



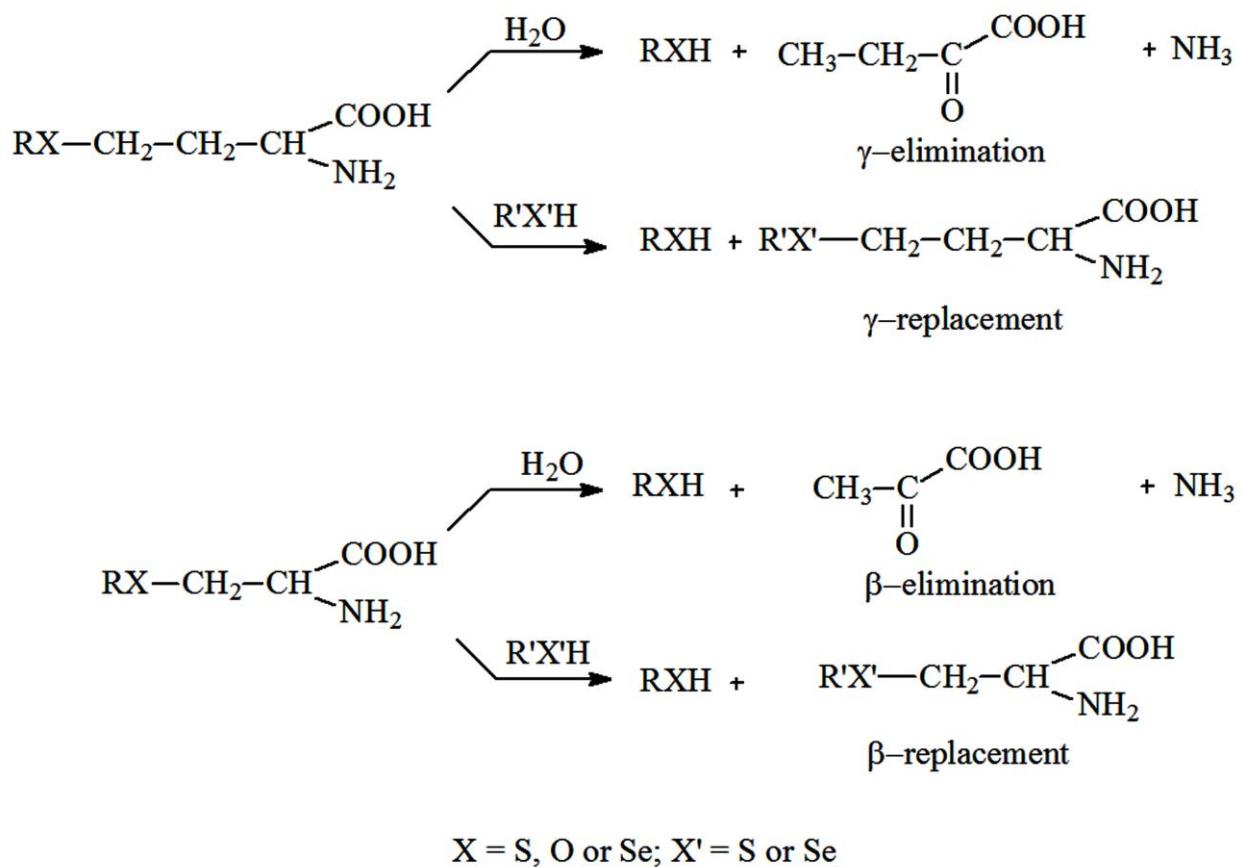
STRUCTURAL BIOLOGY  
COMMUNICATIONS

Volume 72 (2016)

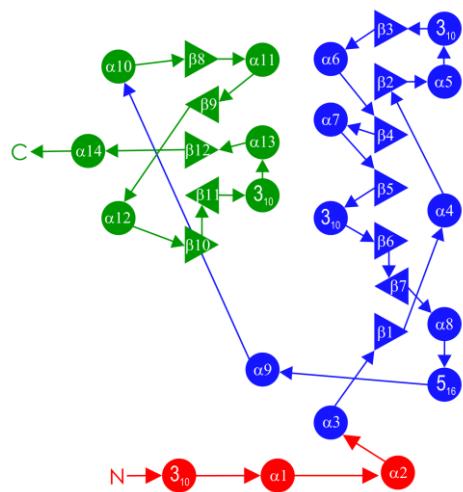
Supporting information for article:

