

Supplementary

Table S1. Comparison of the subunit–subunit interface area.

| μ -GST | Interface Area (Å ²) |
|------------------|----------------------------------|
| <i>CdGSTM1-1</i> | 1379.5 |
| 1xw6 | 1249.2 |
| 1ab6 | 1383.6 |
| 4gtu | 1353.6 |
| 2dc5 | 1358.8 |
| 1gsu | 1212.2 |
| 5an1 | 1157.5 |
| 6gst | 1328.5 |

Table S2. Salt bridges between the *CdGSMT1* subunits (cut-off distance 4.0 Å).

| Subunit C | Distance (Å) | Subunit A |
|-------------|--------------|-----------|
| Arg82 NE | 3.47 | Glu91 OE1 |
| Arg82 NH2 | 3.21 | Glu91 OE1 |
| Arg82 NE | 3.00 | Glu91 OE2 |
| Arg82 NH2 | 3.99 | Glu91 OE2 |
| His68 NE2 | 3.18 | Glu92 OE1 |
| Arg78 NH2 | 2.98 | Asp98 OD1 |
| Arg78 NE | 3.10 | Asp98 OD1 |
| Arg78 NH2 | 3.59 | Asp98 OD2 |
| Arg78 NE | 2.74 | Asp98 OD2 |
| Arg82 NH1 | 2.86 | Asp98 OD2 |
| Arg82 NH2 | 3.81 | Asp98 OD2 |
| Glu91 OE1 | 3.97 | Arg82 NH2 |
| Glu91 OE1 | 3.17 | Arg82 NE |
| Glu91 OE2 | 2.76 | Arg82 NH2 |
| Glu91 OE2 | 3.02 | Arg82 NE |
| Asp98 OD1 | 3.00 | Arg78 NH1 |
| Asp98 OD2 | 2.83 | Arg82 NH1 |
| Asp98 OD2 | 3.99 | Arg82 NH2 |
| Glu101 OE1 | 3.27 | Arg78 NH1 |
| Glu101 OE1 | 3.94 | Arg78 NH2 |
| Glu101 OE2 | 3.96 | Arg78 NH1 |
| Glu 101 OE2 | 3.24 | Arg78 NH2 |
| Subunit F | Distance (Å) | Subunit B |
| Arg78 NE | 3.20 | Asp98 OD1 |
| Arg78 NE | 2.95 | Asp98 OD2 |
| Arg78 NH2 | 3.27 | Asp98 OD1 |
| Arg78 NH2 | 3.89 | Asp98 OD2 |
| Arg82 NE | 2.85 | Glu91 OE1 |
| Arg82 NE | 3.09 | Glu91 OE2 |
| Arg82 NH1 | 3.06 | Asp98 OD2 |
| Arg82 NH2 | 3.70 | Glu91 OE1 |

| | | |
|------------|------|------------|
| Arg82 NH2 | 2.60 | Glu91 OE2 |
| Glu91 OE1 | 2.98 | Arg82 NE |
| Glu91 OE2 | 3.16 | Arg82 NE |
| Glu91 OE2 | 2.90 | Arg82 NH2 |
| Glu92 OE2 | 3.68 | His68 NE2 |
| Asp98 OD1 | 2.77 | Arg78 NH1 |
| Asp98 OD2 | 2.83 | Arg82 NH1 |
| Asp98 OD2 | 3.80 | Arg82 NH2] |
| Glu101 OE1 | 3.27 | Arg78 NH1 |
| Glu101 OE1 | 3.85 | Arg78 NH2 |
| Glu101 OE2 | 3.89 | Arg78 NH1 |
| Glu101 OE2 | 3.08 | Arg78 NH2 |
