

# CITATION REPORT

List of articles citing

**Crystallography & NMR system: A new software suite for macromolecular structure determination**

**DOI: 10.1107/s0907444998003254**

**Acta Crystallographica Section D: Biological Crystallography, 1998, 54, 905-21.**

**Source:** <https://exaly.com/paper-pdf/29146755/citation-report.pdf>

**Version:** 2024-04-24

This report has been generated based on the citations recorded by exaly.com for the above article. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

#	Paper	IF	Citations
2286	Molecular basis of double-stranded RNA-protein interactions: structure of a dsRNA-binding domain complexed with dsRNA. <b>1998</b> , 17, 7505-13		392
2285	Crystal structure of the ATP-binding subunit of an ABC transporter. <b>1998</b> , 396, 703-7		632
2284	Crystal structure of a SNARE complex involved in synaptic exocytosis at 2.4 Å resolution. <b>1998</b> , 395, 347-53		1929
2283	Crystal structure of a hepatitis delta virus ribozyme. <b>1998</b> , 395, 567-74		660
2282	An excitatory scorpion toxin with a distinctive feature: an additional alpha helix at the C terminus and its implications for interaction with insect sodium channels. <b>1998</b> , 6, 1095-103		70
2281	Direct structure refinement against residual dipolar couplings in the presence of rhombicity of unknown magnitude. <b>1998</b> , 131, 159-62		292
2280	Solution structure of the His12 → Cys mutant of the N-terminal zinc binding domain of HIV-1 integrase complexed to cadmium. <b>1998</b> , 7, 2669-74		37
2279	Recent developments for the efficient crystallographic refinement of macromolecular structures. <b>1998</b> , 8, 606-11		80
2278	Crystal structure of the Ebola virus membrane fusion subunit, GP2, from the envelope glycoprotein ectodomain. <b>1998</b> , 2, 605-16		366
2277	Transmembrane signaling across the ligand-gated FhuA receptor: crystal structures of free and ferrichrome-bound states reveal allosteric changes. <b>1998</b> , 95, 771-8		484
2276	Crystal structure of the human high-affinity IgE receptor. <b>1998</b> , 95, 951-61		145
2275	Crystal structure of the <i>Oxytricha nova</i> telomere end binding protein complexed with single strand DNA. <b>1998</b> , 95, 963-74		236
2274	NMR structure and mutagenesis of the N-terminal Dbl homology domain of the nucleotide exchange factor Trio. <b>1998</b> , 95, 269-77		161
2273	Ca <sup>2+</sup> -dependent structural changes in C-type mannose-binding proteins. <b>1998</b> , 37, 17965-76		65
2272	Crystal structure of GCN4-pIQ1, a trimeric coiled coil with buried polar residues. <b>1998</b> , 284, 859-65		84
2271	Conserved structural features of the synaptic fusion complex: SNARE proteins reclassified as Q- and R-SNAREs. <b>1998</b> , 95, 15781-6		734
2270	Crystal structure of the ligand binding domain of the human nuclear receptor PPARγ. <b>1998</b> , 273, 31108-12		210

2269	Structure-based assignment of the biochemical function of a hypothetical protein: a test case of structural genomics. <b>1998</b> , 95, 15189-93	276
2268	Distinct Metal Environment in Fe-Substituted Manganese Superoxide Dismutase Provides a Structural Basis of Metal Specificity. <b>1998</b> , 120, 9684-9685	53
2267	A sulfate pocket formed by three GoU pairs in the 0.97 Å resolution X-ray structure of a nonameric RNA. <b>1999</b> , 5, 1384-95	28
2266	Crystallographic structure of the amino terminal domain of yeast initiation factor 4A, a representative DEAD-box RNA helicase. <b>1999</b> , 5, 1526-34	68
2265	Antibody C219 recognizes an alpha-helical epitope on P-glycoprotein. <b>1999</b> , 96, 13679-84	42
2264	Bactericidal antibody recognition of meningococcal PorA by induced fit. Comparison of liganded and unliganded Fab structures. <b>1999</b> , 274, 1495-501	24
2263	A structural snapshot of base-pair opening in DNA. <b>1999</b> , 96, 11809-14	30
2262	Lys13 plays a crucial role in the functional adaptation of the thermophilic triose-phosphate isomerase from <i>Bacillus stearothermophilus</i> to high temperatures. <b>1999</b> , 274, 19181-7	13
2261	The structural basis for the oriented assembly of a TBP/TFB/promoter complex. <b>1999</b> , 96, 13668-73	127
2260	Crystal structure of <i>Bacillus subtilis</i> YabJ, a purine regulatory protein and member of the highly conserved YjgF family. <b>1999</b> , 96, 13074-9	67
2259	Monomeric structure of the human EphB2 sterile alpha motif domain. <b>1999</b> , 274, 37301-6	35
2258	Crystal structure of the cytosolic C2A-C2B domains of synaptotagmin III. Implications for Ca <sup>2+</sup> -independent snare complex interaction. <b>1999</b> , 147, 589-98	157
2257	Structure of human histocompatibility leukocyte antigen (HLA)-Cw4, a ligand for the KIR2D natural killer cell inhibitory receptor. <b>1999</b> , 190, 113-23	48
2256	Structure-based design of Taq DNA polymerases with improved properties of dideoxynucleotide incorporation. <b>1999</b> , 96, 9491-6	111
2255	Crystal structure of the DNA nucleotide excision repair enzyme UvrB from <i>Thermus thermophilus</i> . <b>1999</b> , 96, 11717-22	87
2254	Core structure of the envelope glycoprotein GP2 from Ebola virus at 1.9-Å resolution. <b>1999</b> , 96, 2662-7	242
2253	Structure of the HIV-1 integrase catalytic domain complexed with an inhibitor: a platform for antiviral drug design. <b>1999</b> , 96, 13040-3	454
2252	Crystal structure of human p32, a doughnut-shaped acidic mitochondrial matrix protein. <b>1999</b> , 96, 3572-7	219

2251	A bicarbonate ion as a general base in the mechanism of peptide hydrolysis by dizinc leucine aminopeptidase. <b>1999</b> , 96, 11151-5	86
2250	Absence of interdomain contacts in the crystal structure of the RNA recognition motifs of Sex-lethal. <b>1999</b> , 96, 4892-7	52
2249	Crystal structure of the Sec18p N-terminal domain. <b>1999</b> , 96, 14759-64	40
2248	Crystal structure of the RNA-dependent RNA polymerase of hepatitis C virus. <b>1999</b> , 96, 13034-9	520
2247	Optical detection of cytochrome P450 by sensitizer-linked substrates. <b>1999</b> , 96, 12987-90	55
2246	Crystal structure and mechanism of CO dehydrogenase, a molybdo iron-sulfur flavoprotein containing S-selanylcyysteine. <b>1999</b> , 96, 8884-9	208
2245	N- and C-terminal residues combine in the fusion-pH influenza hemagglutinin HA(2) subunit to form an N cap that terminates the triple-stranded coiled coil. <b>1999</b> , 96, 8967-72	251
2244	The cytochrome c oxidase from <i>Paracoccus denitrificans</i> does not change the metal center ligation upon reduction. <b>1999</b> , 274, 33296-9	112
2243	Crystallographic analysis of CD40 recognition and signaling by human TRAF2. <b>1999</b> , 96, 8408-13	170
2242	Crystal structures of intermediates in the dehalogenation of haloalkanoates by L-2-haloacid dehalogenase. <b>1999</b> , 274, 30672-8	65
2241	Crystal structure of human type II inosine monophosphate dehydrogenase: implications for ligand binding and drug design. <b>1999</b> , 96, 3531-6	138
2240	Methods for X-ray diffraction analysis of macromolecular structures. <b>1999</b> , 3, 525-9	10
2239	The role of high-resolution structural studies in the development of commercial enzymes. <b>1999</b> , 10, 391-7	4
2238	Evaluation of macromolecular electron-density map quality using the correlation of local r.m.s. density. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>1999</b> , 55, 1872-7	52
2237	Structure of the Janus-faced C2B domain of rabphilin. <b>1999</b> , 1, 106-12	60
2236	Crystal structure of the amino-terminal domain of N-ethylmaleimide-sensitive fusion protein. <b>1999</b> , 1, 175-82	85
2235	Crystal structure of 2-oxoisovalerate and dehydrogenase and the architecture of 2-oxo acid dehydrogenase multienzyme complexes. <b>1999</b> , 6, 785-92	98
2234	Crystal structure of human heme oxygenase-1. <b>1999</b> , 6, 860-7	254

2233	Structure and mechanism of the glycol radical enzyme pyruvate formate-lyase. <b>1999</b> , 6, 969-75	159
2232	Structural basis for self-association and receptor recognition of human TRAF2. <b>1999</b> , 398, 533-8	304
2231	Structural basis for initiation of transcription from an RNA polymerase-promoter complex. <b>1999</b> , 399, 80-3	267
2230	Structure of the nuclear transport complex karyopherin-beta2-Ran x GppNHp. <b>1999</b> , 399, 230-7	300
2229	Clathrin self-assembly is mediated by a tandemly repeated superhelix. <b>1999</b> , 399, 371-5	134
2228	Structure of Cdc42 in complex with the GTPase-binding domain of the 'Wiskott-Aldrich syndrome' protein. <b>1999</b> , 399, 379-83	289
2227	Structure of cytochrome c nitrite reductase. <b>1999</b> , 400, 476-80	287
2226	Placement of protein and RNA structures into a 5 A-resolution map of the 50S ribosomal subunit. <b>1999</b> , 400, 841-7	352
2225	Structure of the TRAIL-DR5 complex reveals mechanisms conferring specificity in apoptotic initiation. <b>1999</b> , 6, 1048-53	214
2224	Structure of Tetrahymena GCN5 bound to coenzyme A and a histone H3 peptide. <b>1999</b> , 401, 93-8	244
2223	Structures of a histone deacetylase homologue bound to the TSA and SAHA inhibitors. <b>1999</b> , 401, 188-93	1430
2222	High-resolution X-ray structure of an early intermediate in the bacteriorhodopsin photocycle. <b>1999</b> , 401, 822-6	302
2221	A triple beta-spiral in the adenovirus fibre shaft reveals a new structural motif for a fibrous protein. <b>1999</b> , 401, 935-8	279
2220	Crystal structure of a lectin-like natural killer cell receptor bound to its MHC class I ligand. <b>1999</b> , 402, 623-31	231
2219	Structural changes linked to proton translocation by subunit c of the ATP synthase. <b>1999</b> , 402, 263-8	408
2218	Structural insights into phosphoinositide 3-kinase catalysis and signalling. <b>1999</b> , 402, 313-20	413
2217	Structure of fumarate reductase from Wolinella succinogenes at 2.2 A resolution. <b>1999</b> , 402, 377-85	316
2216	Structure of the C2 domain of human factor VIII at 1.5 A resolution. <b>1999</b> , 402, 439-42	300

