Geometric considerations support the double-displacement catalytic mechanism of L-asparaginase

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Supplementary Material

Table S1. Equivalent residues in the active sites of L-asparaginases from different organisms

EcAII	Thr12	Tyr25	Thr89	Asp90	Lys162
ErA	Thr15	Tyr29	Thr95	Asp96	Lys168
W. succinogenes	Thr14	Tyr27	Thr93	Asp94	Lys166
Guinea pig (AB)[&]	Thr19	Tyr308	Thr116	Asp117	Lys188
H. pylori	Thr16	Tyr29	Thr95	Asp96	Lys168
***P. furiosus* (AB)[&]**	Thr11	Tyr273	Thr83	Asp84	Lys154

[&]In these enzymes the active site tyrosine residue is contributed by another monomer

Table S2. Details of the crystallization conditions for structures determined in this study

Structure	Crystallization and Freezing Conditions
$EcAII^{wt}{}_1$	0.17 M NH_4-citrate, pH 7, 17-18% PEG3350, 30 mM L-Asp (co-crystallization) Flash-freezing in mother liquid but PEG3350 content increased to 38%
$EcAII^{wt}{}_2$	0.17 M NH_4-citrate, pH 5.6, 17-18% PEG3350 (1 min soaking in solution with 5 mM L-Asp) Flash-freezing in mother liquid but PEG3350 content increased to 38%
$EcAII^{T12V}{}_1$	0.17 M NH_4-citrate, pH 5.5, 17-18% PEG3350, 5 mM L-Asp (co-crystallization) Flash-freezing in mother liquid enriched with 25% (v/v) glycerol
$EcAII^{T12V}{}_2$	0.17 M NH_4-citrate, pH 7.0, 17-18% PEG3350, 5 mM L-Asp (co-crystallization) Flash-freezing in mother liquid enriched with 25% (v/v) glycerol
$EcAII^{T89V/K162T}{}_1$	0.17 M NH_4-citrate, pH 7.0, 17-18% PEG3350, 10 mM L-Asn (co-crystallization) Flash-freezing in mother liquid but PEG3350 content increased to 38%
$EcAII^{T89V/K162T}{}_2$	0.17 M NH_4-citrate, pH 7.0, 17-18% PEG3350 (1 min soaking in solution with 0.5 mM L-Asn) Flash-freezing in mother liquid but PEG3350 content increased to 38%
$EcAII^{T89V/K162T}{}_3$	0.17 M NH_4-citrate, pH 7.0, 17-18% PEG3350, 5 mM L-Asp (co-crystallization) Flash-freezing in mother liquid but PEG3350 content increased to 38%
$EcAII^{T89V/K162T}{}_4$	0.17 M NH_4-citrate, pH 7.0, 17-18% PEG3350 Transfer to 0.1 M Tris, pH 8.3, 19-20% PEG3350 with 5 mM L-Asn Flash-freezing in mother liquid but PEG3350 content increased to 38%
$EcAII^{T89V/K162T}{}_5$	0.17 M NH_4-citrate, pH 7.0, 17-18% PEG3350 Transfer to 0.1 M Tris, pH 8.3, 19-20% PEG3350 with 5 mM L-Asn Flash-freezing in mother liquid but PEG3350 content increased to 38%
$EcAII^{K162M}{}_1$	0.17 M NH_4-citrate, pH 5.6, 17-18% PEG3350, 10 mM L-Asp (co-crystallization) Flash-freezing in mother liquid enriched with 25% (v/v) glycerol
$EcAII^{K162M}{}_2$	0.17 M NH_4-citrate, pH 5.6, 17-18% PEG3350, 10 mM L-Asp (co-crystallization) Flash-freezing in mother liquid but PEG3350 content increased to 38%
ErA	Described in ref.[32]