 85.1 | 76.7 | 75.9 | 74.7 | 87.9 | 85.6 | 90.1 | 84.3 | 82.3 | 90.4 | 83.0 | 91.1 | 85.1 | 83.5 | 100 | |

Table S3 Comparison of the overall structure (tetramer) and dimer of mouse with human and other small animals Hbs.

| | | Mouse | BRat | DMouse (AM) | DMouse (D) | GPig (O) | GPig (M) | Mongoose (O) | APika | Rabbit (O) | EHare (O) | Cat | Human (O) | Human (CO) | Human (D) | Human (M) |
|--------------|------------------------------|---------------------------------|-------|-------------|------------|----------|----------|--------------|-------|------------|-----------|-------|-----------|------------|-----------|-----------|
| | | Tetramer (r.m.s.d. values in Å) | | | | | | | | | | | | | | |
| Mouse | Dimer (r.m.s.d. values in Å) | 100 | 2.178 | 0.615 | 1.883 | 2.044 | 1.947 | 1.799 | 1.788 | 2.242 | 2.100 | 2.278 | 0.904 | 0.938 | 2.005 | 1.729 |
| Brat | | 0.671 | 100 | 2.165 | 0.584 | 0.539 | 0.540 | 0.615 | 0.561 | 0.456 | 0.531 | 3.998 | 1.596 | 1.542 | 2.005 | 1.729 |
| DMouse AM | | 0.535 | 0.744 | 100 | 1.893 | 2.093 | 1.987 | 1.805 | 1.776 | 2.256 | 2.033 | 2.355 | 0.890 | 0.974 | 1.957 | 1.766 |
| DMouse (D) | | 0.647 | 0.534 | 0.402 | 100 | 0.615 | 0.582 | 0.483 | 0.505 | 0.671 | 0.552 | 3.659 | 1.307 | 1.203 | 3.040 | 1.282 |
| GPig (O) | | 0.709 | 0.487 | 0.642 | 0.551 | 100 | 0.240 | 0.521 | 0.513 | 0.630 | 0.619 | 3.757 | 1.513 | 1.455 | 3.160 | 1.423 |
| GPig (M) | | 0.745 | 0.524 | 0.643 | 0.553 | 0.225 | 100 | 0.472 | 0.549 | 0.649 | 0.595 | 3.737 | 1.468 | 1.336 | 3.147 | 1.442 |
| Mongoose (O) | | 0.692 | 0.443 | 0.584 | 0.553 | 0.460 | 0.425 | 100 | 0.442 | 0.679 | 0.566 | 3.522 | 1.176 | 1.122 | 2.878 | 1.185 |
| APika | | 0.556 | 0.463 | 0.586 | 0.497 | 0.433 | 0.462 | 0.366 | 100 | 0.671 | 0.591 | 3.642 | 1.099 | 1.048 | 3.103 | 1.236 |
| Rabbit (O) | | 0.744 | 0.385 | 0.753 | 0.584 | 0.525 | 0.533 | 0.480 | 0.422 | 100 | 0.504 | 3.982 | 1.616 | 1.542 | 3.396 | 1.256 |
| EHare (O) | | 0.696 | 0.468 | 0.665 | 0.542 | 0.600 | 0.613 | 0.534 | 0.465 | 0.374 | 100 | 3.884 | 1.470 | 1.419 | 3.263 | 1.272 |
| Cat | | 0.805 | 0.620 | 0.695 | 0.536 | 0.728 | 0.702 | 0.557 | 0.606 | 0.529 | 0.561 | 100 | 2.690 | 2.647 | 1.525 | 3.049 |
| Human (O) | | 0.572 | 0.570 | 0.600 | 0.654 | 0.711 | 0.705 | 0.578 | 0.493 | 0.476 | 0.557 | 0.621 | 100 | 0.411 | 2.261 | 1.408 |
| Human (CO) | | 0.622 | 0.591 | 0.636 | 0.702 | 0.736 | 0.742 | 0.656 | 0.555 | 0.412 | 0.554 | 0.658 | 0.338 | 100 | 2.310 | 1.252 |
| Human (D) | | 0.689 | 0.855 | 0.757 | 0.839 | 1.039 | 1.055 | 0.815 | 0.961 | 0.728 | 0.875 | 0.781 | 0.597 | 0.528 | 100 | 2.522 |
| Human (M) | | 0.737 | 0.639 | 0.759 | 0.772 | 0.756 | 0.770 | 0.630 | 0.644 | 0.524 | 0.666 | 0.724 | 0.563 | 0.485 | 0.615 | 100 |