2215	Crystal structure of the novel aspartic proteinase zymogen proplasmepsin II from plasmodium falciparum. <b>1999</b> , 6, 32-7	55
2214	Crystal structure of the outer membrane active transporter FepA from Escherichia coli. <b>1999</b> , 6, 56-63	463
2213	Solution structure of the 40,000 Mr phosphoryl transfer complex between the N-terminal domain of enzyme I and HPr. <b>1999</b> , 6, 166-73	171
2212	Crystal structure of a lead-dependent ribozyme revealing metal binding sites relevant to catalysis. <b>1999</b> , 6, 261-8	83
2211	Structural and mechanistic mapping of a unique fumarate reductase. <b>1999</b> , 6, 1108-12	127
2210	Automated protein model building combined with iterative structure refinement. <b>1999</b> , 6, 458-63	2261
2209	Self-consistent 3J coupling analysis for the joint calibration of Karplus coefficients and evaluation of torsion angles. <b>1999</b> , 14, 1-12	85
2208	StarDOM: from STAR format to XML. <b>1999</b> , 15, 169-72	1
2207	Pig heart short chain L-3-hydroxyacyl-CoA dehydrogenase revisited: sequence analysis and crystal structure determination. <b>1999</b> , 8, 2010-8	16
2206	Crystal structure of the human protein kinase CK2 regulatory subunit reveals its zinc finger-mediated dimerization. <b>1999</b> , 18, 2930-40	119
2205	Structure-specific tRNA-binding protein from the extreme thermophile Aquifex aeolicus. <b>1999</b> , 18, 3475-83	65
2204	The three-dimensional structure of the RNA-binding domain of ribosomal protein L2; a protein at the peptidyl transferase center of the ribosome. <b>1999</b> , 18, 1459-67	51
2203	Crystal structure of a heparin- and integrin-binding segment of human fibronectin. <b>1999</b> , 18, 1468-79	165
2202	The pre-hydrolysis state of p21(ras) in complex with GTP: new insights into the role of water molecules in the GTP hydrolysis reaction of ras-like proteins. <b>1999</b> , 7, 1311-24	167
2201	The 2 A structure of helix 6 of the human signal recognition particle RNA. <b>1999</b> , 7, 1345-52	42
2200	Crystal structure of colicin E3 immunity protein: an inhibitor of a ribosome-inactivating RNase. <b>1999</b> , 7, 1365-72	12
2199	The crystal structure of the minus-end-directed microtubule motor protein ncd reveals variable dimer conformations. <b>1999</b> , 7, 1407-16	47
2198	The crystal structure of the dimerization initiation site of genomic HIV-1 RNA reveals an extended duplex with two adenine bulges. <b>1999</b> , 7, 1439-49	136

2197	Crystal structure of an archaeobacterial DNA polymerase. <b>1999</b> , 7, 1189-99	81
2196	The structure of bacteriophage T4 gene product 9: the trigger for tail contraction. <b>1999</b> , 7, 1213-22	52
2195	The crystal structure of methenyltetrahydromethanopterin cyclohydrolase from the hyperthermophilic archaeon <i>Methanopyrus kandleri</i> . <b>1999</b> , 7, 1257-68	41
2194	Metal-ion affinity and specificity in EF-hand proteins: coordination geometry and domain plasticity in parvalbumin. <b>1999</b> , 7, 1269-78	69
2193	Structure of the <i>Escherichia coli</i> TolB protein determined by MAD methods at 1.95 Å resolution. <b>1999</b> , 7, 1291-300	64
2192	<i>Helianthus tuberosus</i> lectin reveals a widespread scaffold for mannose-binding lectins. <b>1999</b> , 7, 1473-82	95
2191	Crystal structure of a transcriptionally active Smad4 fragment. <b>1999</b> , 7, 1493-503	59
2190	Conformational changes induced by phosphorylation of the FixJ receiver domain. <b>1999</b> , 7, 1505-15	177
2189	Structural transitions in the FixJ receiver domain. <b>1999</b> , 7, 1517-26	50
2188	The three-dimensional structure of the HRDC domain and implications for the Werner and Bloom syndrome proteins. <b>1999</b> , 7, 1557-66	110
2187	The active conformation of plasminogen activator inhibitor 1, a target for drugs to control fibrinolysis and cell adhesion. <b>1999</b> , 7, 111-8	136
2186	Crystal structures of Nova-1 and Nova-2 K-homology RNA-binding domains. <b>1999</b> , 7, 191-203	98
2185	Crystal structure of the human p58 killer cell inhibitory receptor (KIR2DL3) specific for HLA-Cw3-related MHC class I. <b>1999</b> , 7, 391-8	77
2184	Crystal structure of human bleomycin hydrolase, a self-compartmentalizing cysteine protease. <b>1999</b> , 7, 619-27	52
2183	Crystal structure of the ATPase domain of translation initiation factor 4A from <i>Saccharomyces cerevisiae</i> --the prototype of the DEAD box protein family. <b>1999</b> , 7, 671-9	102
2182	Selenium-based MAD phasing: setting the sites on larger structures. <b>1999</b> , 7, R161-6	31
2181	Pyruvate formate lyase is structurally homologous to type I ribonucleotide reductase. <b>1999</b> , 7, 733-44	36
2180	Protein, lipid and water organization in bacteriorhodopsin crystals: a molecular view of the purple membrane at 1.9 Å resolution. <b>1999</b> , 7, 909-17	396

2179	Crystallographic evidence for substrate ring distortion and protein conformational changes during catalysis in cellobiohydrolase Ce16A from trichoderma reesei. <b>1999</b> , 7, 1035-45	150
2178	The structure of phosphorylated p38gamma is monomeric and reveals a conserved activation-loop conformation. <b>1999</b> , 7, 1057-65	113
2177	Crystal structure of human glyoxalase II and its complex with a glutathione thiolester substrate analogue. <b>1999</b> , 7, 1067-78	152
2176	X-ray crystal structure of aminoimidazole ribonucleotide synthetase (PurM), from the Escherichia coli purine biosynthetic pathway at 2.5 A resolution. <b>1999</b> , 7, 1155-66	61
2175	Effective Computational Strategies for Determining Structures of Carcinogen-Damaged DNA. <b>1999</b> , 151, 313-332	4
2174	The crystal structure of triosephosphate isomerase (TIM) from Thermotoga maritima: A comparative thermostability structural analysis of ten different TIM structures. <b>1999</b> , 37, 441-453	119
2173	Crystal structure of a thermophilic alcohol dehydrogenase substrate complex suggests determinants of substrate specificity and thermostability. <b>1999</b> , 37, 619-27	52
2172	Non-Boltzmann thermodynamic integration (NBTI) for macromolecular systems: relative free energy of binding of trypsin to benzamidine and benzylamine. <b>1999</b> , 37, 641-53	30
2171	Crystal structures of aged phosphonylated acetylcholinesterase: nerve agent reaction products at the atomic level. <b>1999</b> , 38, 7032-9	248
2170	Oligomeric structure of the human EphB2 receptor SAM domain. <b>1999</b> , 283, 833-6	198
2169	Crystal structure of human ZAG, a fat-depleting factor related to MHC molecules. <b>1999</b> , 283, 1914-9	113
2168	Structure of the VHL-ElonginC-ElonginB complex: implications for VHL tumor suppressor function. <b>1999</b> , 284, 455-61	680
2167	X-ray crystal structures of 70S ribosome functional complexes. <b>1999</b> , 285, 2095-104	528
2166	Structure of an E6AP-UbcH7 complex: insights into ubiquitination by the E2-E3 enzyme cascade. <b>1999</b> , 286, 1321-6	429
2165	Structural analysis of the mechanism of adenovirus binding to its human cellular receptor, CAR. <b>1999</b> , 286, 1579-83	370
2164	Domain movement in gelsolin: a calcium-activated switch. <b>1999</b> , 286, 1939-42	127
2163	Structure of a transcribing T7 RNA polymerase initiation complex. <b>1999</b> , 286, 2305-9	307
2162	Conformational flexibility of the acetylcholinesterase tetramer suggested by x-ray crystallography. <b>1999</b> , 274, 30370-6	122



2161	Mapping the role of active site residues for transducing an ATP-induced conformational change in the bovine 70-kDa heat shock cognate protein. <b>1999</b> , 38, 10823-30	45
2160	Crystal structure of the MHC class I homolog MIC-A, a gammadelta T cell ligand. <b>1999</b> , 10, 577-84	152
2159	Melatonin biosynthesis: the structure of serotonin N-acetyltransferase at 2.5 A resolution suggests a catalytic mechanism. <b>1999</b> , 3, 23-32	107
2158	Structure of the InlB leucine-rich repeats, a domain that triggers host cell invasion by the bacterial pathogen <i>L. monocytogenes</i> . <b>1999</b> , 4, 1063-72	144
2157	The structural basis for the recognition of diverse receptor sequences by TRAF2. <b>1999</b> , 4, 321-30	237
2156	Crystal structure of Hck in complex with a Src family-selective tyrosine kinase inhibitor. <b>1999</b> , 3, 639-48	384
2155	A molecular mechanism for the phosphorylation-dependent regulation of heterotrimeric G proteins by phosducin. <b>1999</b> , 3, 649-60	77
2154	Tick histamine-binding proteins: isolation, cloning, and three-dimensional structure. <b>1999</b> , 3, 661-71	279
2153	Structural basis for paramyxovirus-mediated membrane fusion. <b>1999</b> , 3, 309-19	341
2152	The structural basis for terminator recognition by the Rho transcription termination factor. <b>1999</b> , 3, 487-93	120
2151	New strategies for protein crystal growth. <b>1999</b> , 1, 505-34	53
2150	Characteristics and crystal structure of bacterial inosine-5'-monophosphate dehydrogenase. <b>1999</b> , 38, 4691-700	157
2149	NMR structure of a minimized human agouti related protein prepared by total chemical synthesis. <b>1999</b> , 451, 125-31	68
2148	Mutations in the Ca <sup>2+</sup> binding site of the <i>Paracoccus denitrificans</i> cytochrome c oxidase. <b>1999</b> , 456, 365-9	18
2147	Structure of acetylcholinesterase complexed with (-)-galanthamine at 2.3 A resolution. <b>1999</b> , 463, 321-6	220
2146	Structural basis for FGF receptor dimerization and activation. <b>1999</b> , 98, 641-50	505
2145	The structure of the ligand-binding domain of neuexin Ibeta: regulation of LNS domain function by alternative splicing. <b>1999</b> , 99, 93-101	121
2144	Inhibiting HIV-1 entry: discovery of D-peptide inhibitors that target the gp41 coiled-coil pocket. <b>1999</b> , 99, 103-15	406

