



STRUCTURAL  
BIOLOGY

**Volume 79 (2023)**

**Supporting information for article:**

**Structural basis for the allosteric pathway of 4-amino-4-deoxychorismate synthase**

**Yusuke Nakamichi, Jyumpei Kobayashi, Koichi Toyoda, Masako Suda, Kazumi Hiraga, Masayuki Inui and Masahiro Watanabe**

**Table S1** Comparison of PabA domain structures.

|           | Crystal 0  | Crystal 1  | Crystal 2  | Crystal 3  |
|-----------|--|--|--|--|
| Crystal 0 |  | Q-score: 0.972<br>RMSD: 0.239<br>Aligned residues: 181 | Q-score: 0.931<br>RMSD: 0.257<br>Aligned residues: 182 | Q-score: 0.789<br>RMSD: 0.887<br>Aligned residues: 174 |
| Crystal 1 | Q-score: 0.972<br>RMSD: 0.239<br>Aligned residues: 181 |  | Q-score: 0.935<br>RMSD: 0.354<br>Aligned residues: 184 | Q-score: 0.775<br>RMSD: 0.920<br>Aligned residues: 174 |
| Crystal 2 | Q-score: 0.931<br>RMSD: 0.257<br>Aligned residues: 182 | Q-score: 0.935<br>RMSD: 0.354<br>Aligned residues: 184 |  | Q-score: 0.742<br>RMSD: 1.045<br>Aligned residues: 177 |
| Crystal 3 | Q-score: 0.789<br>RMSD: 0.887<br>Aligned residues: 174 | Q-score: 0.775<br>RMSD: 0.920<br>Aligned residues: 174 | Q-score: 0.742<br>RMSD: 1.045<br>Aligned residues: 177 |  |

Q-score and RMSD were calculated by GESAMT program in the CCP4 suite (Krissinel, 2012).

**Table S2** Comparison of PabB domain structures.

|           | Crystal 0  | Crystal 1  | Crystal 2  | Crystal 3  |
|-----------|--|--|--|--|
| Crystal 0 |  | Q-score: 0.982<br>RMSD: 0.227<br>Aligned residues: 467 | Q-score: 0.962<br>RMSD: 0.417<br>Aligned residues: 468 | Q-score: 0.969<br>RMSD: 0.359<br>Aligned residues: 469 |
| Crystal 1 | Q-score: 0.982<br>RMSD: 0.227<br>Aligned residues: 467 |  | Q-score: 0.959<br>RMSD: 0.415<br>Aligned residues: 466 | Q-score: 0.970<br>RMSD: 0.353<br>Aligned residues: 468 |
| Crystal 2 | Q-score: 0.962<br>RMSD: 0.417<br>Aligned residues: 468 | Q-score: 0.959<br>RMSD: 0.415<br>Aligned residues: 466 |  | Q-score: 0.944<br>RMSD: 0.490<br>Aligned residues: 467 |
| Crystal 3 | Q-score: 0.969<br>RMSD: 0.359<br>Aligned residues: 469 | Q-score: 0.970<br>RMSD: 0.353<br>Aligned residues: 468 | Q-score: 0.944<br>RMSD: 0.490<br>Aligned residues: 467 |  |

**Table S3** Polar interactions between PabA and PabB domains.

| Crystal 2 |                |     |         |                |      |  |  | Crystal 3 |                |     |         |              |      |  |  |     |          |        |          |     |         |                |            |      |     |
|-----------|----------------|-----|---------|----------------|------|--|--|-----------|----------------|-----|---------|--------------|------|--|--|-----|----------|--------|----------|-----|---------|----------------|------------|------|-----|
| PabA      |                |     |         | PabB           |      |  |  | Distance  | PabA           |     |         |              | PabB |  |  |     | Distance |        |          |     |         |                |            |      |     |
|           |                |     |         |                |      |  |  |           |                |     |         |              |      |  |  | (Å) |          |        |          |     |         |                |            |      | (Å) |
|           |                |     |         |                |      |  |  |           |                |     |         |              |      |  |  |     |          | Tyr 9  | O $\eta$ | ... | Glu 603 | O $\epsilon$ 2 | 2.57       |      |     |
|           |                |     |         |                |      |  |  |           |                |     |         |              |      |  |  |     |          | Asp 10 | O        | ... | Asn 538 | N $\delta$ 2   | 2.79       |      |     |
| Ser 11    | O $\gamma$     | ... | Lys 598 | N              | 3.06 |  |  |           |                |     |         |              |      |  |  |     |          | Ser 11 | O        | ... | Asn 538 | N $\delta$ 2   | 3.28       |      |     |
| Thr 13    | N              | ... | Asn 538 | O $\delta$ 1   | 3.06 |  |  |           |                |     |         |              |      |  |  |     |          |        |          |     |         |                |            |      |     |
| His 14    | N              | ... | Asn 538 | O $\delta$ 1   | 2.71 |  |  | His 14    | N              | ... | Asn 538 | O $\delta$ 1 | 2.81 |  |  |     |          |        |          |     |         |                |            |      |     |
| Asn 15    | O $\delta$ 1   | ... | Asn 541 | N $\delta$ 2   | 2.83 |  |  | Asn 15    | O $\delta$ 1   | ... | Asn 541 | N $\delta$ 2 | 2.76 |  |  |     |          |        |          |     |         |                |            |      |     |
|           |                |     |         |                |      |  |  |           |                |     |         |              |      |  |  |     |          |        |          |     | ...     | Asn 538        | N          | 3.15 |     |
| Asn 15    | N $\delta$ 2   | ... | Asp 534 | O              | 2.73 |  |  | Asn 15    | N $\delta$ 2   | ... | Asp 534 | O            | 2.79 |  |  |     |          |        |          |     |         |                |            |      |     |
|           |                |     |         |                |      |  |  |           |                |     |         |              |      |  |  |     |          | Asn 15 | N        | ... | Asn 538 | O $\delta$ 1   | 3.16       |      |     |
| Gln 18    | O $\epsilon$ 1 | ... | Asn 541 | N $\delta$ 2   | 2.69 |  |  | Gln 18    | O $\epsilon$ 1 | ... | Asn 541 | N $\delta$ 2 | 2.86 |  |  |     |          |        |          |     |         |                |            |      |     |
| Gln 18    | N $\epsilon$ 2 | ... | Val 549 | O              | 2.97 |  |  | Gln 18    | N $\epsilon$ 2 | ... | Val 549 | O            | 3.04 |  |  |     |          |        |          |     |         |                |            |      |     |
| Gly 53    | O              | ... | Tyr 435 | O $\eta$       | 3.13 |  |  | Gly 53    | O              | ... | Tyr 435 | O $\eta$     | 2.60 |  |  |     |          |        |          |     |         |                |            |      |     |
| Gly 55    | N              | ... | Gly 432 | O              | 2.59 |  |  |           |                |     |         |              |      |  |  |     |          |        |          |     |         |                |            |      |     |
| Asp 62    | O $\delta$ 1   | ... | Arg 600 | N $\eta$ 2     | 2.73 |  |  |           |                |     |         |              |      |  |  |     |          |        |          |     |         |                |            |      |     |
| Arg 105   | N $\epsilon$   | ... | Glu 523 | O $\epsilon$ 2 | 3.16 |  |  |           |                |     |         |              |      |  |  |     |          |        |          |     |         |                |            |      |     |
| Tyr 129   | O $\eta$       | ... | Asp 534 | O $\delta$ 2   | 2.65 |  |  | Tyr 129   | O $\eta$       | ... | Asp 534 | O $\delta$ 2 | 2.41 |  |  |     |          |        |          |     |         |                |            |      |     |
| Glu 170   | O              | ... | Arg 537 | N $\eta$ 1     | 3.20 |  |  | Glu 170   | O              | ... | Arg 537 | N $\eta$ 1   | 2.94 |  |  |     |          |        |          |     |         |                |            |      |     |
|           |                |     |         |                |      |  |  |           |                |     |         |              |      |  |  |     |          |        |          |     | ...     | Arg 537        | N $\eta$ 2 | 2.88 |     |
|           |                |     |         |                |      |  |  |           |                |     |         |              |      |  |  |     |          |        |          |     |         |                |            |      |     |
| Ser 171   | O $\gamma$     | ... | Asp 534 | O $\delta$ 2   | 2.56 |  |  | Ser 171   | O $\gamma$     | ... | Asp 534 | O $\delta$ 2 | 2.64 |  |  |     |          |        |          |     |         |                |            |      |     |
| Ile 172   | N              | ... | Asp 534 | O $\delta$ 1   | 3.00 |  |  | Ile 172   | N              | ... | Asp 534 | O $\delta$ 1 | 2.88 |  |  |     |          |        |          |     |         |                |            |      |     |

