

# Molecular dynamics simulations for three-dimensional structures of orotate phosphoribosyltransferases constructed from a simplified amino acid set

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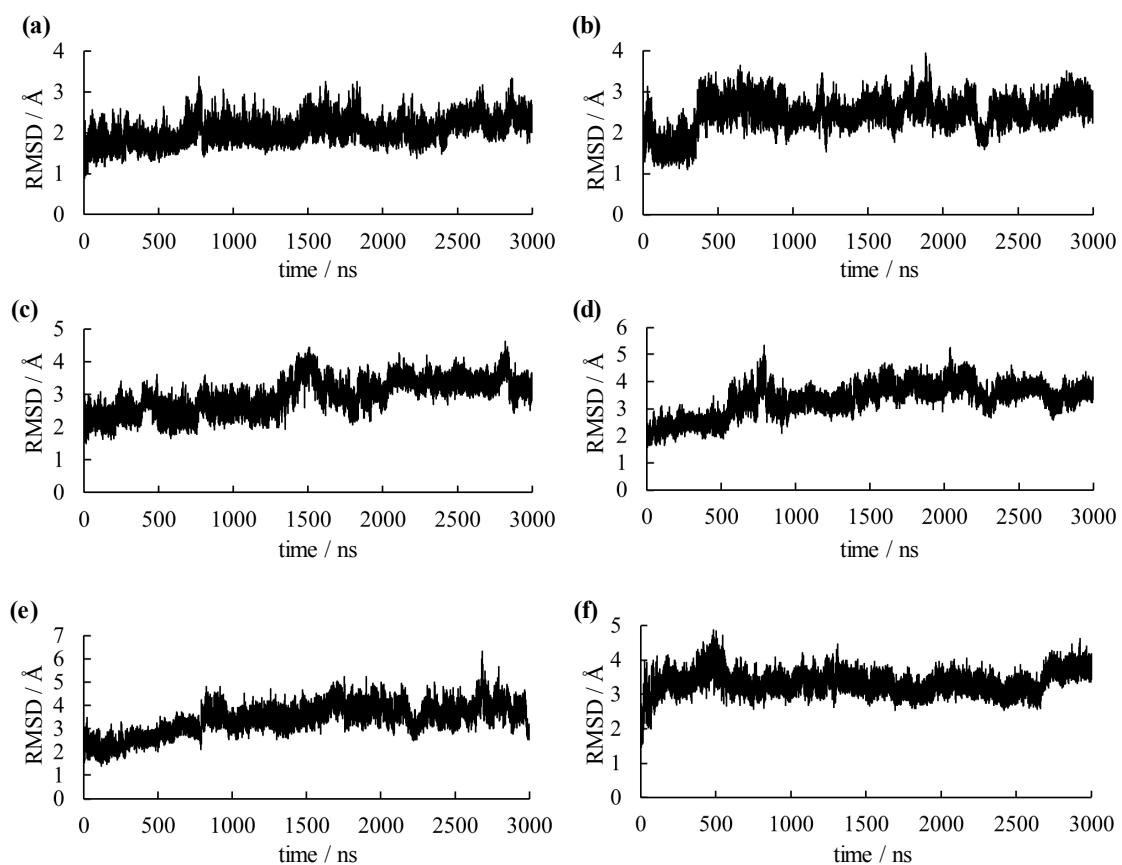
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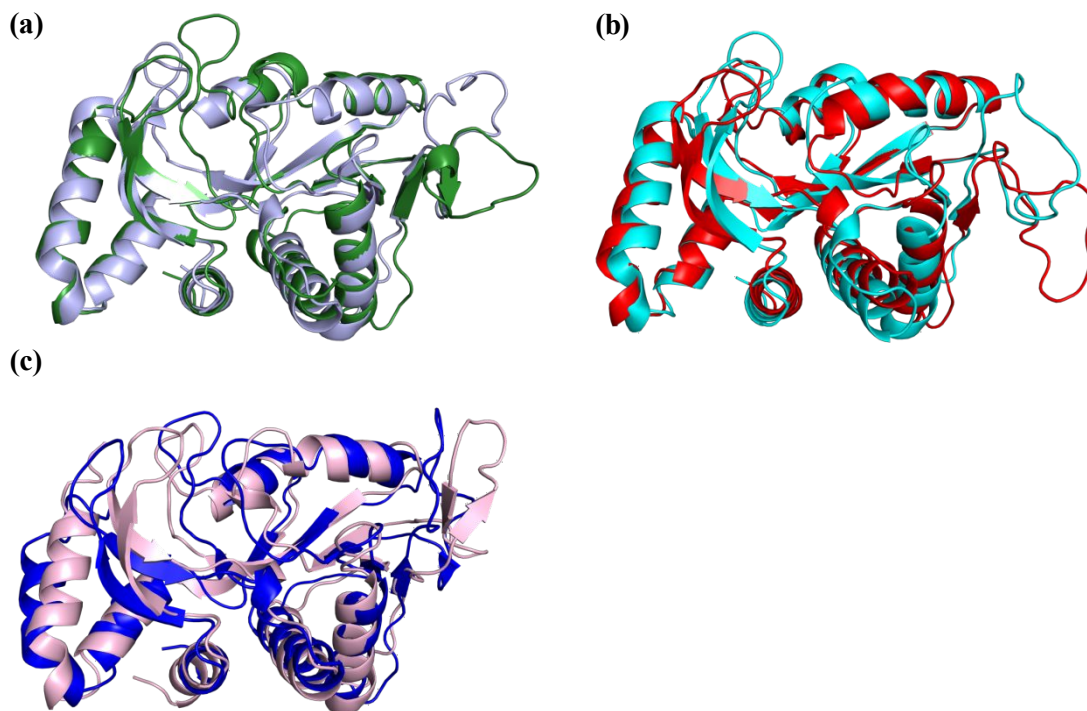
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**Figure S1.** Root mean square deviation (RMSD) plots for the main chain atom of OPRase monomers. RMSD plots of (a) wild-type 1, (b) wild-type 2, (c) middle-variant 1, (d) middle-variant 2, (e) Simp-2 1, and (f) Simp-2 2 in monomers.