2143	Crystal structure of the cytoplasmic domain of the type I TGF beta receptor in complex with FKBP12. <b>1999</b> , 96, 425-36	375
2142	Structure of a HoxB1-Pbx1 heterodimer bound to DNA: role of the hexapeptide and a fourth homeodomain helix in complex formation. <b>1999</b> , 96, 587-97	290
2141	Transformation of MutL by ATP binding and hydrolysis: a switch in DNA mismatch repair. <b>1999</b> , 97, 85-97	348
2140	The 2.8 Å crystal structure of visual arrestin: a model for arrestin's regulation. <b>1999</b> , 97, 257-69	370
2139	The structure of threonyl-tRNA synthetase-tRNA(Thr) complex enlightens its repressor activity and reveals an essential zinc ion in the active site. <b>1999</b> , 97, 371-81	264
2138	Structure of the enabled/VASP homology 1 domain-peptide complex: a key component in the spatial control of actin assembly. <b>1999</b> , 97, 471-80	218
2137	Crystal structure of a phosphatidylinositol 3-phosphate-specific membrane-targeting motif, the FYVE domain of Vps27p. <b>1999</b> , 97, 657-66	229
2136	Structure of a voltage-dependent K <sup>+</sup> channel beta subunit. <b>1999</b> , 97, 943-52	244
2135	The structure of the protein phosphatase 2A PR65/A subunit reveals the conformation of its 15 tandemly repeated HEAT motifs. <b>1999</b> , 96, 99-110	359
2134	Recognition of polyadenylate RNA by the poly(A)-binding protein. <b>1999</b> , 98, 835-45	412
2133	Three-dimensional structure of a complex between the death domains of Pelle and Tube. <b>1999</b> , 99, 545-55	156
2132	Crystal structure of the vinculin tail suggests a pathway for activation. <b>1999</b> , 99, 603-13	163
2131	Recognition of a TG mismatch: the crystal structure of very short patch repair endonuclease in complex with a DNA duplex. <b>1999</b> , 99, 615-23	92
2130	Building a replisome from interacting pieces: sliding clamp complexed to a peptide from DNA polymerase and a polymerase editing complex. <b>1999</b> , 99, 155-66	331
2129	Crystal structure of the helicase domain from the replicative helicase-primase of bacteriophage T7. <b>1999</b> , 99, 167-77	256
2128	Crystal structure of the PTEN tumor suppressor: implications for its phosphoinositide phosphatase activity and membrane association. <b>1999</b> , 99, 323-34	850
2127	The crystal structure of a GroEL/peptide complex: plasticity as a basis for substrate diversity. <b>1999</b> , 99, 757-68	214
2126	Structure of the DNA repair enzyme endonuclease IV and its DNA complex: double-nucleotide flipping at abasic sites and three-metal-ion catalysis. <b>1999</b> , 98, 397-408	237

2125	Structures of two repeats of spectrin suggest models of flexibility. <b>1999</b> , 98, 523-35	214
2124	Structure of the alpha-actinin rod: molecular basis for cross-linking of actin filaments. <b>1999</b> , 98, 537-46	218
2123	vpu transmembrane peptide structure obtained by site-specific fourier transform infrared dichroism and global molecular dynamics searching. <b>1999</b> , 77, 1594-601	93
2122	Comparison of the crystal and solution structures of two RNA oligonucleotides. <b>1999</b> , 76, 65-75	33
2121	Structure of a triple helical DNA with a triplex-duplex junction. <b>1999</b> , 38, 16810-5	66
2120	The structural mechanism for half-the-sites reactivity in an enzyme, thymidylate synthase, involves a relay of changes between subunits. <b>1999</b> , 38, 13829-36	69
2119	Structure-function correlations of the reaction of reduced nicotinamide analogues with p-hydroxybenzoate hydroxylase substituted with a series of 8-substituted flavins. <b>1999</b> , 38, 16636-47	27
2118	Structure and recognition of sheared tandem G x A base pairs associated with human centromere DNA sequence at atomic resolution. <b>1999</b> , 38, 16452-60	42
2117	Crystal structure of the proenzyme domain of plasminogen. <b>1999</b> , 38, 11180-8	37
2116	R-factor, Free R, and Complete Cross-Validation for Dipolar Coupling Refinement of NMR Structures. <b>1999</b> , 121, 9008-9012	225
2115	Model for lentivirus capsid core assembly based on crystal dimers of EIAV p26. <b>1999</b> , 286, 83-93	100
2114	Structure of D-allose binding protein from Escherichia coli bound to D-allose at 1.8 A resolution. <b>1999</b> , 286, 1519-31	49
2113	Crystal structure of human bone morphogenetic protein-2 at 2.7 A resolution. <b>1999</b> , 287, 103-15	302
2112	Crystal structure of cyanovirin-N, a potent HIV-inactivating protein, shows unexpected domain swapping. <b>1999</b> , 288, 403-12	152
2111	The 2.2 A structure of the rRNA methyltransferase ErmC' and its complexes with cofactor and cofactor analogs: implications for the reaction mechanism. <b>1999</b> , 289, 277-91	85
2110	Crystal structure of a mammalian purple acid phosphatase. <b>1999</b> , 290, 201-11	108
2109	Induced fit on sugar binding activates ribokinase. <b>1999</b> , 290, 1009-18	68
2108	Three-dimensional structure of a mammalian purple acid phosphatase at 2.2 A resolution with a mu-(hydr)oxo bridged di-iron center. <b>1999</b> , 291, 135-47	119

2107	Structure of recombinant mouse collagenase-3 (MMP-13). <b>1999</b> , 292, 837-44	38
2106	Crystal structure of enteropeptidase light chain complexed with an analog of the trypsinogen activation peptide. <b>1999</b> , 292, 361-73	87
2105	Structure of the complex of the antistasin-type inhibitor bdellastasin with trypsin and modelling of the bdellastasin-microplasmin system. <b>1999</b> , 293, 93-106	15
2104	Crystal structure of Apaf-1 caspase recruitment domain: an alpha-helical Greek key fold for apoptotic signaling. <b>1999</b> , 293, 439-47	70
2103	The variable region-1 from tissue-type plasminogen activator confers specificity for plasminogen activator inhibitor-1 to thrombin by facilitating catalysis: release of a kinetic block by a heterologous protein surface loop. <b>1999</b> , 293, 613-27	24
2102	A 2.6 Å structure of a serpin polymer and implications for conformational disease. <b>1999</b> , 293, 449-55	108
2101	Crystal structure of chondroitinase B from <i>Flavobacterium heparinum</i> and its complex with a disaccharide product at 1.7 Å resolution. <b>1999</b> , 294, 1257-69	95
2100	Structural analysis of an RNase T1 variant with an altered guanine binding segment. <b>1999</b> , 294, 1231-8	7
2099	Crystal structure of the purine nucleoside phosphorylase (PNP) from <i>Cellulomonas</i> sp. and its implication for the mechanism of trimeric PNPs. <b>1999</b> , 294, 1239-55	60
2098	Structural basis of DNA recognition by the heterodimeric cell cycle transcription factor E2F-DP. <b>1999</b> , 13, 666-74	207
2097	Crystal structure of the two-RRM domain of hnRNP A1 (UP1) complexed with single-stranded telomeric DNA. <b>1999</b> , 13, 1102-15	259
2096	Crystal structure of CHO reductase, a member of the aldo-keto reductase superfamily. <b>2000</b> , 38, 41-8	11
2095	Crystal structure of human ubiquitous mitochondrial creatine kinase. <b>2000</b> , 39, 216-25	59
2094	Crystal structure of YbaK protein from <i>Haemophilus influenzae</i> (HI1434) at 1.8 Å resolution: functional implications. <b>2000</b> , 40, 86-97	42
2093	The duplication of an eight-residue helical stretch in Staphylococcal nuclease is not helical: a model for evolutionary change. <b>2000</b> , 40, 465-72	2
2092	Functional aspects of the heme bound hemophore HasA by structural analysis of various crystal forms. <b>2000</b> , 41, 202-10	33
2091	A comparative structural analysis of the ADF/cofilin family. <b>2000</b> , 41, 374-84	66
2090	Crystal structure of the W35A mutant thioredoxin h from <i>Chlamydomonas reinhardtii</i> : the substitution of the conserved active site Trp leads to modifications in the environment of the two catalytic cysteines. <b>2000</b> , 56, 1-7	14

2089	Quadruplex structures in nucleic acids. <b>2000</b> , 56, 123-46	286
2088	The crystal structure of the complex of Zea mays alpha subunit with a fragment of human beta subunit provides the clue to the architecture of protein kinase CK2 holoenzyme. <b>2000</b> , 267, 5184-90	29
2087	Selective boron-containing thrombin inhibitors--X-ray analysis reveals surprising binding mode. <b>2000</b> , 8, 2291-303	15
2086	Crystal structure of the hereditary haemochromatosis protein HFE complexed with transferrin receptor. <b>2000</b> , 403, 46-53	287
2085	Design of single-layer beta-sheets without a hydrophobic core. <b>2000</b> , 403, 456-60	54
2084	Shiga-like toxins are neutralized by tailored multivalent carbohydrate ligands. <b>2000</b> , 403, 669-72	772
2083	The structures of HslU and the ATP-dependent protease HslU-HslV. <b>2000</b> , 403, 800-5	378
2082	Structural basis for recognition and repair of the endogenous mutagen 8-oxoguanine in DNA. <b>2000</b> , 403, 859-66	787
2081	Structure of the winged-helix protein hRFX1 reveals a new mode of DNA binding. <b>2000</b> , 403, 916-21	261
2080	Autoinhibition and activation mechanisms of the Wiskott-Aldrich syndrome protein. <b>2000</b> , 404, 151-8	616
2079	Three-dimensional structure of the neuronal-Sec1-syntaxin 1a complex. <b>2000</b> , 404, 355-62	613
2078	Structure of the reovirus core at 3.6 A resolution. <b>2000</b> , 404, 960-7	392
2077	The crystal structure of the photoprotein aequorin at 2.3 A resolution. <b>2000</b> , 405, 372-6	262
2076	Crystal structure of an NK cell immunoglobulin-like receptor in complex with its class I MHC ligand. <b>2000</b> , 405, 537-43	339
2075	Crystal structure of the calcium pump of sarcoplasmic reticulum at 2.6 A resolution. <b>2000</b> , 405, 647-55	1626
2074	Crystal structure of the bacterial membrane protein TolC central to multidrug efflux and protein export. <b>2000</b> , 405, 914-9	926
2073	Crystal structure of enteropathogenic Escherichia coli intimin-receptor complex. <b>2000</b> , 405, 1073-7	263
2072	Structure of the dimerized hormone-binding domain of a guanylyl-cyclase-coupled receptor. <b>2000</b> , 406, 101-4	142