**Table S4** Residues at PabA-PabB interface within 4.5 Å.

| Crystal 2 |    |     |     |     | Crystal 3 |    |     |     |     |
|-----------|----|-----|-----|-----|-----------|----|-----|-----|-----|
|           |    |     |     |     | Tyr       | 9  | ... | Lys | 599 |
|           |    |     |     |     |           |    |     | Arg | 600 |
|           |    |     |     |     |           |    |     | Glu | 603 |
| Asp       | 10 | ... | Tyr | 435 | Asp       | 10 | ... | Asn | 538 |
|           |    |     | Asn | 538 |           |    |     |     |     |
|           |    |     | Pro | 597 |           |    |     |     |     |
| Ser       | 11 | ... | Asp | 534 | Ser       | 11 | ... |     |     |
|           |    |     | Leu | 535 |           |    |     |     |     |
|           |    |     | Asn | 538 |           |    |     | Asn | 538 |
|           |    |     | Pro | 597 |           |    |     | Pro | 597 |
|           |    |     | Lys | 598 |           |    |     |     |     |
| Phe       | 12 | ... | Tyr | 435 | Phe       | 12 | ... | Tyr | 435 |
|           |    |     | Met | 531 |           |    |     |     |     |
|           |    |     | Asp | 534 |           |    |     |     |     |
|           |    |     | Leu | 535 |           |    |     |     |     |
|           |    |     | Asn | 538 |           |    |     | Asn | 538 |
|           |    |     | Ala | 596 |           |    |     |     |     |
| Thr       | 13 | ... | Asn | 538 | Thr       | 13 | ... | Asn | 538 |
| His       | 14 | ... | Asn | 538 | His       | 14 | ... | Asn | 538 |
|           |    |     | Asn | 541 |           |    |     | Asn | 541 |
|           |    |     | Ser | 542 |           |    |     | Ser | 542 |
| Asn       | 15 | ... | Asn | 541 | Asn       | 15 | ... | Asp | 534 |
|           |    |     | Asp | 534 |           |    |     |     |     |
|           |    |     | Arg | 537 |           |    |     | Arg | 537 |
|           |    |     | Asn | 538 |           |    |     | Asn | 538 |
|           |    |     |     |     |           |    |     | Asn | 541 |
| Phe       | 17 | ... | Ile | 546 | Phe       | 17 | ... | Ile | 546 |

