

Vladimir I Timofeev

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	The comparative analysis of the properties and structures of purine nucleoside phosphorylases from thermophilic bacterium <i>Thermus thermophilus</i> HB27. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 3626-3641.	2.0	4
2	Immunoinformatics analysis to design novel epitope based vaccine candidate targeting the glycoprotein and nucleoprotein of Lassa mammarenavirus (LASMV) using strains from Nigeria. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 7283-7302.	2.0	9
3	Identification of the Precursor Cluster in the Crystallization Solution of Proteinase K Protein by Molecular Dynamics Methods. <i>Crystals</i> , 2022, 12, 484.	1.0	4
4	Elucidation of the Conformational Transition of Oligopeptidase B by an Integrative Approach Based on the Combination of X-ray, SAXS, and Essential Dynamics Sampling Simulation. <i>Crystals</i> , 2022, 12, 712.	1.0	2
5	The Role of Cations and Anions in the Formation of Crystallization Oligomers in Protein Solutions as Revealed by Combination of Small-Angle X-ray Scattering and Molecular Dynamics. <i>Crystals</i> , 2022, 12, 751.	1.0	1
6	Precipitant ions influence on lysozyme oligomers stability investigated by molecular dynamics simulation at different temperatures. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 7223-7230.	2.0	10
7	Structure of the microbial carboxypeptidase T complexed with the transition state analog N-sulfamoyl-L-lysine. <i>Biophysical Chemistry</i> , 2021, 270, 106535.	1.5	1
8	Preparation, Crystallization, and Preliminary X-Ray Diffraction Study of Mutant Carboxypeptidase T Bearing the Hydrophilized Primary Specificity Pocket. <i>Crystallography Reports</i> , 2021, 66, 476-478.	0.1	0
9	Effect of the Simulation Box Size and Precipitant Concentration on the Behavior of Tetragonal Lysozyme Dimer. <i>Crystallography Reports</i> , 2021, 66, 525-528.	0.1	0
10	Simulation of A Bilayer Imitating the Inner Mitochondrial Membrane Using Coarse-Grained Molecular Dynamics. <i>Journal of Surface Investigation</i> , 2021, 15, 652-654.	0.1	1
11	Study of the Interaction of Sorption and Catalytic Centers in Carboxypeptidase T by X-ray Analysis. <i>Crystals</i> , 2021, 11, 1088.	1.0	0
12	Comparison of Spatial Structures and Packaging of Phosphorybosyl Pyrophosphate Synthetase 2 from <i>Thermus thermophilus</i> HB27 in Rhombohedral and Tetragonal Crystals. <i>Crystals</i> , 2021, 11, 1128.	1.0	1
13	Free Energy Change during the Formation of Crystalline Contact between Lysozyme Monomers under Different Physical and Chemical Conditions. <i>Crystals</i> , 2021, 11, 1121.	1.0	5
14	Effect of Disruption of the Interface between Monomers in a Dimer on the Structural and Dynamic Properties of the HU Protein from <i>Spiroplasma Melliferum</i> . <i>Journal of Surface Investigation</i> , 2021, 15, 1020-1023.	0.1	1
15	Three-Dimensional Structure of Recombinant Thermophilic Ribokinase from <i>Thermus speñies</i> 2.9 in Complex with Adenosine Diphosphate. <i>Crystallography Reports</i> , 2021, 66, 769-776.	0.1	1
16	Molecular Dynamics of the Self-Organization of Dilinoleoyl Phosphatidylethanolamine Molecules. <i>Journal of Surface Investigation</i> , 2021, 15, 1012-1014.	0.1	0
17	First Crystal Structure of Bacterial Oligopeptidase B in an Intermediate State: The Roles of the Hinge Region Modification and Spermine. <i>Biology</i> , 2021, 10, 1021.	1.3	7
18	The Crystal Structure of N ¹ -p-tosyl-lysyl Chloromethylketone-Bound Oligopeptidase B from <i>Serratia Proteamaculans</i> Revealed a New Type of Inhibitor Binding. <i>Crystals</i> , 2021, 11, 1438.	1.0	4

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19	Molecular Dynamics Study of Escherichia coli Thymidine Phosphorylase in a Complex with 3'-Azidothymidine Inhibitor and Phosphate. Russian Journal of Bioorganic Chemistry, 2021, 47, 1231-1240.	0.3	1
20	Modeling of the Lipid Bilayer Mimicking the Inner Mitochondrial Membrane. Crystallography Reports, 2021, 66, 1006-1009.	0.1	0