2071	Structure of the Fc fragment of human IgE bound to its high-affinity receptor Fc epsilonRI alpha. <b>2000</b> , 406, 259-66	291
2070	Mimicry of ice structure by surface hydroxyls and water of a beta-helix antifreeze protein. <b>2000</b> , 406, 322-4	362
2069	Helix deformation is coupled to vectorial proton transport in the photocycle of bacteriorhodopsin. <b>2000</b> , 406, 645-8	215
2068	Structural alterations for proton translocation in the M state of wild-type bacteriorhodopsin. <b>2000</b> , 406, 649-53	305
2067	Molecular mechanism of vectorial proton translocation by bacteriorhodopsin. <b>2000</b> , 406, 653-7	394
2066	Structural and biochemical basis of apoptotic activation by Smac/DIABLO. <b>2000</b> , 406, 855-62	699
2065	Structure of the 30S ribosomal subunit. <b>2000</b> , 407, 327-39	1682
2064	Functional insights from the structure of the 30S ribosomal subunit and its interactions with antibiotics. <b>2000</b> , 407, 340-8	1296
2063	Crystal structures of mismatch repair protein MutS and its complex with a substrate DNA. <b>2000</b> , 407, 703-10	538
2062	The crystal structure of DNA mismatch repair protein MutS binding to a G x T mismatch. <b>2000</b> , 407, 711-7	540
2061	Structure of a serpin-protease complex shows inhibition by deformation. <b>2000</b> , 407, 923-6	916
2060	Crystal structure of fibroblast growth factor receptor ectodomain bound to ligand and heparin. <b>2000</b> , 407, 1029-34	659
2059	Structural basis of glutamate recognition by a dimeric metabotropic glutamate receptor. <b>2000</b> , 407, 971-7	1089
2058	Structural basis for signal transduction by the Toll/interleukin-1 receptor domains. <b>2000</b> , 408, 111-5	613
2057	Structure and assembly of the Alu domain of the mammalian signal recognition particle. <b>2000</b> , 408, 167-73	164
2056	Insights into SCF ubiquitin ligases from the structure of the Skp1-Skp2 complex. <b>2000</b> , 408, 381-6	487
2055	Crystal structure of Rac1 in complex with the guanine nucleotide exchange region of Tiam1. <b>2000</b> , 408, 682-8	310
2054	Directed evolution of an enantioselective lipase. <b>2000</b> , 7, 709-18	204

2053	Sexual attraction in the silkworm moth: structure of the pheromone-binding-protein-bombykol complex. <b>2000</b> , 7, 143-51	362
2052	Recent developments in software for the automation of crystallographic macromolecular structure determination. <b>2000</b> , 10, 564-8	15
2051	Crystal structure of the worm NitFhit Rosetta Stone protein reveals a Nit tetramer binding two Fhit dimers. <b>2000</b> , 10, 907-17	107
2050	The high-resolution structure of the NADP(H)-binding component (dIII) of proton-translocating transhydrogenase from human heart mitochondria. <b>2000</b> , 8, 1-12	162
2049	Structures of human dihydroorotate dehydrogenase in complex with antiproliferative agents. <b>2000</b> , 8, 25-33	246
2048	The crystal structure of the formiminotransferase domain of formiminotransferase-cyclodeaminase: implications for substrate channeling in a bifunctional enzyme. <b>2000</b> , 8, 35-46	37
2047	The structure of TolB, an essential component of the tol-dependent translocation system, and its protein-protein interaction with the translocation domain of colicin E9. <b>2000</b> , 8, 57-66	75
2046	A new scaffold for binding haem in the cytochrome domain of the extracellular flavocytochrome cellobiose dehydrogenase. <b>2000</b> , 8, 79-88	126
2045	Structure of <i>Aspergillus niger</i> epoxide hydrolase at 1.8 Å resolution: implications for the structure and function of the mammalian microsomal class of epoxide hydrolases. <b>2000</b> , 8, 111-22	161
2044	Structural and kinetic analysis of <i>Escherichia coli</i> GDP-mannose 4,6 dehydratase provides insights into the enzyme's catalytic mechanism and regulation by GDP-fucose. <b>2000</b> , 8, 123-35	77
2043	The structure of adenylosuccinate lyase, an enzyme with dual activity in the de novo purine biosynthetic pathway. <b>2000</b> , 8, 163-74	65
2042	The coiled-coil trigger site of the rod domain of cortexillin I unveils a distinct network of interhelical and intrahelical salt bridges. <b>2000</b> , 8, 223-30	110
2041	Crystal structure of Rab geranylgeranyltransferase at 2.0 Å resolution. <b>2000</b> , 8, 241-51	98
2040	A mutant Shiga-like toxin IIe bound to its receptor Gb(3): structure of a group II Shiga-like toxin with altered binding specificity. <b>2000</b> , 8, 253-64	32
2039	Crystal structure of human branched-chain alpha-ketoacid dehydrogenase and the molecular basis of multienzyme complex deficiency in maple syrup urine disease. <b>2000</b> , 8, 277-91	132
2038	Crystallographic analysis of the specific yet versatile recognition of distinct nuclear localization signals by karyopherin alpha. <b>2000</b> , 8, 329-38	247
2037	The 'fingerprint' that X-rays can leave on structures. <b>2000</b> , 8, 315-28	264
2036	The 1.8 Å crystal structure of catechol 1,2-dioxygenase reveals a novel hydrophobic helical zipper as a subunit linker. <b>2000</b> , 8, 429-40	116

2035	Structure of cyanase reveals that a novel dimeric and decameric arrangement of subunits is required for formation of the enzyme active site. <b>2000</b> , 8, 505-14	50
2034	A potential target enzyme for trypanocidal drugs revealed by the crystal structure of NAD-dependent glycerol-3-phosphate dehydrogenase from <i>Leishmania mexicana</i> . <b>2000</b> , 8, 541-52	45
2033	Crystal structure of the ffh and EF-G binding sites in the conserved domain IV of <i>Escherichia coli</i> 4.5S RNA. <b>2000</b> , 8, 527-40	52
2032	A conserved structural motif for lipopolysaccharide recognition by procaryotic and eucaryotic proteins. <b>2000</b> , 8, 585-92	173
2031	Structure and self-association of the Rous sarcoma virus capsid protein. <b>2000</b> , 8, 617-28	104
2030	Structure at 2.3 Å resolution of the cytochrome bc(1) complex from the yeast <i>Saccharomyces cerevisiae</i> co-crystallized with an antibody Fv fragment. <b>2000</b> , 8, 669-84	510
2029	A water channel in the core of the vitamin B(12) RNA aptamer. <b>2000</b> , 8, 719-27	21
2028	Crystal structure of N-carbamyl-D-amino acid amidohydrolase with a novel catalytic framework common to amidohydrolases. <b>2000</b> , 8, 729-37	118
2027	X-ray structure of <i>Escherichia coli</i> pyridoxine 5'-phosphate oxidase complexed with FMN at 1.8 Å resolution. <b>2000</b> , 8, 751-62	26
2026	How a protein generates a catalytic radical from coenzyme B(12): X-ray structure of a diol-dehydratase-adeninylpentylcobalamin complex. <b>2000</b> , 8, 775-88	126
2025	Luxury accommodations: the expanding role of structural plasticity in protein-protein interactions. <b>2000</b> , 8, R137-42	65
2024	The crystal structure of the peptide-binding fragment from the yeast Hsp40 protein Sis1. <b>2000</b> , 8, 799-807	140
2023	Crystal structure of a methyltetrahydrofolate- and corrinoid-dependent methyltransferase. <b>2000</b> , 8, 817-30	62
2022	Crystal structure and mutational analysis of the <i>Saccharomyces cerevisiae</i> cell cycle regulatory protein Cks1: implications for domain swapping, anion binding and protein interactions. <b>2000</b> , 8, 841-50	33
2021	Crystal structures of substrate binding to <i>Bacillus subtilis</i> holo-(acyl carrier protein) synthase reveal a novel trimeric arrangement of molecules resulting in three active sites. <b>2000</b> , 8, 883-95	189
2020	Crystal structure of archaeal RNase HII: a homologue of human major RNase H. <b>2000</b> , 8, 897-904	60
2019	Inhibition of a ribosome-inactivating ribonuclease: the crystal structure of the cytotoxic domain of colicin E3 in complex with its immunity protein. <b>2000</b> , 8, 949-60	39
2018	Crystal structure of Omp32, the anion-selective porin from <i>Comamonas acidovorans</i> , in complex with a periplasmic peptide at 2.1 Å resolution. <b>2000</b> , 8, 981-92	100



2017	Crystal structure of a nonsymbiotic plant hemoglobin. <b>2000</b> , 8, 1005-14	148
2016	Structure of a PH domain from the <i>C. elegans</i> muscle protein UNC-89 suggests a novel function. <b>2000</b> , 8, 1079-87	25
2015	Crystal structure of hyaluronidase, a major allergen of bee venom. <b>2000</b> , 8, 1025-35	229
2014	Crystal structure of saccharopine reductase from <i>Magnaporthe grisea</i> , an enzyme of the alpha-aminoadipate pathway of lysine biosynthesis. <b>2000</b> , 8, 1037-47	37
2013	Structural basis for the resilience of efavirenz (DMP-266) to drug resistance mutations in HIV-1 reverse transcriptase. <b>2000</b> , 8, 1089-94	231
2012	A duplicated fold is the structural basis for polynucleotide phosphorylase catalytic activity, processivity, and regulation. <b>2000</b> , 8, 1215-26	226
2011	Crystal structure of protein isoaspartyl methyltransferase: a catalyst for protein repair. <b>2000</b> , 8, 1189-201	49
2010	Does NMR mean "not for molecular replacement"? Using NMR-based search models to solve protein crystal structures. <b>2000</b> , 8, R213-20	29
2009	Structure of the molybdate/tungstate binding protein mop from <i>Sporomusa ovata</i> . <b>2000</b> , 8, 1127-36	33
2008	Crystal structure of the <i>Escherichia coli</i> peptide methionine sulphoxide reductase at 1.9 Å resolution. <b>2000</b> , 8, 1167-78	82
2007	Solution structures of two CCHC zinc fingers from the FOG family protein U-shaped that mediate protein-protein interactions. <b>2000</b> , 8, 1157-66	36
2006	Structure of dihydroorotate dehydrogenase B: electron transfer between two flavin groups bridged by an iron-sulphur cluster. <b>2000</b> , 8, 1227-38	59
2005	Structural and biochemical properties show ARL3-GDP as a distinct GTP binding protein. <b>2000</b> , 8, 1239-45	49
2004	Structure and mechanism of homoserine kinase: prototype for the GHMP kinase superfamily. <b>2000</b> , 8, 1247-57	100
2003	A cluster exposed: structure of the Rieske ferredoxin from biphenyl dioxygenase and the redox properties of Rieske Fe-S proteins. <b>2000</b> , 8, 1267-78	105
2002	Curling of flap tips in HIV-1 protease as a mechanism for substrate entry and tolerance of drug resistance. <b>2000</b> , 8, 1259-65	172
2001	Dramatic structural and thermodynamic consequences of repacking a protein's hydrophobic core. <b>2000</b> , 8, 1319-28	41
2000	Structures of HIV-1 gp120 envelope glycoproteins from laboratory-adapted and primary isolates. <b>2000</b> , 8, 1329-39	341