Abbreviations: Aquo-met (AM); deoxy (D); oxy (O); met (M); carboxy or carbonmonoxy (CO)

Table S4 Comparison of α - and β -subunits of mouse met Hb with human and other small animals Hbs in terms of r.m.s.d.

| | Mouse | BRat | DMouse (AM) | DMouse (D) | GPig (O) | GPig (M) | Mongoose (O) | APika | Rabbit (O) | EHare (O) | Cat | Human (O) | Human (CO) | Human (D) | Human (M) |
|--------------|---|-------|-------------|------------|----------|----------|--------------|-------|------------|-----------|-------|-----------|------------|-----------|-----------|
| | α - subunit (r.m.s.d. values in Å) | | | | | | | | | | | | | | |
| Mouse | 100 | 0.595 | 0.457 | 0.661 | 0.624 | 0.608 | 0.614 | 0.528 | 0.707 | 0.691 | 0.676 | 0.519 | 0.549 | 0.652 | 0.675 |
| BRat | 0.584 | 100 | 0.526 | 0.407 | 0.404 | 0.449 | 0.326 | 0.383 | 0.287 | 0.417 | 0.422 | 0.512 | 0.531 | 0.498 | 0.534 |
| DMouse (AM) | 0.494 | 0.485 | 100 | 0.466 | 0.545 | 0.499 | 0.434 | 0.402 | 0.540 | 0.483 | 0.534 | 0.477 | 0.458 | 0.544 | 0.584 |
| DMouse (D) | 0.537 | 0.460 | 0.282 | 100 | 0.487 | 0.453 | 0.335 | 0.367 | 0.440 | 0.442 | 0.470 | 0.575 | 0.595 | 0.689 | 0.654 |
| GPig (O) | 0.757 | 0.428 | 0.464 | 0.510 | 100 | 0.161 | 0.354 | 0.399 | 0.471 | 0.518 | 0.500 | 0.531 | 0.553 | 0.635 | 0.611 |
| GPig (M) | 0.763 | 0.496 | 0.441 | 0.600 | 0.274 | 100 | 0.344 | 0.351 | 0.480 | 0.534 | 0.508 | 0.529 | 0.557 | 0.636 | 0.598 |
| Mongoose (O) | 0.623 | 0.389 | 0.453 | 0.444 | 0.455 | 0.483 | 100 | 0.312 | 0.281 | 0.354 | 0.378 | 0.524 | 0.524 | 0.503 | 0.548 |
| APika | 0.598 | 0.479 | 0.466 | 0.532 | 0.404 | 0.516 | 0.363 | 100 | 0.397 | 0.414 | 0.467 | 0.364 | 0.486 | 0.710 | 0.530 |
| Rabbit (O) | 0.597 | 0.380 | 0.592 | 0.516 | 0.377 | 0.439 | 0.391 | 0.341 | 100 | 0.332 | 0.428 | 0.518 | 0.474 | 0.533 | 0.483 |
| EHare (O) | 0.602 | 0.428 | 0.535 | 0.525 | 0.422 | 0.495 | 0.459 | 0.399 | 0.322 | 100 | 0.467 | 0.608 | 0.564 | 0.548 | 0.629 |
| Cat | 0.580 | 0.518 | 0.387 | 0.415 | 0.484 | 0.470 | 0.319 | 0.390 | 0.404 | 0.499 | 100 | 0.483 | 0.551 | 0.612 | 0.627 |
| Human (O) | 0.524 | 0.446 | 0.475 | 0.519 | 0.517 | 0.555 | 0.432 | 0.415 | 0.383 | 0.408 | 0.450 | 100 | 0.316 | 0.479 | 0.514 |
| Human (CO) | 0.566 | 0.450 | 0.556 | 0.551 | 0.540 | 0.529 | 0.453 | 0.486 | 0.296 | 0.390 | 0.462 | 0.328 | 100 | 0.401 | 0.421 |
| Human (D) | 0.644 | 0.877 | 0.568 | 0.654 | 0.747 | 0.723 | 0.521 | 0.759 | 0.671 | 0.769 | 0.532 | 0.745 | 0.653 | 100 | 0.513 |
| Human (M) | 0.640 | 0.566 | 0.521 | 0.581 | 0.536 | 0.563 | 0.447 | 0.534 | 0.410 | 0.451 | 0.528 | 0.451 | 0.455 | 0.687 | 100 |