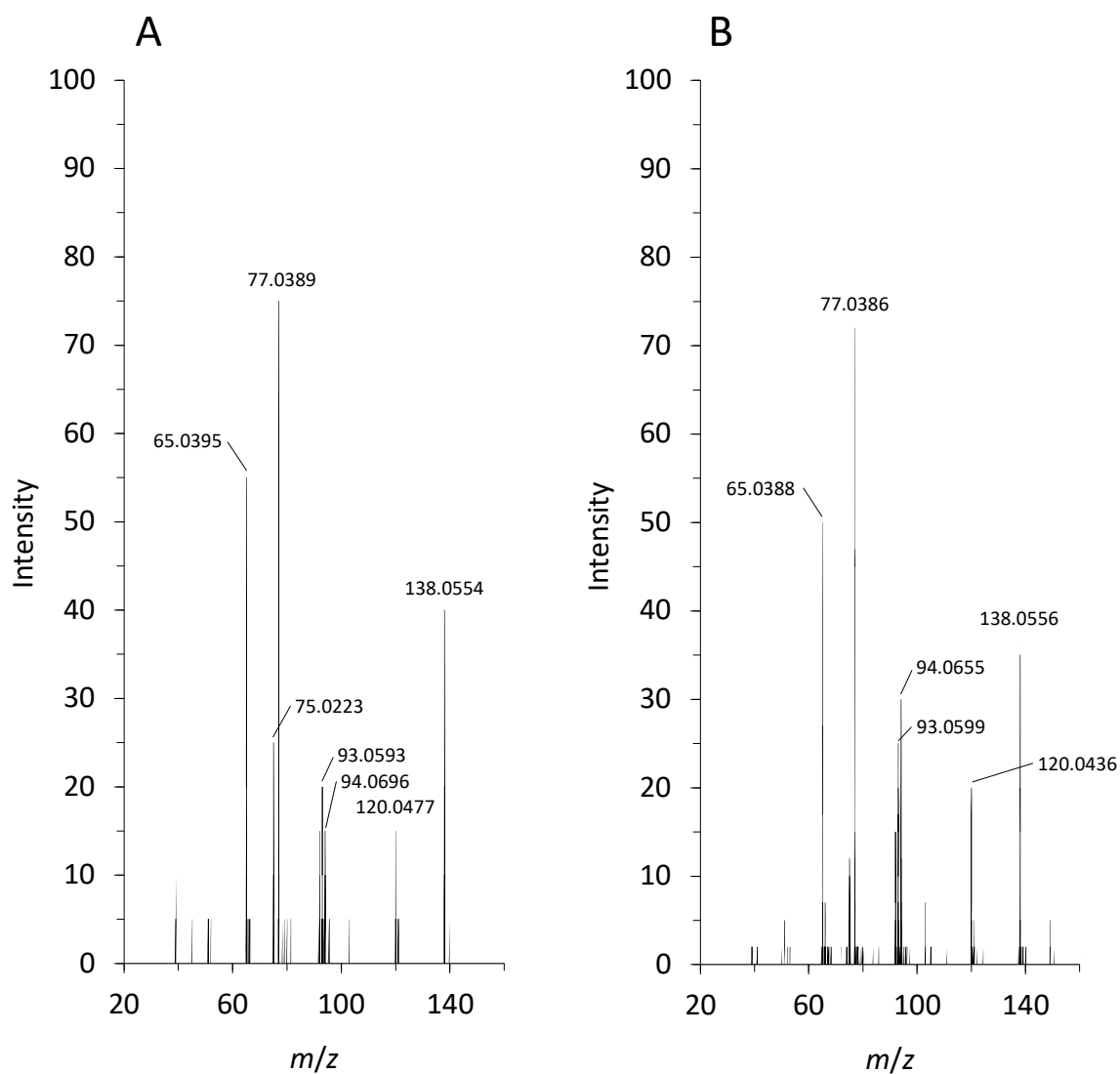
|     |    |     |     |     |     |    |     |     |     |
|-----|----|-----|-----|-----|-----|----|-----|-----|-----|
|     |    |     | Arg | 575 |     |    | Arg | 575 |     |
| Gln | 18 | ... |     |     | Gln | 18 | ... | Arg | 537 |
|     |    |     | Asn | 541 |     |    |     | Asn | 541 |
|     |    |     | Ile | 546 |     |    |     | Ile | 546 |
|     |    |     | Gly | 547 |     |    |     | Gly | 547 |
|     |    |     | Val | 549 |     |    |     | Val | 549 |
| Tyr | 19 | ... | Arg | 537 | Tyr | 19 | ... | Arg | 537 |
| Gly | 21 | ... | Ile | 546 | Gly | 21 | ... | Ile | 546 |
| Glu | 22 | ... | Ile | 546 | Glu | 22 | ... | Ile | 546 |
|     |    |     | Gly | 547 |     |    |     | Gly | 547 |
| Pro | 27 | ... | Ile | 546 | Pro | 27 | ... | Ile | 546 |
| Gly | 53 | ... | Tyr | 435 | Gly | 53 | ... | Tyr | 435 |
|     |    |     |     |     |     |    |     | Pro | 597 |
| Pro | 54 | ... | Gly | 432 | Pro | 54 | ... | Gly | 432 |
|     |    |     | Glu | 433 |     |    |     | Glu | 433 |
|     |    |     | Tyr | 435 |     |    |     | Ser | 434 |
|     |    |     | Pro | 597 |     |    |     | Tyr | 435 |
|     |    |     | Arg | 600 |     |    |     | Pro | 597 |
|     |    |     |     |     |     |    |     | Arg | 600 |
| Gly | 55 | ... | Asn | 431 | Gly | 55 | ... |     |     |
|     |    |     | Gly | 432 |     |    |     | Glu | 433 |
|     |    |     | Glu | 433 |     |    |     |     |     |
|     |    |     | Arg | 600 |     |    |     | Arg | 600 |
|     |    |     |     |     | Ser | 56 | ... | Arg | 600 |
|     |    |     |     |     | Pro | 57 | ... | Glu | 433 |
|     |    |     |     |     |     |    |     | Arg | 600 |
|     |    |     |     |     | Glu | 60 | ... | Glu | 433 |
| Arg | 61 | ... | Arg | 600 |     |    |     |     |     |
| Asp | 62 | ... | Arg | 600 |     |    |     |     |     |
| Cys | 81 | ... | Tyr | 435 |     |    |     |     |     |

|     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Glu | 100 | ... | Leu | 656 |     |     |     |     |     |
| Pro | 101 | ... | Ser | 655 |     |     |     |     |     |
|     |     |     |     |     | Met | 102 | ... | Glu | 523 |
|     |     |     |     |     |     |     |     | Lys | 524 |
|     |     |     |     |     |     |     |     | Ala | 527 |
|     |     |     |     |     |     |     |     | Ser | 655 |
|     |     |     |     |     |     |     |     | Leu | 656 |
| His | 103 | ... | Ile | 429 | His | 103 | ... | Ile | 429 |
|     |     |     | Tyr | 435 |     |     |     | Tyr | 435 |
|     |     |     | Ala | 527 |     |     |     | Ala | 527 |
|     |     |     | Met | 531 |     |     |     | Met | 531 |
|     |     |     | Ser | 655 |     |     |     | Ser | 655 |
| Gly | 104 | ... | Ala | 527 | Gly | 104 | ... | Ala | 527 |
|     |     |     | Leu | 530 |     |     |     |     |     |
|     |     |     | Met | 531 |     |     |     | Met | 531 |
| Arg | 105 | ... | Glu | 523 |     |     |     |     |     |
|     |     |     | Ala | 527 |     |     |     |     |     |
|     |     |     | Leu | 656 |     |     |     |     |     |
| Val | 127 | ... | Leu | 530 | Val | 127 | ... | Leu | 530 |
| Tyr | 129 | ... | Tyr | 435 | Tyr | 129 | ... | Tyr | 435 |
|     |     |     | Leu | 530 |     |     |     | Leu | 530 |
|     |     |     | Met | 531 |     |     |     | Met | 531 |
|     |     |     | Asp | 534 |     |     |     | Asp | 534 |
|     |     |     |     |     | His | 130 | ... | Gly | 432 |
|     |     |     |     |     |     |     |     | Tyr | 435 |
| Ser | 131 | ... | Arg | 430 |     |     |     |     |     |
| Glu | 170 | ... | Arg | 537 | Glu | 170 | ... | Asp | 534 |
|     |     |     |     |     |     |     |     | Arg | 537 |
| Ser | 171 | ... | Leu | 530 | Ser | 171 | ... | Leu | 530 |
|     |     |     | Asp | 534 |     |     |     | Asp | 534 |