1999	Refinement of the protein backbone angle psi in NMR structure calculations. <b>2000</b> , 16, 47-58	25
1998	Rapid fold and structure determination of the archaeal translation elongation factor 1beta from <i>Methanobacterium thermoautotrophicum</i> . <b>2000</b> , 17, 187-94	12
1997	Structure of a rat $\mu$ macroglobulin receptor-binding domain dimer. <b>2000</b> , 9, 1889-97	17
1996	Structure of the Ca <sup>2+</sup> -regulated photoprotein obelin at 1.7 Å resolution determined directly from its sulfur substructure. <b>2000</b> , 9, 2085-93	152
1995	Proline in alpha-helical kink is required for folding kinetics but not for kinked structure, function, or stability of heat shock transcription factor. <b>2000</b> , 9, 2128-41	21
1994	Design of a minimal protein oligomerization domain by a structural approach. <b>2000</b> , 9, 2294-301	81
1993	Crystal structure of the antibiotic albomycin in complex with the outer membrane transporter FhuA. <b>2000</b> , 9, 956-63	128
1992	The 1.9 Å crystal structure of <i>Escherichia coli</i> MurG, a membrane-associated glycosyltransferase involved in peptidoglycan biosynthesis. <b>2000</b> , 9, 1045-52	218
1991	Three-dimensional structures of <i>Drosophila melanogaster</i> acetylcholinesterase and of its complexes with two potent inhibitors. <b>2000</b> , 9, 1063-72	246
1990	Crystal structure of viral serpin crmA provides insights into its mechanism of cysteine proteinase inhibition. <b>2000</b> , 9, 1423-7	44
1989	Structure of a (Cys3His) zinc ribbon, a ubiquitous motif in archaeal and eucaryal transcription. <b>2000</b> , 9, 1743-52	53
1988	Crystal structure of the catalytic domain of human bile salt activated lipase. <b>2000</b> , 9, 1783-90	46
1987	Structure of streptococcal pyrogenic exotoxin A reveals a novel metal cluster. <b>2000</b> , 9, 1847-51	26
1986	Change in dimerization mode by removal of a single unsatisfied polar residue located at the interface. <b>2000</b> , 9, 1852-5	6
1985	Structural basis of the Axin-adenomatous polyposis coli interaction. <b>2000</b> , 19, 2270-9	163
1984	Crystal structure of the ribosome recycling factor from <i>Escherichia coli</i> . <b>2000</b> , 19, 2362-70	80
1983	A novel two-over-two alpha-helical sandwich fold is characteristic of the truncated hemoglobin family. <b>2000</b> , 19, 2424-34	199
1982	Crystal structure of the human RXRalpha ligand-binding domain bound to its natural ligand: 9-cis retinoic acid. <b>2000</b> , 19, 2592-601	265

1981	The crystal structures of chloramphenicol phosphotransferase reveal a novel inactivation mechanism. <b>2000</b> , 19, 2690-700	51
1980	Crystal structure of a gamma-herpesvirus cyclin-cdk complex. <b>2000</b> , 19, 2877-88	41
1979	Structural basis for the heterodimeric interaction between the acute leukaemia-associated transcription factors AML1 and CBFbeta. <b>2000</b> , 19, 3004-15	85
1978	Structure of the C-terminal domain of Tup1, a corepressor of transcription in yeast. <b>2000</b> , 19, 3016-27	94
1977	Crystal structure of NaeI-an evolutionary bridge between DNA endonuclease and topoisomerase. <b>2000</b> , 19, 3110-8	63
1976	Crystal structure of cystalysin from <i>Treponema denticola</i> : a pyridoxal 5'-phosphate-dependent protein acting as a haemolytic enzyme. <b>2000</b> , 19, 3168-78	64
1975	The bacterial cell-division protein ZipA and its interaction with an FtsZ fragment revealed by X-ray crystallography. <b>2000</b> , 19, 3179-91	213
1974	Structural basis for activation of alpha-boranophosphate nucleotide analogues targeting drug-resistant reverse transcriptase. <b>2000</b> , 19, 3520-9	60
1973	Charged residues dominate a unique interlocking topography in the heterodimeric cytokine interleukin-12. <b>2000</b> , 19, 3530-41	119
1972	Crystal structures of the metal-dependent 2-dehydro-3-deoxy-galactarate aldolase suggest a novel reaction mechanism. <b>2000</b> , 19, 3849-56	41
1971	Crystal structure of a repair enzyme of oxidatively damaged DNA, MutM (Fpg), from an extreme thermophile, <i>Thermus thermophilus</i> HB8. <b>2000</b> , 19, 3857-69	116
1970	The structure of L-amino acid oxidase reveals the substrate trajectory into an enantiomerically conserved active site. <b>2000</b> , 19, 4204-15	198
1969	Crystal structure of the matrix protein VP40 from Ebola virus. <b>2000</b> , 19, 4228-36	131
1968	Structural basis of the membrane-targeting and unmasking mechanisms of the radixin FERM domain. <b>2000</b> , 19, 4449-62	302
1967	Triphosphate structure of guanylate-binding protein 1 and implications for nucleotide binding and GTPase mechanism. <b>2000</b> , 19, 4555-64	119
1966	Crystal structure of a eukaryote/archaeon-like protyl-tRNA synthetase and its complex with tRNA <sup>Pro</sup> (CGG). <b>2000</b> , 19, 4745-58	73
1965	Structure of the ArsA ATPase: the catalytic subunit of a heavy metal resistance pump. <b>2000</b> , 19, 4838-45	140
1964	Dual epitope recognition by the VASP EVH1 domain modulates polyproline ligand specificity and binding affinity. <b>2000</b> , 19, 4903-14	103

1963	Crystal structure of the GAP domain of Gyp1p: first insights into interaction with Ypt/Rab proteins. <b>2000</b> , 19, 5105-13	82
1962	Crystal structure of FadR, a fatty acid-responsive transcription factor with a novel acyl coenzyme A-binding fold. <b>2000</b> , 19, 5167-77	110
1961	New structural motifs on the chymotrypsin fold and their potential roles in complement factor B. <b>2000</b> , 19, 164-73	40
1960	Flexibility, conformational diversity and two dimerization modes in complexes of ribosomal protein L12. <b>2000</b> , 19, 174-86	79
1959	X-ray crystal structure of rabbit N-acetylglucosaminyltransferase I: catalytic mechanism and a new protein superfamily. <b>2000</b> , 19, 5269-80	207
1958	Structure of the GAF domain, a ubiquitous signaling motif and a new class of cyclic GMP receptor. <b>2000</b> , 19, 5288-99	238
1957	Crystal structure of the cell division protein FtsA from <i>Thermotoga maritima</i> . <b>2000</b> , 19, 5300-7	163
1956	The structure of the mRNA export factor TAP reveals a cis arrangement of a non-canonical RNP domain and an LRR domain. <b>2000</b> , 19, 5587-98	108
1955	tRNA aminoacylation by arginyl-tRNA synthetase: induced conformations during substrates binding. <b>2000</b> , 19, 5599-610	144
1954	Structure of a covalently stabilized complex of a human alphabeta T-cell receptor, influenza HA peptide and MHC class II molecule, HLA-DR1. <b>2000</b> , 19, 5611-24	211
1953	Crystal structure of MalK, the ATPase subunit of the trehalose/maltose ABC transporter of the archaeon <i>Thermococcus litoralis</i> . <b>2000</b> , 19, 5951-61	255
1952	Crystal structure of the Xrcc4 DNA repair protein and implications for end joining. <b>2000</b> , 19, 5962-70	137
1951	Eukaryotic chaperonin CCT stabilizes actin and tubulin folding intermediates in open quasi-native conformations. <b>2000</b> , 19, 5971-9	163
1950	Structure and mechanism of activity of the cyclic phosphodiesterase of <i>Appr&gt;p</i> , a product of the tRNA splicing reaction. <b>2000</b> , 19, 6207-17	51
1949	Crystal structure of trbp111: a structure-specific tRNA-binding protein. <b>2000</b> , 19, 6287-98	44
1948	Crystal structure of the peptidyl-cysteine decarboxylase EpiD complexed with a pentapeptide substrate. <b>2000</b> , 19, 6299-310	80
1947	The structural basis of the catalytic mechanism and regulation of glucose-1-phosphate thymidyltransferase (RmlA). <b>2000</b> , 19, 6652-63	158
1946	Crystal structure of a fibrillarlin homologue from <i>Methanococcus jannaschii</i> , a hyperthermophile, at 1.6 Å resolution. <b>2000</b> , 19, 317-23	140