21	The Role of Cations of the Precipitant in the Interaction of Protein Molecules in the Lysozyme Oligomers in Crystallization Solutions. Crystals, 2021, 11, 1534.	1.0	3
22	Dodecamers derived from the crystal structure were found in the pre-crystallization solution of the transaminase from the thermophilic bacterium <i>Thermobaculum terrenum</i> by small-angle X-ray scattering. Journal of Biomolecular Structure and Dynamics, 2020, 38, 2939-2944.	2.0	9
23	Molecular dynamics complemented by site-directed mutagenesis reveals significant difference between the interdomain salt bridge networks stabilizing oligopeptidases B from bacteria and protozoa in their active conformations. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4868-4882.	2.0	8
24	The binding of precipitant ions in the tetragonal crystals of hen egg white lysozyme. Journal of Biomolecular Structure and Dynamics, 2020, 38, 5159-5172.	2.0	8
25	Features of Optical Activity in Inorganic and Organic Materials. Crystallography Reports, 2020, 65, 653-677.	0.1	3
26	Three-Dimensional Structure of Branched-Chain Amino Acid Transaminase from <i>Thermoproteus uzoniensis</i> in Complex with L-Norvaline. Crystallography Reports, 2020, 65, 740-743.	0.1	2
27	Structure-based inhibitors targeting the alpha-helical domain of the <i>Spiroplasma melliferum</i> histone-like HU protein. Scientific Reports, 2020, 10, 15128.	1.6	11
28	Molecular Packing of a Mutant of L-Asparaginase from <i>Wolinella succinigenes</i> in Two Crystal Modifications. Crystallography Reports, 2020, 65, 586-592.	0.1	2
29	Features of the Three Dimensional Structure of the Mutant Form of <i>Wolinella succinigenes</i> L-Asparaginase in Complexes with L-Aspartic and L-Glutamic Acids. Russian Journal of Bioorganic Chemistry, 2020, 46, 171-180.	0.3	4
30	Screening of Conditions that Facilitate Crystallization of Oligopeptidase B from <i>Serratia Proteamaculans</i> by Differential Scanning Fluorimetry. Crystallography Reports, 2020, 65, 264-268.	0.1	5
31	Crystal Packing of Phosphopantetheine Adenylyltransferase from <i>Mycobacterium tuberculosis</i> in Two Crystal Modifications. Crystallography Reports, 2020, 65, 84-90.	0.1	0
32	Molecular Dynamics Calculations of the Interaction Energy of Imidazole Glycerol Phosphate Dehydratase from <i>Mycobacterium tuberculosis</i> with Triazole Derivatives. Crystallography Reports, 2020, 65, 755-756.	0.1	0
33	Inhibitor Targeting the Interface between Monomers of HU Protein from <i>Spiroplasma melliferum</i> Disrupts Conformational Dynamics and DNA-Binding Properties of the Protein. Crystallography Reports, 2020, 65, 903-908.	0.1	2
34	Preparation, Crystallization, and Preliminary X-Ray Diffraction Study of Mutant Carboxypeptidase T Bearing the Primary Specificity Pocket and the Active-Site Loop of Carboxypeptidase B. Crystallography Reports, 2020, 65, 900-902.	0.1	1
35	Crystallographic Study of Mutants and Complexes of Oligopeptidase B from <i>Serratia proteamaculans</i> . Crystallography Reports, 2020, 65, 909-914.	0.1	3
36	Modeling of Phosphoribosylpyrophosphate Synthetase from <i>Thermus Thermophilus</i> in Complex with ATP and Ribose 5-Phosphate. Crystallography Reports, 2019, 64, 94-97.	0.1	0

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37	Molecular Dynamics Study of Triazole Derivative Binding to the Active Site of Imidazole Glycerol Phosphate Dehydratase from <i>Mycobacterium tuberculosis</i> . <i>Crystallography Reports</i> , 2019, 64, 608-610.	0.1	3
38	Virtual Screening Targeting Dimerization Signals of Two <i>Mycoplasma HU</i> Proteins Revealed Different Types of Inhibitors Interacting with Common Binding Determinants. <i>Crystallography Reports</i> , 2019, 64, 602-607.	0.1	4
39	Molecular Dynamics Study of Binding of Substrates Bearing Two Positively Charged Residues to Oligopeptidase B from <i>Serratia proteamaculans</i> . <i>Crystallography Reports</i> , 2019, 64, 758-764.	0.1	3