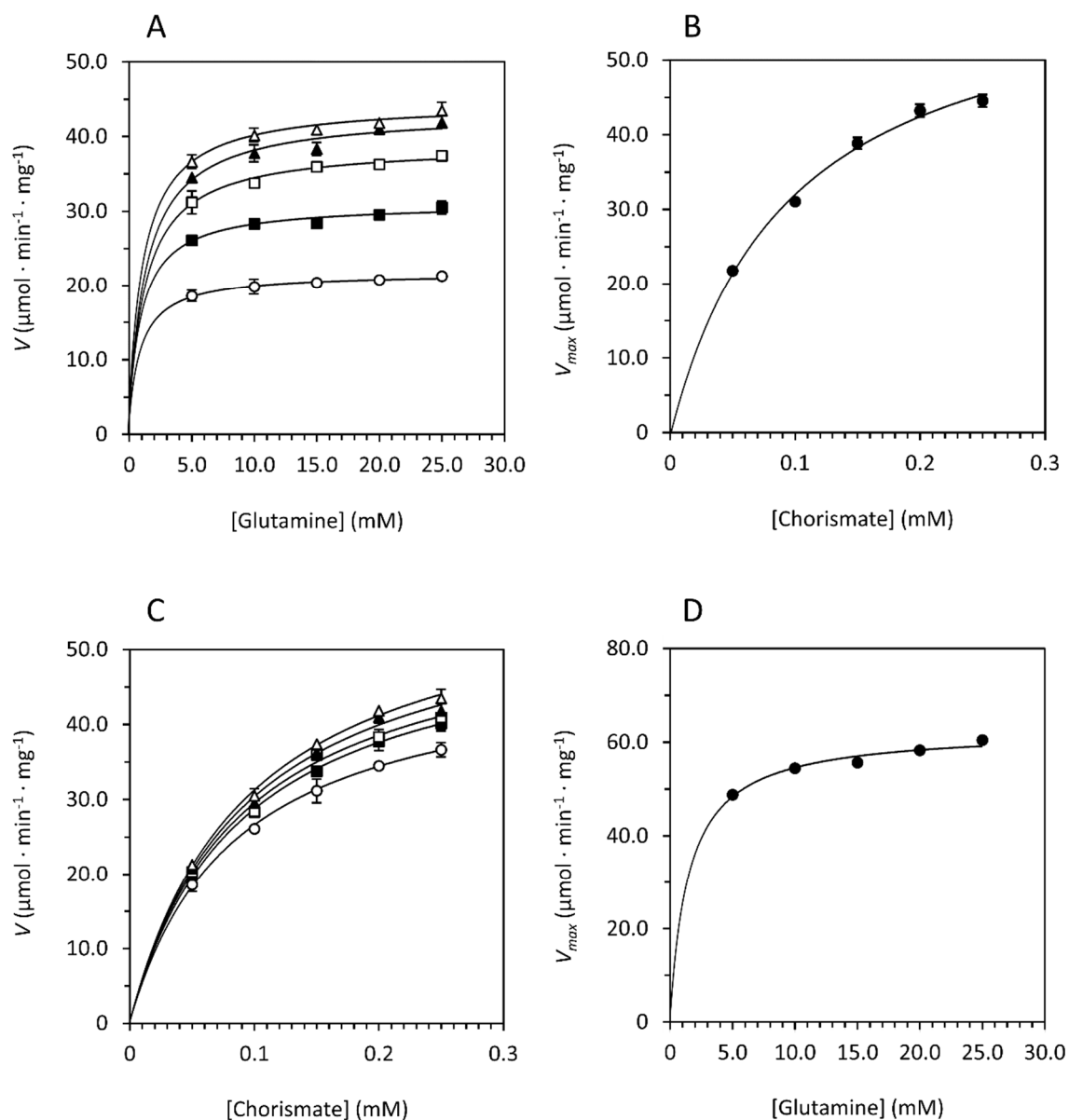
|     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
|     |     |     | Arg | 537 |     |     |     | Arg | 537 |
| Ile | 172 | ... | Leu | 530 | Ile | 172 | ... | Leu | 530 |
|     |     |     | Val | 533 |     |     |     | Val | 533 |
|     |     |     | Asp | 534 |     |     |     | Asp | 534 |
|     |     |     | Arg | 537 |     |     |     | Arg | 537 |
|     |     |     | Val | 551 |     |     |     | Val | 551 |
| Gly | 173 | ... | Leu | 530 | Gly | 173 | ... | Leu | 530 |

---





**Figure S1** MS/MS spectrum of standard *p*ABA and *p*ABA produced by catalyzation of SvPapA and EcPabC. (A) MS/MS spectrum of 5 μM *p*ABA standard. The retention time of *p*ABA was 1.620 min. (B) MS/MS spectrum of *p*ABA in reaction mixture using 250 mM glutamine and 250 μM chorismate as substrates. The retention time of *p*ABA was 1.621 min.