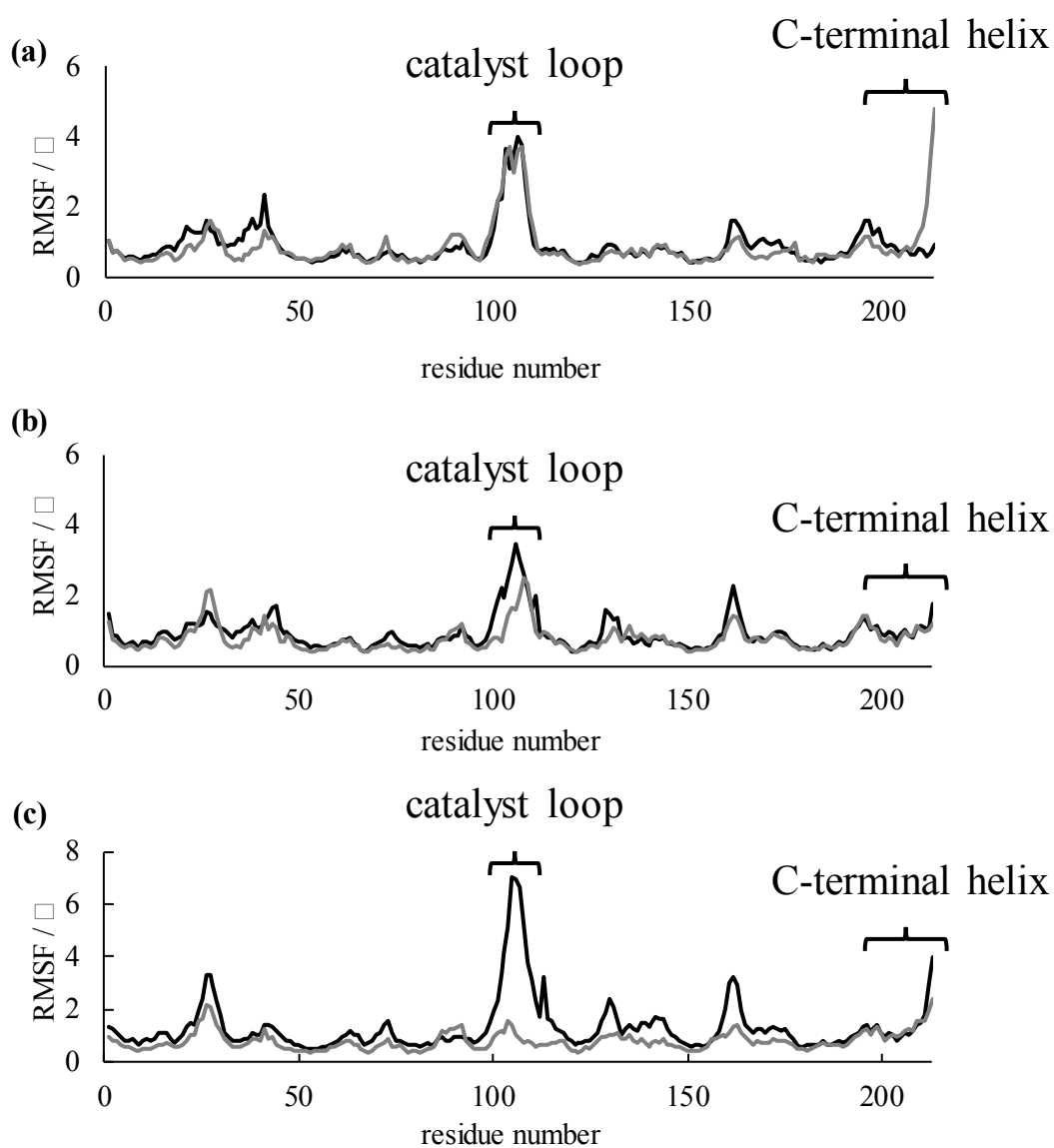
**Figure S2.** Comparison between the calculated monomer structures. The structural superposition of the calculated structures for (a) wild-type 1–wild-type 2, (b) middle-variant 1–middle-variant 2, and (c) Simp-2 1–Simp-2 2. Wild-type 1: green, wild-type 2: light blue, middle variant 1: red, middle variant 2: cyan, Simp-2 1: blue, Simp-2 2: pink.