40	Three-Dimensional Structure of a Mutant of Carboxypeptidase T from <i>Thermoactinomyces vulgaris</i> Bearing an Implanted S1' Subsite of Pancreatic Carboxypeptidase B Complexed with a Product Analog. <i>Crystallography Reports</i> , 2019, 64, 750-757.	0.1	0
41	Molecular Dynamics Study of Thymidine Phosphorylase from <i>E. coli</i> in the Apo Form and in Complexes with Substrates. <i>Crystallography Reports</i> , 2019, 64, 98-104.	0.1	2
42	Study of the Influence of a Precipitant Cation on the Formation of Oligomers in Crystallization Solutions of Lysozyme Protein. <i>Crystallography Reports</i> , 2019, 64, 11-15.	0.1	13
43	Functional characterization of PLP fold type IV transaminase with a mixed type of activity from <i>Haliangium ochraceum</i> . <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2019, 1867, 575-585.	1.1	11
44	The nature of the ligand's side chain interacting with the S1'-subsite of metallo-carboxypeptidase T (from <i>Thermoactinomyces vulgaris</i>) determines the geometry of the tetrahedral transition complex. <i>PLoS ONE</i> , 2019, 14, e0226636.	1.1	4
45	Crystallization and Preliminary X-ray Diffraction Study of a Mutant of L-Asparaginase from <i>Wolinella succinogenes</i> . <i>Crystallography Reports</i> , 2019, 64, 910-913.	0.1	2
46	Pre-crystallization phase formation of thermolysin hexamers in solution close to crystallization conditions. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 3058-3064.	2.0	12
47	An explanation for the narrow carbohydrate substrate specificity of adenine phosphoribosyltransferase from <i>Thermus thermophilus</i> from the model of the enzyme, substrate, and magnesium cation cofactor complex. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 4460-4464.	2.0	0
48	Discovery of Selective Inhibitors of Imidazoleglycerol-Phosphate Dehydratase from <i>Mycobacterium tuberculosis</i> by Virtual Screening. <i>Crystallography Reports</i> , 2018, 63, 74-78.	0.1	3
49	Structural plasticity and thermal stability of the histone-like protein from <i>Spiroplasma melliferum</i> are due to phenylalanine insertions into the conservative scaffold. <i>Journal of Biomolecular Structure and Dynamics</i> , 2018, 36, 4392-4404.	2.0	7
50	Enhanced conformational flexibility of the histone-like (HU) protein from <i>Mycoplasma gallisepticum</i> . <i>Journal of Biomolecular Structure and Dynamics</i> , 2018, 36, 45-53.	2.0	10
51	Structure of the carboxypeptidase B complex with N-sulfamoyl-L-phenylalanine as a transition state analog of non-specific substrate. <i>Journal of Biomolecular Structure and Dynamics</i> , 2018, 36, 956-965.	2.0	7
52	Crystal structures of carboxypeptidase T complexes with transition-state analogs. <i>Journal of Biomolecular Structure and Dynamics</i> , 2018, 36, 3958-3966.	2.0	3
53	Study of the Behavior of Lysozyme Oligomers in Solutions by the Molecular Dynamics Method. <i>Crystallography Reports</i> , 2018, 63, 947-950.	0.1	14
54	Mobile Loop in the Active Site of Metallo-carboxypeptidases as an Underestimated Determinant of Substrate Specificity. <i>Biochemistry (Moscow)</i> , 2018, 83, 1594-1602.	0.7	1

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55	Crystal structure of mutant carboxypeptidase T from <i>Thermoactinomyces vulgaris</i> with an implanted S1 \hat{e} 2 subsite from pancreatic carboxypeptidase B. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2018, 74, 638-643.	0.4	4
56	Crystallization and Preliminary X-ray Diffraction Study of Purine Nucleoside Phosphorylase from the Thermophilic Bacterium <i>Thermus thermophilus</i> Strain HB27. <i>Crystallography Reports</i> , 2018, 63, 761-764.	0.1	1
57	Three-Dimensional Structure of Recombinant Adenine Phosphoribosyltransferase from Thermophilic Bacterial Strain <i>Thermus thermophilus</i> HB27. <i>Russian Journal of Bioorganic Chemistry</i> , 2018, 44, 504-510.	0.3	2