**Figure S2** Michaelis–Menten kinetic analysis of SvPapA using glutamine and chorismate as substrates. The enzyme was incubated for 5 min at 28 °C and pH 7.5 with various concentrations of glutamine and chorismate. (A) Nonlinear regression curves of initial velocity against glutamine concentration at several fixed concentrations of chorismate (hollow circles: 50  $\mu\text{M}$ , solid squares: 100  $\mu\text{M}$ , hollow squares: 150  $\mu\text{M}$ , solid triangles: 200  $\mu\text{M}$ , hollow triangles: 250  $\mu\text{M}$ ;  $n = 5$ ). (B) Secondary curve between  $V_{\text{max}}$  values for glutamine, which was calculated in (A), and chorismate concentrations. The final  $V_{\text{max}}$  value for glutamine was calculated by curve fitting using GraphPad Prism ver.9.5.1 for Windows (GraphPad Software, San Diego California, USA). (C) Nonlinear regression curves of initial velocity against chorismate concentration at several fixed concentrations of glutamine (hollow circles: 5.0 mM, solid squares: 10.0 mM, hollow squares: 15.0 mM, solid triangles: 20.0 mM, hollow triangles: 25.0 mM;  $n = 5$ ). (D) Secondary curve between  $V_{\text{max}}$  values for