**Structure of methionine  $\gamma$ -lyase from *Clostridium sporogenes***

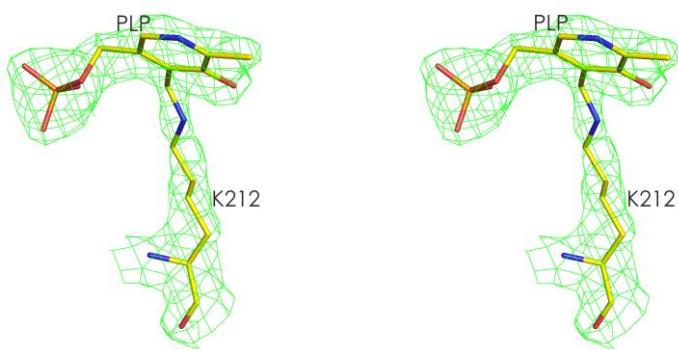
**Svetlana Revtovich, Natalya Anufrieva, Elena Morozova, Vitalia Kulikova, Alexey Nikulin and Tatyana Demidkina**



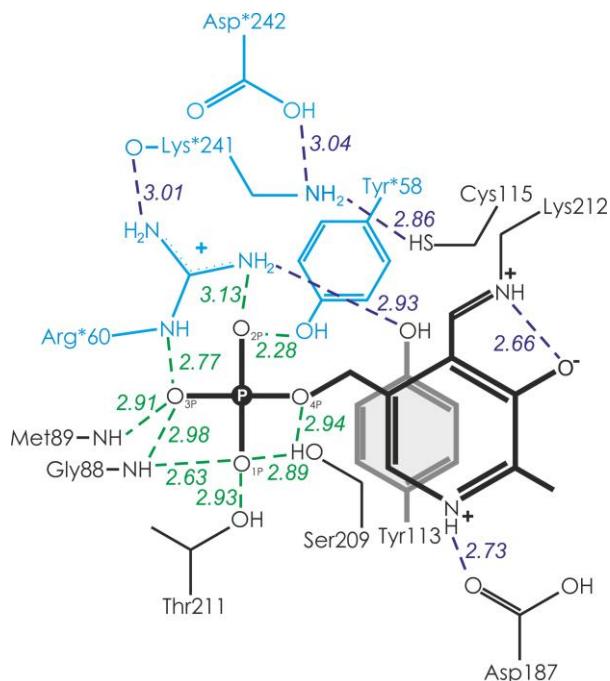
**Figure S1** Reactions catalyzed by MGL.



**Figure S2** Topology diagram of a monomer. The N-terminal domain is shown in red, the PLP-binding domain is in blue, and the C-terminal domain is in green.



**Figure S3** Stereoview of a  $2F_0 - F_c$  electron-density fragment of internal aldimine contoured at  $1.5\sigma$ .



**Figure S4** The network of H-bonds at the PLP-binding site. Residues of the neighboring subunit are colored in cyan. Hydrogen bonds of the PLP phosphate handle are indicated by green.

**Table S1** Hydrogen bonds between the subunit molecules of the tetramer.

| Molecule A<br>(chain A) | Molecule B<br>(chain B) | Bond<br>length (Å) |  | Bond<br>length (Å) | Molecule A<br>(chain A) | Molecule B<br>(chain B) |
|-------------------------|-------------------------|--------------------|--|--------------------|-------------------------|-------------------------|
| Gln33 NE2               | Glu252 OE2              | 3.04               |  | 2.85               | Glu252 OE2              | Gln33 NE2               |
| Gln33 NE2               | Asp219 O                | 2.99               |  | 2.85               | Asp219 O                | Gln33 NE2               |
| Ser35 N                 | Gly218 O                | 2.91               |  | 2.73               | Gly218 O                | Ser35 N                 |
| Thr36 OG1               | Val340 O                | 2.80               |  | 2.88               | Val340 O                | Thr36 OG1               |
| Phe39 N                 | Leu338 O                | 2.88               |  | 2.94               | Leu338 O                | Phe39 N                 |
| Ala42 N                 | Asn331 OD1              | 2.69               |  | 2.73               | Asn331 OD1              | Ala42 N                 |
| Glu43 OE1               | Asn331 ND2              | 3.32               |  | 2.88               | Asn331 ND2              | Glu43 OE1               |
| Glu43 OE2               | Lys327 NZ               | 3.09               |  | 3.13               | Lys327 NZ               | Glu43 OE2               |
| Tyr58 OH                | LLP212 OP2              | 2.47               |  | 2.28               | LLP212 OP2              | Tyr58 OH                |
| Arg60 NE                | LLP212 OP3              | 2.80               |  | 2.77               | LLP212 OP3              | Arg60 NE                |
| Arg60 NH2               | LLP212 OP2              | 3.00               |  | 3.11               | LLP212 OP2              | Arg60 NH2               |
| Arg60 NH2               | Tyr113 OH               | 2.76               |  | 2.93               | Tyr113 OH               | Arg60 NH2               |
| Ser87 OG                | Gly245 O                | 2.79               |  | 2.80               | Gly245 O                | Ser87 OG                |
| Trp97 NE1               | Met243 O                | 2.97               |  | 2.95               | Met243 O                | Trp97 NE1               |
| Trp97 O                 | Tyr127 OH               | 2.67               |  | 2.63               | Tyr127 OH               | Trp97 O                 |
| Leu100 O                | Tyr127 OH               | 2.74               |  | 2.53               | Tyr127 OH               | Leu100 O                |
| Leu100 O                | Arg126 NH2              | 2.29               |  | 2.79               | Arg126 NH2              | Leu100 O                |
| Ser102 N                | Arg126 O                | 2.76               |  | 2.95               | Arg126 O                | Ser102 N                |
| Cys115 SG               | Lys241 NZ               | 2.86               |  | 3.01               | Lys241 NZ               | Cys115 SG               |
| Arg126 NH2              | Ser98 O                 | 3.02               |  | 3.91               | Ser98 O                 | Arg126 NH2              |
| Arg126 NE               | Leu100 O                | 3.11               |  | 3.43               | Leu100 O                | Arg126 NE               |
| Gly245 O                | Ser246 OG               | 2.87               |  | 2.82               | Ser246 OG               | Gly245 O                |