1945	Crystal structure of a class I alpha1,2-mannosidase involved in N-glycan processing and endoplasmic reticulum quality control. <b>2000</b> , 19, 581-8	91
1944	Structure of Hsp15 reveals a novel RNA-binding motif. <b>2000</b> , 19, 749-57	50
1943	DNA bending and a flip-out mechanism for base excision by the helix-hairpin-helix DNA glycosylase, Escherichia coli AlkA. <b>2000</b> , 19, 758-66	180
1942	Crystal structure of NAD(+)-dependent DNA ligase: modular architecture and functional implications. <b>2000</b> , 19, 1119-29	154
1941	Crystal structure of ribosomal protein L4 shows RNA-binding sites for ribosome incorporation and feedback control of the S10 operon. <b>2000</b> , 19, 807-18	35
1940	Crystal structure of the catalytic portion of human HMG-CoA reductase: insights into regulation of activity and catalysis. <b>2000</b> , 19, 819-30	217
1939	The active site architecture of Pisum sativum beta-carbonic anhydrase is a mirror image of that of alpha-carbonic anhydrases. <b>2000</b> , 19, 1407-18	200
1938	The alpha-subunit of the mitochondrial F(1) ATPase interacts directly with the assembly factor Atp12p. <b>2000</b> , 19, 1486-93	41
1937	Multiple modes of peptide recognition by the PTB domain of the cell fate determinant Numb. <b>2000</b> , 19, 1505-15	77
1936	The structure of mouse HP1 suggests a unique mode of single peptide recognition by the shadow chromo domain dimer. <b>2000</b> , 19, 1587-97	230
1935	Structure and mechanism of the aberrant ba(3)-cytochrome c oxidase from thermus thermophilus. <b>2000</b> , 19, 1766-76	403
1934	Assessment of molecular structure using frame-independent orientational restraints derived from residual dipolar couplings. <b>2000</b> , 18, 239-52	35
1933	Ansig for Windows: an interactive computer program for semiautomatic assignment of protein NMR spectra. <b>2000</b> , 18, 329-36	81
1932	A method for incorporating dipolar couplings into structure calculations in cases of (near) axial symmetry of alignment. <b>2000</b> , 18, 183-8	13
1931	Identification of substituted 3-[(4,5,6,7-tetrahydro-1H-indol-2-yl)methylene]-1,3-dihydroindol-2-ones as growth factor receptor inhibitors for VEGF-R2 (Flk-1/KDR), FGF-R1, and PDGF-Rbeta tyrosine kinases. <b>2000</b> , 43, 2655-63	104
1930	The complete atomic structure of the large ribosomal subunit at 2.4 A resolution. <b>2000</b> , 289, 905-20	2807
1929	Crystal structure of the ribonucleoprotein core of the signal recognition particle. <b>2000</b> , 287, 1232-9	338
1928	The three-dimensional structure of the antigen-binding fragment of a monoclonal antibody to human interleukin-2 in two crystal forms at 2.2 and 2.9 Å resolution. <b>2000</b> , 26, 512-519	1

1927	The crystal structure of yeast phenylalanine tRNA at 1.93 Å resolution: a classic structure revisited. <b>2000</b> , 6, 1091-105	336
1926	Two crystal forms of helix II of <i>Xenopus laevis</i> 5S rRNA with a cytosine bulge. <b>2000</b> , 6, 1316-24	30
1925	The crystal structure of HIV reverse-transcription primer tRNA(Lys,3) shows a canonical anticodon loop. <b>2000</b> , 6, 1347-55	78
1924	(4-aminomethyl)phenylguanidine derivatives as nonpeptidic highly selective inhibitors of human urokinase. <b>2000</b> , 97, 5113-8	64
1923	Molecular basis for CD40 signaling mediated by TRAF3. <b>2000</b> , 97, 10395-10399	118
1922	Structural basis for the impaired channeling and allosteric inter-subunit communication in the beta A169L/beta C170W mutant of tryptophan synthase. <b>2000</b> , 275, 41058-63	18
1921	Three-dimensional structure of the Fab from a human IgM cold agglutinin. <b>2000</b> , 165, 6422-8	26
1920	Determination of the binding sites of the proton transfer inhibitors Cd <sup>2+</sup> and Zn <sup>2+</sup> in bacterial reaction centers. <b>2000</b> , 97, 1542-7	119
1919	The x-ray structure of D-amino acid oxidase at very high resolution identifies the chemical mechanism of flavin-dependent substrate dehydrogenation. <b>2000</b> , 97, 12463-8	165
1918	Anatomy of a proficient enzyme: the structure of orotidine 5'-monophosphate decarboxylase in the presence and absence of a potential transition state analog. <b>2000</b> , 97, 2011-6	182
1917	The crystal structure of palmitoyl protein thioesterase 1 and the molecular basis of infantile neuronal ceroid lipofuscinosis. <b>2000</b> , 97, 4573-8	131
1916	Specific chemical and structural damage to proteins produced by synchrotron radiation. <b>2000</b> , 97, 623-8	383
1915	Maurotoxin versus Pi1/HsTx1 scorpion toxins. Toward new insights in the understanding of their distinct disulfide bridge patterns. <b>2000</b> , 275, 39394-402	36
1914	Structural basis for the insensitivity of a serine enzyme (palmitoyl-protein thioesterase) to phenylmethylsulfonyl fluoride. <b>2000</b> , 275, 23847-51	42
1913	Epsin 1 undergoes nucleocytoplasmic shuttling and its eps15 interactor NH(2)-terminal homology (ENTH) domain, structurally similar to Armadillo and HEAT repeats, interacts with the transcription factor promyelocytic leukemia Zn(2)+ finger protein (PLZF). <b>2000</b> , 149, 537-46	152
1912	Solvent organization in an oligonucleotide crystal. The structure of d(GCGAATTCG) <sub>2</sub> at atomic resolution. <b>2000</b> , 275, 23034-44	46
1911	Uracil-DNA glycosylase-DNA substrate and product structures: conformational strain promotes catalytic efficiency by coupled stereoelectronic effects. <b>2000</b> , 97, 5083-8	223
1910	Zinc plays a key role in human and bacterial GTP cyclohydrolase I. <b>2000</b> , 97, 13567-72	117

1909	Nonstandard peptide binding revealed by crystal structures of HLA-B*5101 complexed with HIV immunodominant epitopes. <b>2000</b> , 165, 3260-7	61
1908	Crystal structure of an antibody bound to an immunodominant peptide epitope: novel features in peptide-antibody recognition. <b>2000</b> , 165, 6949-55	24
1907	Essential role of Glu-C66 for menaquinol oxidation indicates transmembrane electrochemical potential generation by <i>Wolinella succinogenes</i> fumarate reductase. <b>2000</b> , 97, 13051-6	70
1906	Revisiting the catalytic CuZ cluster of nitrous oxide (N <sub>2</sub> O) reductase. Evidence of a bridging inorganic sulfur. <b>2000</b> , 275, 41133-6	138
1905	Structural insights into the protein splicing mechanism of PI-SceI. <b>2000</b> , 275, 16408-13	124
1904	The retro-GCN4 leucine zipper sequence forms a stable three-dimensional structure. <b>2000</b> , 97, 2562-6	61
1903	Inactive conformation of the serpin alpha(1)-antichymotrypsin indicates two-stage insertion of the reactive loop: implications for inhibitory function and conformational disease. <b>2000</b> , 97, 67-72	166
1902	Crystal structure of a DNA.RNA hybrid duplex with a polypurine RNA r(gaagaagag) and a complementary polypyrimidine DNA d(CTCTTCTTC). <b>2000</b> , 28, 2171-6	54
1901	Crystal structures of apo- and holo-bovine alpha-lactalbumin at 2. 2-A resolution reveal an effect of calcium on inter-lobe interactions. <b>2000</b> , 275, 37021-9	193
1900	Cytochrome c nitrite reductase from <i>Wolinella succinogenes</i> . Structure at 1.6 A resolution, inhibitor binding, and heme-packing motifs. <b>2000</b> , 275, 39608-16	166
1899	Annexin 24 from <i>Capsicum annuum</i> . X-ray structure and biochemical characterization. <b>2000</b> , 275, 8072-82	88
1898	Structural characterization of the human respiratory syncytial virus fusion protein core. <b>2000</b> , 97, 14172-7	232
1897	Crystal structure of the functional domain of the splicing factor Prp18. <b>2000</b> , 97, 3022-7	21
1896	The crystal structure of 3alpha -hydroxysteroid dehydrogenase/carbonyl reductase from <i>Comamonas testosteroni</i> shows a novel oligomerization pattern within the short chain dehydrogenase/reductase family. <b>2000</b> , 275, 41333-9	76
1895	Mechanism of pH-dependent N-acetylgalactosamine binding by a functional mimic of the hepatocyte asialoglycoprotein receptor. <b>2000</b> , 275, 35176-84	57
1894	The structural features of concanavalin A governing non-proline peptide isomerization. <b>2000</b> , 275, 19778-87	56
1893	Crystal structure of human frataxin. <b>2000</b> , 275, 30753-6	164
1892	Structure of GATE-16, membrane transport modulator and mammalian ortholog of autophagocytosis factor Aut7p. <b>2000</b> , 275, 25445-50	119

1891	Crystal structure of 1-aminocyclopropane-1-carboxylate deaminase from <i>Hansenula saturnus</i> . <b>2000</b> , 275, 34557-65	47
1890	Structure of <i>Escherichia coli</i> ribosomal protein L25 complexed with a 5S rRNA fragment at 1.8-Å resolution. <b>2000</b> , 97, 2023-8	84
1889	Poliovirus RNA-dependent RNA polymerase (3Dpol): structural, biochemical, and biological analysis of conserved structural motifs A and B. <b>2000</b> , 275, 25523-32	97
1888	The structure of a stable intermediate in the A B DNA helix transition. <b>2000</b> , 97, 2035-9	90
1887	A two B-Z junction containing DNA resolves into an all right-handed double-helix. <b>2000</b> , 28, 4403-9	3
1886	Structure of HAP1-PC7 bound to DNA: implications for DNA recognition and allosteric effects of DNA-binding on transcriptional activation. <b>2000</b> , 28, 3853-63	9
1885	Crystal structures of <i>Mycobacterium tuberculosis</i> RecA and its complex with ADP-ALF(4): implications for decreased ATPase activity and molecular aggregation. <b>2000</b> , 28, 4964-73	78
1884	The functional implications of the dimerization of the catalytic subunits of the mammalian brain platelet-activating factor acetylhydrolase (Ib). <b>2000</b> , 13, 865-71	11
1883	Crystal structure of dTDP-4-keto-6-deoxy-D-hexulose 3,5-epimerase from <i>Methanobacterium thermoautotrophicum</i> complexed with dTDP. <b>2000</b> , 275, 24608-12	48
1882	Mechanism of inactivation of ornithine transcarbamoylase by Ndelta-(N'-Sulfodiaminophosphinyl)-L-ornithine, a true transition state analogue? Crystal structure and implications for catalytic mechanism. <b>2000</b> , 275, 20012-9	33
1881	The high resolution crystal structure for class A beta-lactamase PER-1 reveals the bases for its increase in breadth of activity. <b>2000</b> , 275, 28075-82	55
1880	The replacement of ATP by the competitive inhibitor emodin induces conformational modifications in the catalytic site of protein kinase CK2. <b>2000</b> , 275, 29618-22	124
1879	Crystal structure of the zymogen form of the group A <i>Streptococcus</i> virulence factor SpeB: an integrin-binding cysteine protease. <b>2000</b> , 97, 2235-40	89
1878	A compact x-ray system for macromolecular crystallography. <b>2000</b> , 71, 3900	4
1877	Crystal structure of the HIV-1 integrase catalytic core and C-terminal domains: a model for viral DNA binding. <b>2000</b> , 97, 8233-8	350
1876	The crystal structure of D-lactate dehydrogenase, a peripheral membrane respiratory enzyme. <b>2000</b> , 97, 9413-8	86
1875	Probing the catalytic mechanism of the insulin receptor kinase with a tetrafluorotyrosine-containing peptide substrate. <b>2000</b> , 275, 30394-8	27
1874	Structural basis for catalysis and inhibition of N-glycan processing class I alpha 1,2-mannosidases. <b>2000</b> , 275, 41287-98	123