chorismate, which was calculated in (C), and the glutamine concentrations. The final  $V_{\max}$  value for chorismate was calculated by curve fitting.

```

Sequence  MRTLLIDNYDSFTHNLQYIGEATGQPPVVVNDADWSRLPVEDFAIVVSPGPGSPRE 60
0A  MRTLLIDNYDSFTHNLQYIGEATGQPPVVVNDADWSRLPVEDFAIVVSPGPGSP---
0B  MRTLLIDNYDSFTHNLQYIGEATGQPPVVVNDADWSRLPVEDFAIVVSPGP-----
1A  MRTLLIDNYDSFTHNLQYIGEATGQPPVVVNDADWSRLPVEDFAIVVSPG-----
1B  MRTLLIDNYDSFTHNLQYIGEATGQPPVVVNDADWSRLPVEDFAIVVSPG-----
2A  MRTLLIDNYDSFTHNLQYIGEATGQPPVVVNDADWSRLPVEDFAIVVSPGPGSPRE
2B  MRTLLIDNYDSFTHNLQYIGEATGQPPVVVNDADWSRLPVEDFAIVVSPGPGSPRE
3A  MRTLLIDNYDSFTHNLQYIGEATGQPPVVVNDADWSRLPVEDFAIVVSP-----
3B  MRTLLIDNYDSFTHNLQYIGEATGQPPVVVNDADWSRLPVEDFAIVVSPGPGSPRE

Sequence  RDFGISRRAITDSSLVPLGVLGHQGIQALFGTIVGLAPEPMHGRVSEVRHTGEDVFRGL 120
0A  ---GISRRAITDSSLVPLGVLGHQGIQALFGTIVGLAPEPMHGRVSEVRHTGEDVFRGL
0B  --FGISRRAITDSSLVPLGVLGHQGIQALFGTIVGLAPEPMHGRVSEVRHTGEDVFRGL
1A  -DFGISRRAITDSSLVPLGVLGHQGIQALFGTIVGLAPEPMHGRVSEVRHTGEDVFRGL
1B  RDFGISRRAITDSSLVPLGVLGHQGIQALFGTIVGLAPEPMHGRVSEVRHTGEDVFRGL
2A  RDFGISRRAITDSSLVPLGVLGHQGIQALFGTIVGLAPEPMHGRVSEVRHTGEDVFRGL
2B  -----RAITDSSLVPLGVLGHQGIQALFGTIVGLAPEPMHGRVSEVRHTGEDVFRGL
3A  RDFGISRRAITDSSLVPLGVLGHQGIQALFGTIVGLAPEPMHGRVSEVRHTGEDVFRGL
3B  RDFGISRRAITDSSLVPLGVLGHQGIQALFGTIVGLAPEPMHGRVSEVRHTGEDVFRGL

Sequence  PSPFTAVRYHSLAATLDPELEPLAWSDDGVVMLGRHREKPLWGVQFHPESIGSDFGREI 180
0A  PSPFTAVRYHSLAATLDPELEPLAWSDDGVVMLGRHREKPLWGVQFHPESIGSDFGREI
0B  PSPFTAVRYHSLAATLDPELEPLAWSDDGVVMLGRHREKPLWGVQFHPESIGSDFGREI
1A  PSPFTAVRYHSLAATLDPELEPLAWSDDGVVMLGRHREKPLWGVQFHPESIGSDFGREI
1B  PSPFTAVRYHSLAATLDPELEPLAWSDDGVVMLGRHREKPLWGVQFHPESIGSDFGREI
2A  PSPFTAVRYHSLAATLDPELEPLAWSDDGVVMLGRHREKPLWGVQFHPESIGSDFGREI
2B  PSPFTAVRYHSLAATLDPELEPLAWSDDGVVMLGRHREKPLWGVQFHPESIGSDFGREI
3A  PSPFTAVRYH-----DELEPLAWSDDGVVMLGRHREKPLWGVQFHPESIGSDFGREI
3B  PSPFTAVRYHSLAATLDPELEPLAWSDDGVVMLGRHREKPLWGVQFHPESIGSDFGREI

Sequence  MANFRDLALAHRRARRHGADSPYELHVRVVDVLPDAEVRGCLPGEITFWLDSSSVLE 240
0A  MANFRDLALAHRRARRHGADSPYELHVRVVDVLPDAEVRGCLPGEITFWLDSSSVLE
0B  MANFRDLALAHRRARRH-----DSPYELHVRVVDVLPDAEVRGCLPGEITFWLDSSSVLE
1A  MANFRDLALAHRRARR-----SPYELHVRVVDVLPDAEVRGCLPGEITFWLDSSSVLE
1B  MANFRDLALAHRRARR-----DSPYELHVRVVDVLPDAEVRGCLPGEITFWLDSSSVLE
2A  MANFRDLALAHRRARR-----SPYELHVRVVDVLPDAEVRGCLPGEITFWLDSSSVLE
2B  MANFRDLALAHRRARR-----SPYELHVRVVDVLPDAEVRGCLPGEITFWLDSSSVLE
3A  MANFRDLALAHRRARR-----DSPYELHVRVVDVLPDAEVRGCLPGEITFWLDSSSVLE
3B  MANFRDLALAHRRARRHGADSPYELHVRVVDVLPDAEVRGCLPGEITFWLDSSSVLE

Sequence  GASRFSFLGDDRGLAEYLTYRVADGVSVRSGDGTTRTRRPFNYLEQLERRRVPVA 300
0A  GASRFSFLGDDRGLAEYLTYRVADGVSVRSGDGTTRTRRPFNYLEQLERRRVPVA
0B  GASRFSFLGDDRGLAEYLTYRVADGVSVRSGDGTTRTRRPFNYLEQLERRRVPVA
1A  GASRFSFLGDDRGLAEYLTYRVADGVSVRSGDGTTRTRRPFNYLEQLERRRVPVA
1B  GASRFSFLGDDRGLAEYLTYRVADGVSVRSGDGTTRTRRPFNYLEQLERRRVPVA
2A  GASRFSFLGDDRGLAEYLTYRVADGVSVRSGDGTTRTRRPFNYLEQLERRRVPVA
2B  GASRFSFLGDDRGLAEYLTYRVADGVSVRSGDGTTRTRRPFNYLEQLERRRVPVA
3A  GASRFSFLGDDRGLAEYLTYRVADGVSVRSGDGTTRTRRPFNYLEQLERRRVPVA
3B  GASRFSFLGDDRGLAEYLTYRVADGVSVRSGDGTTRTRRPFNYLEQLERRRVPVA

Sequence  PELPFEFNLGVYGLYELKAEITGDPAHRSPHPDAFLFADRAIALDHQEGCCYLALD 360
0A  PELPFEFNLGVYGLYELKAEITGDPAHRSPHPDAFLFADRAIALDHQEGCCYLALD
0B  PELPFEFNLGVYGLYELKAEITGDPAHRSPHPDAFLFADRAIALDHQEGCCYLALD
1A  PELPFEFNLGVYGLYELKAEITGDPAHRSPHPDAFLFADRAIALDHQEGCCYLALD
1B  PELPFEFNLGVYGLYELKAEITGDPAHRSPHPDAFLFADRAIALDHQEGCCYLALD
2A  PELPFEFNLGVYGLYELKAEITGDPAHRSPHPDAFLFADRAIALDHQEGCCYLALD