Abbreviations: Aquo-met (AM); deoxy (D); oxy (O); met (M); carboxy or carbonmonoxy (CO)

Table S5 Switch region comparison of mouse met Hb with human and other small animal Hbs in terms of r.m.s.d. (Å).

| | Mouse | BRat | DMouse (AM) | DMouse (D) | GPig (O) | GPig (M) | Mongoose (O) | APika | Rabbit (O) | EHare (O) | Cat | Human (O) | Human (CO) | Human (D) | Human (M) |
|--------------|-------|-------|-------------|------------|----------|----------|--------------|-------|------------|-----------|-------|-----------|------------|-----------|-----------|
| Mouse | 100 | 0.905 | 0.282 | 0.632 | 0.810 | 0.907 | 0.631 | 0.596 | 0.797 | 0.701 | 1.652 | 0.532 | 0.488 | 1.247 | 0.573 |
| BRat | 0.905 | 100 | 0.765 | 0.371 | 0.201 | 0.154 | 0.351 | 0.362 | 0.207 | 0.407 | 2.154 | 0.488 | 0.556 | 1.889 | 0.307 |
| DMouse (AM) | 0.282 | 0.765 | 100 | 0.510 | 0.668 | 0.782 | 0.475 | 0.449 | 0.664 | 0.594 | 1.719 | 0.419 | 0.395 | 1.317 | 0.526 |
| DMouse (D) | 0.632 | 0.371 | 0.510 | 100 | 0.276 | 0.347 | 0.174 | 0.194 | 0.232 | 0.261 | 1.957 | 0.283 | 0.344 | 1.665 | 0.289 |
| GPig (O) | 0.810 | 0.201 | 0.668 | 0.276 | 100 | 0.137 | 0.270 | 0.282 | 0.132 | 0.319 | 2.071 | 0.300 | 0.449 | 1.798 | 0.260 |
| GPig (M) | 0.907 | 0.154 | 0.782 | 0.347 | 0.137 | 100 | 0.359 | 0.367 | 0.180 | 0.387 | 2.132 | 0.367 | 0.427 | 1.883 | 0.247 |
| Mongoose (O) | 0.631 | 0.351 | 0.475 | 0.174 | 0.270 | 0.359 | 100 | 0.144 | 0.241 | 0.267 | 1.942 | 0.264 | 0.312 | 1.640 | 0.145 |
| APika | 0.596 | 0.362 | 0.449 | 0.194 | 0.282 | 0.367 | 0.144 | 100 | 0.262 | 0.329 | 1.945 | 0.266 | 0.318 | 1.631 | 0.240 |
| Rabbit (O) | 0.797 | 0.207 | 0.664 | 0.232 | 0.132 | 0.180 | 0.241 | 0.262 | 100 | 0.299 | 2.081 | 0.381 | 0.450 | 1.809 | 0.187 |
| EHare (O) | 0.701 | 0.407 | 0.594 | 0.261 | 0.319 | 0.387 | 0.267 | 0.329 | 0.299 | 100 | 1.912 | 0.344 | 0.388 | 1.654 | 0.339 |
| Cat | 1.652 | 2.154 | 1.719 | 1.957 | 2.071 | 2.132 | 1.942 | 1.945 | 2.081 | 1.912 | 100 | 1.779 | 1.714 | 0.444 | 1.818 |
| Human (O) | 0.532 | 0.488 | 0.419 | 0.283 | 0.300 | 0.367 | 0.264 | 0.266 | 0.381 | 0.344 | 1.779 | 100 | 0.152 | 1.473 | 0.267 |
| Human (CO) | 0.488 | 0.556 | 0.395 | 0.344 | 0.449 | 0.427 | 0.312 | 0.318 | 0.450 | 0.388 | 1.714 | 0.152 | 100 | 1.411 | 0.346 |
| Human (D) | 1.247 | 1.889 | 1.317 | 1.665 | 1.798 | 1.883 | 1.640 | 1.631 | 1.809 | 1.654 | 0.444 | 1.473 | 1.411 | 100 | 1.524 |
| Human (M) | 0.573 | 0.307 | 0.526 | 0.289 | 0.260 | 0.247 | 0.145 | 0.240 | 0.187 | 0.339 | 1.818 | 0.267 | 0.346 | 1.524 | 100 |