1873	Crystal structure of a conformation-selective casein kinase-1 inhibitor. <b>2000</b> , 275, 20052-60	113
1872	Crystal structure of the holliday junction DNA in complex with a single RuvA tetramer. <b>2000</b> , 97, 8257-62	114
1871	Correlated switch binding and signaling in bacterial chemotaxis. <b>2000</b> , 275, 19752-8	25
1870	Structure of the influenza C virus CM2 protein transmembrane domain obtained by site-specific infrared dichroism and global molecular dynamics searching. <b>2000</b> , 275, 4225-9	31
1869	Catalytic roles for two water bridged residues (Asp-98 and His-255) in the active site of copper-containing nitrite reductase. <b>2000</b> , 275, 23957-64	94
1868	Heparan/chondroitin sulfate biosynthesis. Structure and mechanism of human glucuronyltransferase I. <b>2000</b> , 275, 34580-5	134
1867	Characterization of the beta-lactam binding site of penicillin acylase of <i>Escherichia coli</i> by structural and site-directed mutagenesis studies. <b>2000</b> , 13, 857-63	67
1866	The mechanism of substrate (aglycone) specificity in beta -glucosidases is revealed by crystal structures of mutant maize beta -glucosidase-DIMBOA, -DIMBOAGlc, and -dhurrin complexes. <b>2000</b> , 97, 13555-60	148
1865	Structure of a C-type carbohydrate recognition domain from the macrophage mannose receptor. <b>2000</b> , 275, 21539-48	93
1864	Crystal structure of a thermophilic cytochrome P450 from the archaeon <i>Sulfolobus solfataricus</i> . <b>2000</b> , 275, 31086-92	155
1863	The crystal structure and amino acid sequence of dehaloperoxidase from <i>Amphitrite ornata</i> indicate common ancestry with globins. <b>2000</b> , 275, 18712-6	75
1862	Crystal structure of <i>Escherichia coli</i> CyaY protein reveals a previously unidentified fold for the evolutionarily conserved frataxin family. <b>2000</b> , 97, 8932-7	104
1861	Crystal structure of the cystine C-S lyase from <i>Synechocystis</i> : stabilization of cysteine persulfide for FeS cluster biosynthesis. <b>2000</b> , 97, 3856-61	68
1860	An open conformation of switch I revealed by the crystal structure of a Mg <sup>2+</sup> -free form of RHOA complexed with GDP. Implications for the GDP/GTP exchange mechanism. <b>2000</b> , 275, 18311-7	47
1859	Bepidil opens the regulatory N-terminal lobe of cardiac troponin C. <b>2000</b> , 97, 5140-5	68
1858	Structural basis for autorepression of retinoid X receptor by tetramer formation and the AF-2 helix. <b>2000</b> , 14, 2229-41	106
1857	Mutational studies on HslU and its docking mode with HslV. <b>2000</b> , 97, 14103-8	129
1856	Peptide-in-groove interactions link target proteins to the beta -propeller of clathrin. <b>2000</b> , 97, 1096-1100	251

1855	Electrostatic stress in catalysis: structure and mechanism of the enzyme orotidine monophosphate decarboxylase. <b>2000</b> , 97, 2017-22	200
1854	Deletion of a single hydrogen bonding atom from the MS2 RNA operator leads to dramatic rearrangements at the RNA-coat protein interface. <b>2000</b> , 28, 4611-6	17
1853	The structure and stability of an HLA-A*0201/octameric tax peptide complex with an empty conserved peptide-N-terminal binding site. <b>2000</b> , 164, 6398-405	144
1852	Crystal structure of an intracellular protease from <i>Pyrococcus horikoshii</i> at 2-Å resolution. <b>2000</b> , 97, 14079-84	93
1851	Enantiomer discrimination illustrated by high-resolution crystal structures of the human nuclear receptor hRAR $\gamma$ . <b>2000</b> , 97, 6322-7	72
1850	The crystal structure of the Rev binding element of HIV-1 reveals novel base pairing and conformational variability. <b>2000</b> , 97, 5107-12	42
1849	Structure of a two-domain chitotriosidase from <i>Serratia marcescens</i> at 1.9-Å resolution. <b>2000</b> , 97, 5842-7	235
1848	A novel form of intercalation involving four DNA duplexes in an acridine-4-carboxamide complex of d(CGTACG) <sub>2</sub> . <b>2000</b> , 28, 4244-53	23
1847	Structure of RsrI methyltransferase, a member of the N6-adenine beta class of DNA methyltransferases. <b>2000</b> , 28, 3950-61	62
1846	The structure of aspartyl dipeptidase reveals a unique fold with a Ser-His-Glu catalytic triad. <b>2000</b> , 97, 14097-102	31
1845	Synthesis and crystal structure of an octamer RNA r(guguuuac)/r(guaggcac) with G.G/U.U tandem wobble base pairs: comparison with other tandem G.U pairs. <b>2000</b> , 28, 4376-81	13
1844	Structural basis for the interaction of the fluorescence probe 8-anilino-1-naphthalene sulfonate (ANS) with the antibiotic target MurA. <b>2000</b> , 97, 6345-9	139
1843	X-ray crystal structure of an anti-Buckminsterfullerene antibody fab fragment: biomolecular recognition of C(60). <b>2000</b> , 97, 12193-7	115
1842	The crystal structure and mechanism of orotidine 5'-monophosphate decarboxylase. <b>2000</b> , 97, 2005-10	141
1841	Solution structure of the RNA polymerase subunit RPB5 from <i>Methanobacterium thermoautotrophicum</i> . <b>2000</b> , 97, 6311-5	17
1840	Crystal structure of human stem cell factor: implication for stem cell factor receptor dimerization and activation. <b>2000</b> , 97, 7732-7	103
1839	Molecular basis for discriminating between normal and damaged bases by the human alkyladenine glycosylase, AAG. <b>2000</b> , 97, 13573-8	187
1838	Structure and mechanism of 3-deoxy-D-manno-octulosonate 8-phosphate synthase. <b>2000</b> , 275, 9476-84	83

1837	Binding of the second generation non-nucleoside inhibitor S-1153 to HIV-1 reverse transcriptase involves extensive main chain hydrogen bonding. <b>2000</b> , 275, 14316-20	95
1836	Solution structure of the E200K variant of human prion protein. Implications for the mechanism of pathogenesis in familial prion diseases. <b>2000</b> , 275, 33650-4	102
1835	Crystal structure and activity of human p23, a heat shock protein 90 co-chaperone. <b>2000</b> , 275, 23045-52	106
1834	NMR structure of the N-terminal J domain of murine polyomavirus T antigens. Implications for DnaJ-like domains and for mutations of T antigens. <b>2000</b> , 275, 36094-103	31
1833	Structure of the BH domain from graf and its implications for Rho GTPase recognition. <b>2000</b> , 275, 38605-10	16
1832	Crystal structure of the cysteine-rich domain of mannose receptor complexed with a sulfated carbohydrate ligand. <b>2000</b> , 191, 1105-16	109
1831	Structural basis of inhibition of CDK-cyclin complexes by INK4 inhibitors. <b>2000</b> , 14, 3115-25	163
1830	Crystal structure of 4-methyl-5-beta-hydroxyethylthiazole kinase from Bacillus subtilis at 1.5 A resolution. <b>2000</b> , 39, 7868-77	62
1829	Comparison of three methyl-coenzyme M reductases from phylogenetically distant organisms: unusual amino acid modification, conservation and adaptation. <b>2000</b> , 303, 329-44	132
1828	Structures of the flavocytochrome p-cresol methylhydroxylase and its enzyme-substrate complex: gated substrate entry and proton relays support the proposed catalytic mechanism. <b>2000</b> , 295, 357-74	74
1827	NMR structure of tissue inhibitor of metalloproteinases-1 implicates localized induced fit in recognition of matrix metalloproteinases. <b>2000</b> , 295, 257-68	39
1826	Structural effects of DNA sequence on T.A recognition by hydroxypyrrrole/pyrrole pairs in the minor groove. <b>2000</b> , 295, 557-67	63
1825	Structure of the soluble domain of cytochrome c(552) from Paracoccus denitrificans in the oxidized and reduced states. <b>2000</b> , 295, 667-78	35
1824	The structure of the HIV-1 RRE high affinity rev binding site at 1.6 A resolution. <b>2000</b> , 295, 711-7	55
1823	Crystal structure of human procathepsin X: a cysteine protease with the proregion covalently linked to the active site cysteine. <b>2000</b> , 295, 939-51	76
1822	Crystal structure of an active two-domain derivative of Rous sarcoma virus integrase. <b>2000</b> , 296, 535-48	111
1821	Crystal structures of an N-terminal fragment from Moloney murine leukemia virus reverse transcriptase complexed with nucleic acid: functional implications for template-primer binding to the fingers domain. <b>2000</b> , 296, 613-32	45
1820	Conformational flexibility of B-DNA at 0.74 A resolution: d(CCAGTACTGG)(2). <b>2000</b> , 296, 787-801	100