2B  PELPFEFNLGVYGLYELKAEITGDPAHRSPHPDAFLFADRAIALDHQEGCCYLALD
3A  PELPFEFNLGVYGLYELKAEITGDPAHRSPHPDAFLFADRAIALDHQEGCCYLALD
3B  PELPFEFNLGVYGLYELKAEITGDPAHRSPHPDAFLFADRAIALDHQEGCCYLALD

Sequence  RRGHDDGARAWLRETAETLGLAVRAPAEPTAMVFGIPEAAAGFGLARARHKDAYLK 420
0A  RRGHDDGARAWLRETAETLGLAVRAPAEPTAMVFGIPEAAAGFGLARARHKDAYLK
0B  RRGHDDGARAWLRETAETLGLAVRAP-----GFIPEAAAGFGLARARHKDAYLK
1A  RRGHDDGARAWLRETAETLGLAVR-----MVFGIPEAAAGFGLARARHKDAYLK
1B  RRGHDDGARAWLRETAETLGLAVRAPAEPTAMVFGIPEAAAGFGLARARHKDAYLK
2A  RRGHDDGARAWLRETAETLGLAVRAPAEPTAMVFGIPEAAAGFGLARARHKDAYLK
2B  RRGHDDGARAWLRETAETLGLAVRAPAEPTAMVFGIPEAAAGFGLARARHKDAYLK
3A  RRGHDDGARAWLRETAETLGLAVRAP--PTAMVFGIPEAAAGFGLARARHKDAYLK
3B  RRGHDDGARAWLRETAETLGLAVRAPAEPTAMVFGIPEAAAGFGLARARHKDAYLK

Sequence  RIDECLKEIRNGESYEICLNMVTAPEATALPLYSALRAISPVVYGALLEFPELSVSA 480
0A  RIDECLKEIRNGESYEICLNMVTAPEATALPLYSALRAISPVVYGALLEFPELSVSA
0B  RIDECLKEIRNGESYEICLNMVTAPEATALPLYSALRAISPVVYGALLEFPELSVSA
1A  RIDECLKEIRNGESYEICLNMVTAPEATALPLYSALRAISPVVYGALLEFPELSVSA
1B  RIDECLKEIRNGESYEICLNMVTAPEATALPLYSALRAISPVVYGALLEFPELSVSA
2A  RIDECLKEIRNGESYEICLNMVTAPEATALPLYSALRAISPVVYGALLEFPELSVSA
2B  RIDECLKEIRNGESYEICLNMVTAPEATALPLYSALRAISPVVYGALLEFPELSVSA
3A  RIDECLKEIRNGESYEICLNMVTAPEATALPLYSALRAISPVVYGALLEFPELSVSA
3B  RIDECLKEIRNGESYEICLNMVTAPEATALPLYSALRAISPVVYGALLEFPELSVSA

Sequence  SPERFLTIGADGGVSEKPKIGTRPRGCTAEEDERLADLAGREKDRAEMLMIVDLVRNDL 540
0A  SPERFLTIGADGGVSEKPKIGTRPRGCTAEEDERLADLAGREKDRAEMLMIVDLVRNDL
0B  SPERFLTIGADGGVSEKPKIGTRPRGCTAEEDERLADLAGREKDRAEMLMIVDLVRNDL
1A  SPERFLTIGADGGVSEKPKIGTRPRGCTAEEDERLADLAGREKDRAEMLMIVDLVRNDL
1B  SPERFLTIGADGGVSEKPKIGTRPRGCTAEEDERLADLAGREKDRAEMLMIVDLVRNDL
2A  SPERFLTIGADGGVSEKPKIGTRPRGCTAEEDERLADLAGREKDRAEMLMIVDLVRNDL
2B  SPERFLTIGADGGVSEKPKIGTRPRGCTAEEDERLADLAGREKDRAEMLMIVDLVRNDL
3A  SPERFLTIGADGGVSEKPKIGTRPRGCTAEEDERLADLAGREKDRAEMLMIVDLVRNDL
3B  SPERFLTIGADGGVSEKPKIGTRPRGCTAEEDERLADLAGREKDRAEMLMIVDLVRNDL

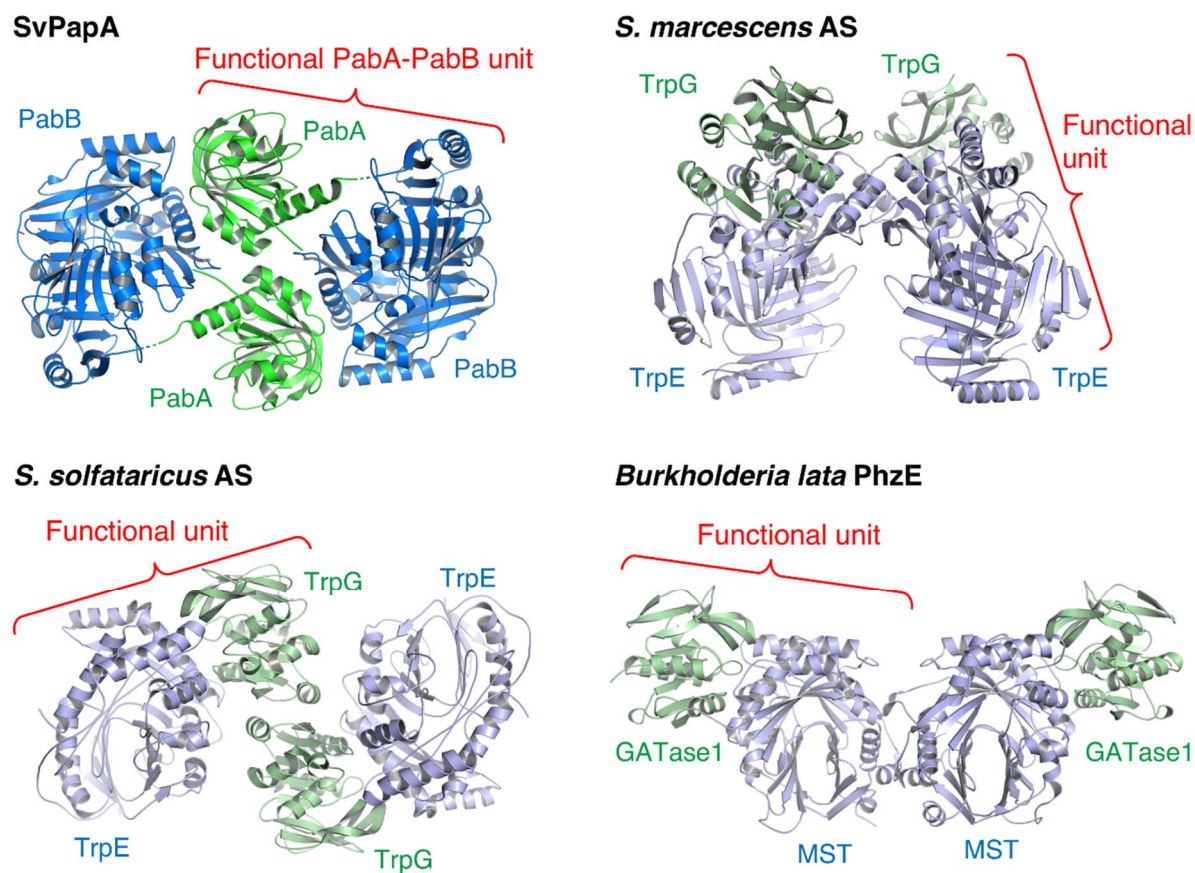
Sequence  NSVCAIGSVHVPRLFEVETAPVHQLVSTIRGRLRPGTSTAACVRAAFPGGSMTGAPKKR 600
0A  NSVCAIGSVHVPRLFEVETAPVHQLVSTIRGRLRPGTSTAACVRAAFPGGSMTGAPKKR
0B  NSVCAIGSVHVPRLFEVETAPVHQLVSTIRGRLRPGTSTAACVRAAFPGGSMTGAPKKR
1A  NSVCAIGSVHVPRLFEVETAPVHQLVSTIRGRLRPGTSTAACVRAAFPGGSMTGAPKKR
1B  NSVCAIGSVHVPRLFEVETAPVHQLVSTIRGRLRPGTSTAACVRAAFPGGSMTGAPKKR
2A  NSVCAIGSVHVPRLFEVETAPVHQLVSTIRGRLRPGTSTAACVRAAFPGGSMTGAPKKR
2B  NSVCAIGSVHVPRLFEVETAPVHQLVSTIRGRLRPGTSTAACVRAAFPGGSMTGAPKKR
3A  NSVCAIGSVHVPRLFEVETAPVHQLVSTIRGRLRPGTSTAACVRAAFPGGSMTGAPKKR
3B  NSVCAIGSVHVPRLFEVETAPVHQLVSTIRGRLRPGTSTAACVRAAFPGGSMTGAPKKR

Sequence  TMEIIDRLEEGRGVYSGALGFALSGAADLSIVRTIVLADGQAEFGVGGAIIVLSDDQE 660
0A  TMEIIDRLEEGRGVYSGALGFALSGAADLSIVRTIVLADGQAEFGVGGAIIVLSDDQE
0B  TMEIIDRLEEGRGVYSGALGFALSGAADLSIVRTIVLADGQAEFGVGGAIIVLSDDQE
1A  TMEIIDRLEEGRGVYSGALGFALSGAADLSIVRTIVLADGQAEFGVGGAIIVLSDDQE
1B  TMEIIDRLEEGRGVYSGALGFALSGAADLSIVRTIVLADGQAEFGVGGAIIVLSDDQE
2A  TMEIIDRLEEGRGVYSGALGFALSGAADLSIVRTIVLADGQAEFGVGGAIIVLSDDQE
2B  TMEIIDRLEEGRGVYSGALGFALSGAADLSIVRTIVLADGQAEFGVGGAIIVLSDDQE
3A  TMEIIDRLEEGRGVYSGALGFALSGAADLSIVRTIVLADGQAEFGVGGAIIVLSDDQE
3B  TMEIIDRLEEGRGVYSGALGFALSGAADLSIVRTIVLADGQAEFGVGGAIIVLSDDQE

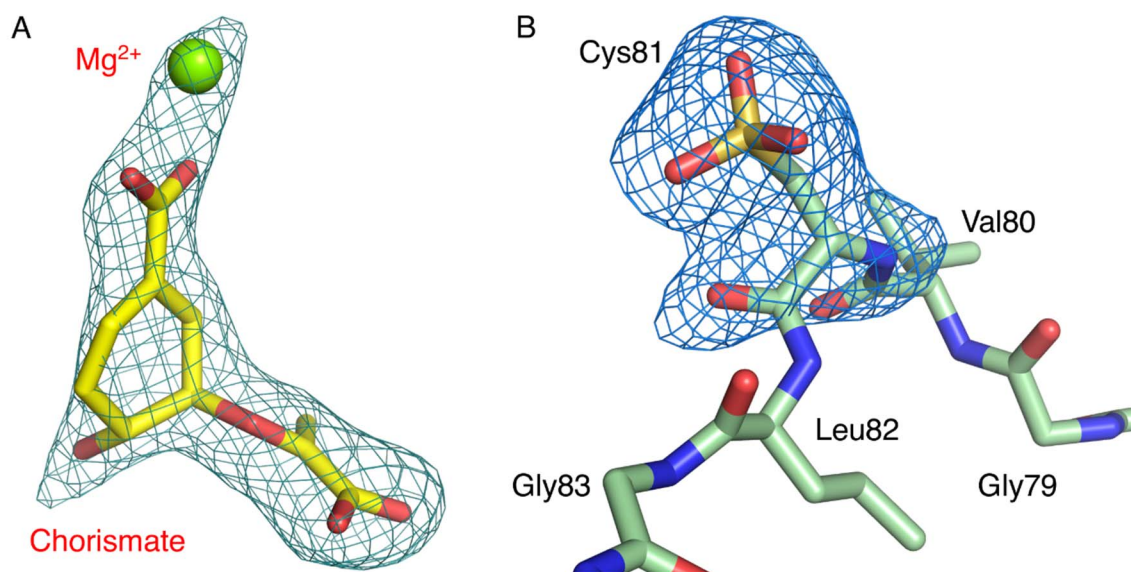
Sequence  EEFTEIVVKARAMVTALDGSVAVGAR686
0A  EEFTEIVVKARAMVTALD-----
0B  EEFTEIVVKARAMVTALD-----
1A  EEFTEIVVKARAMVTALD-----
1B  EEFTEIVVKARAMVTALD-----
2A  EEFTEIVVKARAMVTALDGS-----
2B  EEFTEIVVKARAMVTALD-----
3A  EEFTEIVVKARAMVTALD-----
3B  EEFTEIVVKARAMVTALD-----