Table S1. Secondary structure formation in >50% of trajectories for the last 100 ns of simulation for the monomers

	wild 1	wild 2	middle 1	middle 2	Simp-2 1	Simp-2 2
H1	3-14	3-14	3-14	3-14	3-14	3-14
S1	18-21, 23-24	18-21, 23-24	18-21, 23-24	18-21, 23-24	19-21, 23-24	18-20, 23
S2	30-35	30-35	30-35	30-35	30-34	31-35
H2	37-39	37-39	37-39	37-39	37-39	37-39
H3	43-59	43-59	44-59	43-60	43-59	43-60
S3	66-68	66-68	66-68	66-69	66-68	66-69
H4	75-89	75-89	75-88	74-89	75-88	75-89
S4	95-98	95-98	95-96	95-97	95	95-97
S5	111-113	111-113	not detected	112	109-111	112-113
S6	119-123	119-123	119-123	119-123	119-123	119-123
H5	132-142	134-142	132-142	129-134, 137-142	133-142	134-142
S7	146-147, 149-155	146-147, 149-153	146-147, 149-154	146-147, 149-153, 155	146-147, 149-153	146-147, 149-155
H6	166-173	168-174	166-174	169-173	166-173	167-174
S8	177-183	179-182	177-182	177-181, 183	177-181, 183	177-183
H7	184-191	184-191	184-191	184-192	184-192	184-193
H8	195-211	195-210	195-210	195-210	198-209	195-206, 210-211

H: Helix ( $\alpha$ -helix and 3-10 helix ), S: para and anti  $\beta$ -sheet





**Figure S3.** Comparison of root mean square fluctuations (RMSFs) between monomers 1 and 2. The RMSF plots of monomers in (a) the wild type, (b) the middle variant, and (c) Simp-2. The plots of monomer 1 and monomer 2 are indicated by black and gray lines, respectively.