LLP - N-(5'-phosphopyridoxyl)-L-lysine

| Molecule A<br>(chain A) | Molecule C<br>(chain A symm) | Bond<br>length (Å) | Bond<br>length (Å) | Molecule A<br>(chain A) | Molecule C<br>(chain A symm) |
|-------------------------|------------------------------|--------------------|--------------------|-------------------------|------------------------------|
| Gly8 N                  | Asp386 OD2                   | 2.80               | 2.80               | Asp386 OD2              | Gly8 N                       |
| Phe9 N                  | Asp383 OD2                   | 3.23               | 3.23               | Asp383 OD2              | Phe9 N                       |
| Ala10 N                 | Asp383 OD2                   | 2.89               | 2.89               | Asp383 OD2              | Ala10 N                      |
| Thr11 N                 | Asp383 OD2                   | 3.16               | 3.16               | Asp383 OD2              | Thr11 N                      |
| Thr11 OG1               | Asp383 N                     | 3.11               | 3.11               | Asp383 N                | Thr11 OG1                    |
| Thr11 OG1               | Asp386 OD2                   | 2.74               | 2.74               | Asp386 OD2              | Thr11 OG1                    |
| His15 NE2               | Glu382 OE2                   | 2.84               | 2.84               | Glu382 OE2              | His15 NE2                    |
| Asn215 OD1              | Arg258 NE2                   | 2.83               | 2.83               | Arg258 NE2              | Asn215 OD1                   |
| Asp219 OD1              | Arg258 NE2                   | 2.77               | 2.77               | Arg258 NE2              | Asp219 OD1                   |
| Asp219 OD2              | Arg258 NE                    | 2.57               | 2.57               | Arg258 NE               | Asp219 OD2                   |
| Leu255 O                | Arg258 NH1                   | 3.34               | 3.34               | Arg258 NH1              | Leu255 O                     |
| Lys261 NZ               | Glu346 OE1                   | 2.78               | 2.78               | Glu346 OE1              | Lys261 NZ                    |

| Molecule A<br>(chain A) | Molecule D<br>(chain B symm) | Bond<br>length (Å) | Bond<br>length (Å) | Molecule A<br>(chain A) | Molecule D<br>(chain B symm) |
|-------------------------|------------------------------|--------------------|--------------------|-------------------------|------------------------------|
| Gly20 N                 | Gln23 NE2                    | 2.95               | 3.08               | Gln23 NE2               | Gly20 O                      |
| Lys22 N                 | Gln23 OE1                    | 2.82               | 3.19               | Gln23 OE1               | Lys22 N                      |
| Gly25 O                 | Ile38 N                      | 2.67               | 2.62               | Ile38 N                 | Gly25 O                      |
| Leu27 N                 | Thr36 O                      | 3.01               | 3.10               | Thr36 O                 | Leu27 N                      |
| Ala28 N                 | Thr34 OG1                    | 3.13               | 3.19               | Thr34 OG1               | Ala28 N                      |
| Ile31 N                 | Ile31 O                      | 2.94               | 2.97               | Ile31 O                 | Ile31 N                      |