```

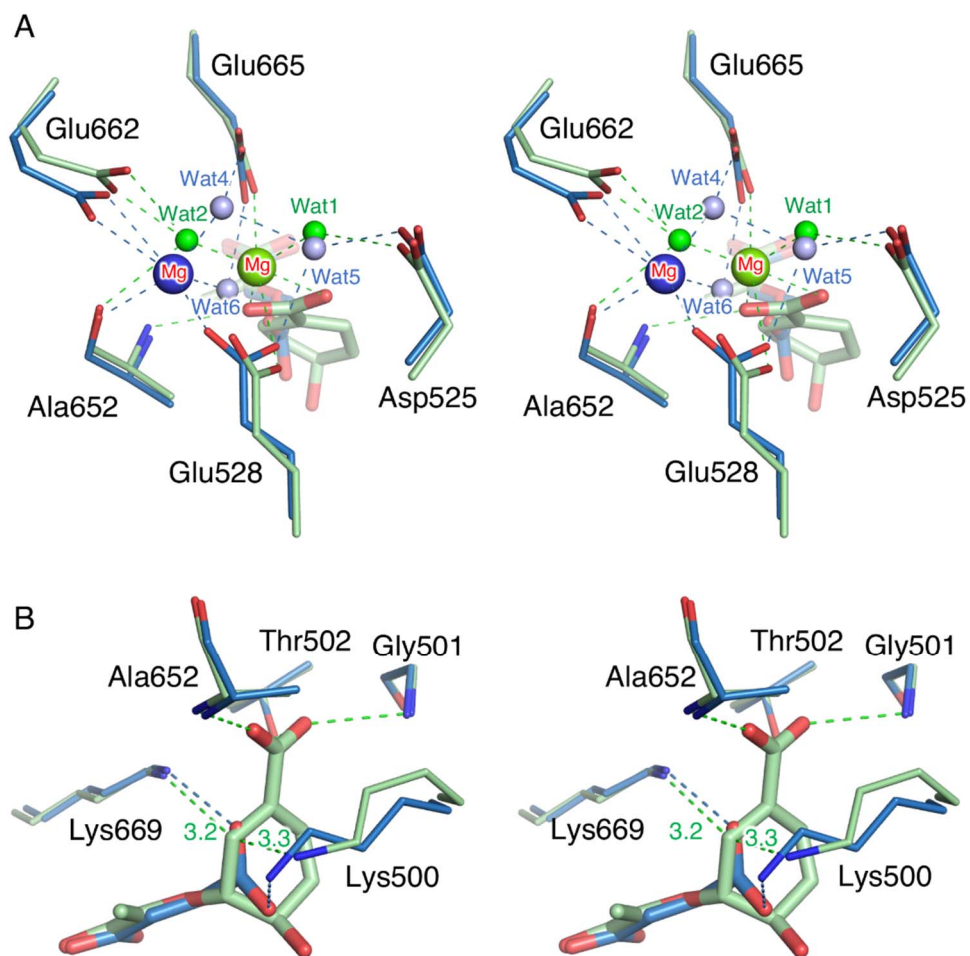
**Figure S3** Assigned residues in each chain of crystals 0–3. Each chain is named based on its chain in the coordinate file and crystal type, e.g., “1A” means chain A in crystal 1. Dashes indicate disordered residues. The line named “Sequence” shows the amino acid sequence of SvPapA.



**Figure S4** Quaternary structures of SvPapA homodimer, AS heterotetramers, and 2-amino-2-deoxychorismate synthase PhzE. TrpE and MST subunits are represented in blue. TrpG and GATase1 subunits are presented in green.



**Figure S5** (A) Fo-Fc Polder omit map ( $5.0 \sigma$ ) for chorismate and  $Mg^{2+}$ . (B) Polder omit map ( $3.0 \sigma$ ) for Cys81, which is oxidized to sulfonic acid.



**Figure S6** (A and B) PabB-active sites with and without chorismate are presented as stereo-diagrams in green and blue, respectively.

## References

Krissinel, E. (2012). *J. Mol. Biochem.* **1**, 76–85.