58	Crystal structure of <i>Escherichia coli</i> purine nucleoside phosphorylase complexed with acyclovir. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2018, 74, 402-409.	0.4	1
59	Crystal structure of <i>Escherichia coli</i> purine nucleoside phosphorylase in complex with 7-deazahypoxanthine. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2018, 74, 355-362.	0.4	2
60	Crystallization and preliminary X-ray diffraction analysis of recombinant phosphoribosylpyrophosphate synthetase from the Thermophilic <i>Thermus thermophilus</i> strain HB27. <i>Crystallography Reports</i> , 2017, 62, 78-81.	0.1	1
61	Crystal structure of recombinant phosphoribosylpyrophosphate synthetase 2 from <i>Thermus thermophilus</i> HB27 complexed with ADP and sulfate ions. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2017, 73, 369-375.	0.4	5
62	Virtual screening of selective inhibitors of phosphopantetheine adenylyltransferase from <i>Mycobacterium tuberculosis</i> . <i>Crystallography Reports</i> , 2017, 62, 405-410.	0.1	1
63	Activity modulation of the oligopeptidase B from <i>Serratia proteamaculans</i> by site-directed mutagenesis of amino acid residues surrounding catalytic triad histidine. <i>Biochimie</i> , 2017, 139, 125-136.	1.3	17
64	Crystallization and preliminary X-ray diffraction study of recombinant adenine phosphoribosyltransferase from the thermophilic bacterium <i>Thermus thermophilus</i> strain HB27. <i>Crystallography Reports</i> , 2017, 62, 580-583.	0.1	2
65	Three-dimensional structure of porcine pancreatic carboxypeptidase B with an acetate ion and two zinc atoms in the active site. <i>Crystallography Reports</i> , 2017, 62, 249-253.	0.1	2
66	Application of virtual screening and molecular dynamics for the analysis of selectivity of inhibitors of HU proteins targeted to the DNA-recognition site. <i>Crystallography Reports</i> , 2017, 62, 903-908.	0.1	3
67	Comparison of histone-like HU protein DNA-binding properties and HU/IHF protein sequence alignment. <i>PLoS ONE</i> , 2017, 12, e0188037.	1.1	37
68	Three-dimensional structure of <i>E. coli</i> purine nucleoside phosphorylase at 0.99 Å... resolution. <i>Crystallography Reports</i> , 2016, 61, 249-257.	0.1	7
69	Protein crystallization under microgravity conditions. Analysis of the results of Russian experiments performed on the International Space Station in 2005~2015. <i>Crystallography Reports</i> , 2016, 61, 718-729.	0.1	18
70	Crystallization and preliminary X-ray diffraction study of recombinant ribokinase from <i>Thermus</i> Species 2.9. <i>Crystallography Reports</i> , 2016, 61, 974-978.	0.1	3
71	Three-dimensional structure of phosphoribosyl pyrophosphate synthetase from <i>E. coli</i> at 2.71 Å... resolution. <i>Crystallography Reports</i> , 2016, 61, 44-54.	0.1	7
72	Investigation of the Initial Crystallization Stage in Lysozyme Solutions by Small-Angle X-ray Scattering. <i>Crystal Growth and Design</i> , 2016, 16, 1792-1797.	1.4	48

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73	In situ study of the state of lysozyme molecules at the very early stage of the crystallization process by small-angle X-ray scattering. <i>Crystallography Reports</i> , 2016, 61, 5-10.	0.1	29
74	Isolation, purification, crystallization, and preliminary X-ray diffraction study of the crystals of HU protein from <i>M. gallisepticum</i> . <i>Crystallography Reports</i> , 2015, 60, 880-883.	0.1	11
75	Crystallization and preliminary X-ray diffraction study of phosphoribosyl pyrophosphate synthetase from <i>E. Coli</i> . <i>Crystallography Reports</i> , 2015, 60, 685-688.	0.1	1
76	Crystallization and preliminary X-ray diffraction study of phosphopantetheine adenylyltransferase from <i>M. tuberculosis</i> crystallizing in space group P32. <i>Crystallography Reports</i> , 2015, 60, 682-684.	0.1	1
77	Structure of the complex of carboxypeptidase B and <i>N</i> -sulfamoyl-L-arginine. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2015, 71, 1335-1340.	0.4	10