Abbreviations: Aquo-met (AM); deoxy (D); oxy (O); met (M); carboxy or carbonmonoxy (CO)

Table S6 The α - and β -heme groups comparison of mouse met Hb with human and other small animal Hbs in terms of r.m.s.d. (Å).

| | | Mouse | BRat | DMouse (AM) | DMouse (D) | GPig (O) | GPig (M) | Mongoose (O) | APika | Rabbit (O) | EHare (O) | Cat | Human (O) | Human (CO) | Human (D) | Human (M) |
|--------------|--|---|-------|-------------|------------|----------|----------|--------------|-------|------------|-----------|-------|-----------|------------|-----------|-----------|
| | | α - subunit (r.m.s.d. values in Å) | | | | | | | | | | | | | | |
| Mouse | β - subunit (r.m.s.d. values in Å) | 100 | 0.191 | 0.356 | 0.327 | 0.352 | 0.343 | 0.370 | 0.212 | 0.292 | 0.358 | 0.307 | 0.271 | 0.205 | 0.494 | 0.305 |
| BRat | | 0.502 | 100 | 0.248 | 0.293 | 0.199 | 0.212 | 0.226 | 0.114 | 0.189 | 0.271 | 0.135 | 0.197 | 0.138 | 0.432 | 0.171 |
| DMouse (AM) | | 0.279 | 0.366 | 100 | 0.476 | 0.158 | 0.131 | 0.338 | 0.302 | 0.373 | 0.428 | 0.252 | 0.287 | 0.341 | 0.412 | 0.382 |
| DMouse (D) | | 0.323 | 0.400 | 0.112 | 100 | 0.358 | 0.376 | 0.264 | 0.246 | 0.213 | 0.263 | 0.294 | 0.239 | 0.208 | 0.632 | 0.254 |
| GPig (O) | | 0.404 | 0.266 | 0.161 | 0.165 | 100 | 0.086 | 0.203 | 0.229 | 0.260 | 0.320 | 0.134 | 0.192 | 0.256 | 0.435 | 0.276 |
| GPig (M) | | 0.437 | 0.343 | 0.177 | 0.160 | 0.085 | 100 | 0.269 | 0.250 | 0.307 | 0.378 | 0.189 | 0.226 | 0.289 | 0.484 | 0.315 |
| Mongoose (O) | | 0.402 | 0.408 | 0.146 | 0.180 | 0.181 | 0.145 | 100 | 0.200 | 0.160 | 0.141 | 0.154 | 0.170 | 0.181 | 0.439 | 0.211 |
| APika | | 0.348 | 0.316 | 0.120 | 0.179 | 0.147 | 0.175 | 0.140 | 100 | 0.118 | 0.233 | 0.182 | 0.188 | 0.093 | 0.475 | 0.184 |
| Rabbit (O) | | 0.342 | 0.316 | 0.115 | 0.198 | 0.154 | 0.183 | 0.149 | 0.056 | 100 | 0.188 | 0.182 | 0.206 | 0.111 | 0.496 | 0.145 |
| EHare (O) | | 0.443 | 0.377 | 0.215 | 0.273 | 0.239 | 0.249 | 0.168 | 0.185 | 0.188 | 100 | 0.248 | 0.207 | 0.172 | 0.426 | 0.251 |
| Cat | | 0.444 | 0.369 | 0.246 | 0.304 | 0.266 | 0.281 | 0.191 | 0.171 | 0.192 | 0.117 | 100 | 0.180 | 0.182 | 0.424 | 0.154 |
| Human (O) | | 0.351 | 0.491 | 0.183 | 0.233 | 0.300 | 0.290 | 0.173 | 0.184 | 0.194 | 0.211 | 0.213 | 100 | 0.149 | 0.431 | 0.267 |
| Human (CO) | | 0.358 | 0.452 | 0.147 | 0.184 | 0.238 | 0.215 | 0.104 | 0.139 | 0.154 | 0.213 | 0.209 | 0.093 | 100 | 0.449 | 0.176 |
| Human (D) | | 0.647 | 0.854 | 0.538 | 0.508 | 0.605 | 0.535 | 0.470 | 0.580 | 0.591 | 0.601 | 0.611 | 0.487 | 0.456 | 100 | 0.509 |
| Human (M) | 0.493 | 0.510 | 0.350 | 0.427 | 0.420 | 0.440 | 0.364 | 0.341 | 0.319 | 0.254 | 0.310 | 0.296 | 0.353 | 0.730 | 100 | |

Abbreviations: Aquo-met (AM); deoxy (D); oxy (O); met (M); carboxy or carbonmonoxy (CO)

Table S7 The Iron to Iron (Fe-Fe) distances of mouse met Hb with human and other small animal Hbs (Å).

| | Mouse | BRat | DMouse (AM) | DMouse (D) | GPig (O) | GPig (M) | Mongoose (O) | APika | Rabbit (O) | EHare (O) | Cat | Human (O) | Human (CO) | Human (D) | Human (M) |
|--------------------|-------|-------|----------------|---------------|-------------|-------------|-----------------|-------|---------------|--------------|-------|--------------|---------------|--------------|--------------|
| $\alpha 1\beta 1$ | 34.9 | 35.1 | 35.5 | 34.7 | 35.4 | 35.8 | 35.4 | 34.8 | 34.5 | 34.8 | 34.4 | 34.7 | 34.8 | 36.5 | 34.9 |
| $\alpha 1\beta 2$ | 25.9 | 26.4 | 25.5 | 25.9 | 26.3 | 26.4 | 25.9 | 26.1 | 26.2 | 26.0 | 24.4 | 25.5 | 25.7 | 24.3 | 26.8 |
| $\alpha 1\alpha 2$ | 34.9 | 35.9 | 35.6 | 35.7 | 35.7 | 35.7 | 35.8 | 35.3 | 35.3 | 35.9 | 32.7 | 34.7 | 34.8 | 34.2 | 36.6 |
| $\beta 1\beta 2$ | 35.4 | 34.0 | 35.1 | 34.6 | 34.7 | 34.9 | 34.9 | 34.2 | 34.3 | 34.2 | 38.6 | 34.6 | 34.7 | 39.5 | 36.6 |
| Total | 131.1 | 131.4 | 131.7 | 130.9 | 132.1 | 132.8 | 132.0 | 130.4 | 130.3 | 130.9 | 130.1 | 129.5 | 130.0 | 134.5 | 134.9 |

Abbreviations: Aquo-met (AM); deoxy (D); oxy (O); met (M); carboxy or carbonmonoxy (CO)