78	Structure of recombinant prolidase from <i>Thermococcus sibiricus</i> in space group $P2_12_12_1$. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2015, 71, 951-957.	0.4	4
79	Structural insights into the broad substrate specificity of carboxypeptidase T from <i>Thermoactinomyces vulgarens</i> . <i>FEBS Journal</i> , 2015, 282, 1214-1224.	2.2	15
80	Purification, crystallization, and preliminary X-ray diffraction study of purine nucleoside phosphorylase from <i>E. coli</i> . <i>Crystallography Reports</i> , 2015, 60, 521-524.	0.1	1
81	Crystallization and preliminary X-ray diffraction study of porcine carboxypeptidase B. <i>Crystallography Reports</i> , 2015, 60, 367-369.	0.1	2
82	3-Azidothymidine in the active site of <i>Escherichia coli</i> thymidine phosphorylase: the peculiarity of the binding on the basis of X-ray study. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2014, 70, 1155-1165.	2.5	17
83	Three-dimensional structure of thymidine phosphorylase from <i>E. coli</i> in complex with $3\text{-azido-2-fluoro-2,3-dideoxyuridine}$. <i>Crystallography Reports</i> , 2013, 58, 842-853.	0.1	20
84	Three-dimensional structure of carboxypeptidase T from <i>Thermoactinomyces vulgarens</i> in complex with N-BOC-L-leucine. <i>Biochemistry (Moscow)</i> , 2013, 78, 252-259.	0.7	4
85	X-ray study of the conformational changes in the molecule of phosphopantetheine adenylyltransferase from <i>Mycobacterium tuberculosis</i> during the catalyzed reaction. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012, 68, 1660-1670.	2.5	28
86	Three-dimensional structure of phosphopantetheine adenylyltransferase from <i>Mycobacterium tuberculosis</i> in the apo form and in complexes with coenzyme A and dephosphocoenzyme A. <i>Crystallography Reports</i> , 2012, 57, 96-104.	0.1	12
87	Three-dimensional structure of recombinant carboxypeptidase T from <i>Thermoactinomyces vulgarens</i> without calcium ions. <i>Crystallography Reports</i> , 2011, 56, 596-602.	0.1	7
88	Crystal growth of phosphopantetheine adenylyltransferase, carboxypeptidase t, and thymidine phosphorylase on the international space station by the capillary counter-diffusion method. <i>Crystallography Reports</i> , 2011, 56, 884-891.	0.1	39
89	Preparation, crystallization, and preliminary X-ray diffraction study of mutant carboxypeptidase T containing the primary specificity pocket of carboxypeptidase B. <i>Crystallography Reports</i> , 2010, 55, 802-805.	0.1	6
90	Recombinant formate dehydrogenase from <i>Arabidopsis thaliana</i> : Preparation, crystal growth in microgravity, and preliminary X-ray diffraction study. <i>Crystallography Reports</i> , 2010, 55, 806-810.	0.1	13

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91	Preparation of the Crystal Complex of Phosphopantetheine Adenylyltransferase from <i>Mycobacterium tuberculosis</i> with Coenzyme A and Investigation of Its Three-Dimensional Structure at 2.1-Å... Resolution. <i>Crystallography Reports</i> , 2010, 55, 1050-1059.	0.1	13
92	X-ray investigation of gene-engineered human insulin crystallized from a solution containing polysialic acid. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2010, 66, 259-263.	0.7	48
93	Protein crystal growth on the Russian segment of the International Space Station. <i>Crystallography Reports</i> , 2009, 54, 901-911.	0.1	13
94	Isolation, crystallization and preliminary crystallographic analysis of <i>Salmonella typhimurium</i> uridine phosphorylase crystallized with 2,2'-anhydrouridine. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2007, 63, 852-854.	0.7	5
95	Structure of the homodimer of uridine phosphorylase from <i>Salmonella typhimurium</i> in the native state at 1.9 Å... resolution. <i>Crystallography Reports</i> , 2007, 52, 1072-1078.	0.1	2
96	Computational designing of a novel subunit vaccine for human cytomegalovirus by employing the immunoinformatics framework. <i>Journal of Biomolecular Structure and Dynamics</i> , 0, , 1-23.	2.0	6