1819	Structure of human neutral endopeptidase (Nepriylsin) complexed with phosphoramidon. <b>2000</b> , 296, 341-9	234
1818	Crystal structure of amyloamylase from <i>Thermus aquaticus</i> , a glycosyltransferase catalysing the production of large cyclic glucans. <b>2000</b> , 296, 873-86	86
1817	Crystal structure of MEF2A core bound to DNA at 1.5 Å resolution. <b>2000</b> , 297, 437-49	98
1816	Structural and mechanistic basis of porphyrin metallation by ferrochelatase. <b>2000</b> , 297, 221-32	105
1815	The crystal structure of dihydrofolate reductase from <i>Thermotoga maritima</i> : molecular features of thermostability. <b>2000</b> , 297, 659-72	90
1814	Crystal structure of a NifS-like protein from <i>Thermotoga maritima</i> : implications for iron sulphur cluster assembly. <b>2000</b> , 297, 451-64	129
1813	The three-dimensional structure of a <i>Plasmodium falciparum</i> cyclophilin in complex with the potent anti-malarial cyclosporin A. <b>2000</b> , 298, 123-33	34
1812	Divergence in macromolecular assembly: X-ray crystallographic structure analysis of lumazine synthase from <i>Brucella abortus</i> . <b>2000</b> , 297, 1031-6	51
1811	Structural basis of recognition of monopartite and bipartite nuclear localization sequences by mammalian importin- $\alpha$ . <b>2000</b> , 297, 1183-94	316
1810	High-resolution crystal structure of <i>S. cerevisiae</i> Ypt51( $\Delta$ C15)-GppNHp, a small GTP-binding protein involved in regulation of endocytosis. <b>2000</b> , 298, 111-21	30
1809	The structure of an insect chymotrypsin. <b>2000</b> , 298, 895-901	51
1808	NMR structure of stem-loop SL2 of the HIV-1 $\psi$ RNA packaging signal reveals a novel A-U-A base-triple platform. <b>2000</b> , 299, 145-56	89
1807	Conservation and variation in superantigen structure and activity highlighted by the three-dimensional structures of two new superantigens from <i>Streptococcus pyogenes</i> . <b>2000</b> , 299, 157-68	64
1806	Crystal structure of an adenine bulge in the RNA chain of a DNA:RNA hybrid, d(CTCCTCTTC).r(gaagagagag). <b>2000</b> , 299, 103-12	13
1805	1.9 Å resolution crystal structure of the <i>Saccharomyces cerevisiae</i> Ran-binding protein Mog1p. <b>2000</b> , 299, 213-23	29
1804	Design, characterization, and structure of a biologically active single-chain mutant of human IFN- $\gamma$ . <b>2000</b> , 299, 169-79	29
1803	The crystal structure of the penicillin-binding protein 2x from <i>Streptococcus pneumoniae</i> and its acyl-enzyme form: implication in drug resistance. <b>2000</b> , 299, 477-85	181
1802	Core structure of the outer membrane lipoprotein from <i>Escherichia coli</i> at 1.9 Å resolution. <b>2000</b> , 299, 1101-12	92

1801	The role of weak protein-protein interactions in multivalent lectin-carbohydrate binding: crystal structure of cross-linked FRIL. <b>2000</b> , 299, 875-83	40
1800	The free yeast aspartyl-tRNA synthetase differs from the tRNA(Asp)-complexed enzyme by structural changes in the catalytic site, hinge region, and anticodon-binding domain. <b>2000</b> , 299, 1313-24	61
1799	Aspartyl tRNA-synthetase from <i>Escherichia coli</i> : flexibility and adaptability to the substrates. <b>2000</b> , 299, 1157-64	35
1798	Crystal structure of <i>Pseudomonas aeruginosa</i> PAK pilin suggests a main-chain-dominated mode of receptor binding. <b>2000</b> , 299, 1005-17	120
1797	The 1.7 Å crystal structure of BPI: a study of how two dissimilar amino acid sequences can adopt the same fold. <b>2000</b> , 299, 1019-34	44
1796	Phosphorylated and dephosphorylated structures of pig heart, GTP-specific succinyl-CoA synthetase. <b>2000</b> , 299, 1325-39	49
1795	Global folds of proteins with low densities of NOEs using residual dipolar couplings: application to the 370-residue maltodextrin-binding protein. <b>2000</b> , 300, 197-212	147
1794	A TOPRIM domain in the crystal structure of the catalytic core of <i>Escherichia coli</i> primase confirms a structural link to DNA topoisomerases. <b>2000</b> , 300, 353-62	88
1793	Crystal structure of a novel germination protease from spores of <i>Bacillus megaterium</i> : structural arrangement and zymogen activation. <b>2000</b> , 300, 1-10	17
1792	Crystal structure of the carbohydrate recognition domain of the H1 subunit of the asialoglycoprotein receptor. <b>2000</b> , 300, 857-65	154
1791	Host range and variability of calcium binding by surface loops in the capsids of canine and feline parvoviruses. <b>2000</b> , 300, 597-610	65
1790	Structure of a thioredoxin-like [2Fe-2S] ferredoxin from <i>Aquifex aeolicus</i> . <b>2000</b> , 300, 587-95	52
1789	Crystal structure of an archaeal intein-encoded homing endonuclease PI-Pful. <b>2000</b> , 300, 889-901	101
1788	The structure of reduced tryparedoxin peroxidase reveals a decamer and insight into reactivity of 2Cys-peroxiredoxins. <b>2000</b> , 300, 903-16	143
1787	Use of a new label, (13) $\Rightarrow$ (18)O, in the determination of a structural model of phospholamban in a lipid bilayer. Spatial restraints resolve the ambiguity arising from interpretations of mutagenesis data. <b>2000</b> , 300, 677-85	91
1786	Crystal structure of the amino-terminal coiled-coil domain of the APC tumor suppressor. <b>2000</b> , 301, 147-56	48
1785	The structure of rhamnose isomerase from <i>Escherichia coli</i> and its relation with xylose isomerase illustrates a change between inter and intra-subunit complementation during evolution. <b>2000</b> , 300, 917-33	57
1784	Structure of coenzyme F(420) dependent methylenetetrahydromethanopterin reductase from two methanogenic archaea. <b>2000</b> , 300, 935-50	59

1783	Structures of type 2 peroxisomal targeting signals in two trypanosomatid aldolases. <b>2000</b> , 300, 697-707	72
1782	Crystal structure of human grancalcin, a member of the penta-EF-hand protein family. <b>2000</b> , 300, 1271-81	39
1781	Substitutions at the P(1) position in BPTI strongly affect the association energy with serine proteinases. <b>2000</b> , 301, 205-17	64
1780	Three-dimensional crystal structure of human eosinophil cationic protein (RNase 3) at 1.75 Å resolution. <b>2000</b> , 300, 1297-307	45
1779	Specificity in protein-protein interactions: the structural basis for dual recognition in endonuclease colicin-immunity protein complexes. <b>2000</b> , 301, 1163-78	131
1778	The crystal structure of yeast phenylalanine tRNA at 2.0 Å resolution: cleavage by Mg(2+) in 15-year old crystals. <b>2000</b> , 301, 401-14	124
1777	2.8 Å crystal structure of the malachite green aptamer. <b>2000</b> , 301, 117-28	163
1776	Crystal structure of the beta-apical domain of the thermosome reveals structural plasticity in the protrusion region. <b>2000</b> , 301, 19-25	23
1775	3-Deoxy-D-manno-octulosonate-8-phosphate synthase from Escherichia coli. Model of binding of phosphoenolpyruvate and D-arabinose-5-phosphate. <b>2000</b> , 301, 233-8	32
1774	Structure of 3-deoxy-d-arabino-heptulosonate-7-phosphate synthase from Escherichia coli: comparison of the Mn(2+)*2-phosphoglycolate and the Pb(2+)*2-phosphoenolpyruvate complexes and implications for catalysis. <b>2000</b> , 301, 389-99	57
1773	Crystals of the urokinase type plasminogen activator variant beta(c)-uPAin complex with small molecule inhibitors open the way towards structure-based drug design. <b>2000</b> , 301, 465-75	67
1772	The crystal structure of adenylosuccinate lyase from Pyrobaculum aerophilum reveals an intracellular protein with three disulfide bonds. <b>2000</b> , 301, 433-50	69
1771	Solution conformation and amyloid-like fibril formation of a polar peptide derived from a beta-hairpin in the OspA single-layer beta-sheet. <b>2000</b> , 301, 477-89	59
1770	Structure of bacteriophage T4 gene product 11, the interface between the baseplate and short tail fibers. <b>2000</b> , 301, 975-85	48
1769	"Open" structures of MurD: domain movements and structural similarities with folylpolyglutamate synthetase. <b>2000</b> , 301, 1257-66	75
1768	Crystal structures of two functionally different thioredoxins in spinach chloroplasts. <b>2000</b> , 302, 135-54	81
1767	Staggered molecular packing in crystals of a collagen-like peptide with a single charged pair. <b>2000</b> , 301, 1191-205	180
1766	How does a symmetric dimer recognize an asymmetric substrate? A substrate complex of HIV-1 protease. <b>2000</b> , 301, 1207-20	145

1765	The effect of intracellular molybdenum in <i>Hydrogenophaga pseudoflava</i> on the crystallographic structure of the seleno-molybdo-iron-sulfur flavoenzyme carbon monoxide dehydrogenase. <b>2000</b> , 301, 1221-35	71
1764	The 1.0 Å crystal structure of Ca(2+)-bound calmodulin: an analysis of disorder and implications for functionally relevant plasticity. <b>2000</b> , 301, 1237-56	263
1763	Structural basis for isotype selectivity of the human retinoic acid nuclear receptor. <b>2000</b> , 302, 155-70	110
1762	Crystal structures of mouse class II alcohol dehydrogenase reveal determinants of substrate specificity and catalytic efficiency. <b>2000</b> , 302, 441-53	44
1761	Caspase-8 specificity probed at subsite S(4): crystal structure of the caspase-8-Z-DEVD-cho complex. <b>2000</b> , 302, 9-16	51
1760	Structural consequences of mono-glucosylation of Ha-Ras by <i>Clostridium sordellii</i> lethal toxin. <b>2000</b> , 301, 1091-5	57
1759	Structures of thermolabile mutants of human glutathione transferase P1-1. <b>2000</b> , 302, 295-302	15
1758	The adoption of a twisted structure of importin-beta is essential for the protein-protein interaction required for nuclear transport. <b>2000</b> , 302, 251-64	59
1757	Functional and crystallographic characterization of <i>Salmonella typhimurium</i> Cu,Zn superoxide dismutase coded by the <i>sodCI</i> virulence gene. <b>2000</b> , 302, 465-78	44
1756	A comparative analysis of 23 structures of the amyloidogenic protein transthyretin. <b>2000</b> , 302, 649-69	179
1755	The three-dimensional structure of the Nudix enzyme diadenosine tetraphosphate hydrolase from <i>Lupinus angustifolius</i> L. <b>2000</b> , 302, 1165-77	43
1754	The crystal structure of staphylococcal enterotoxin H: implications for binding properties to MHC class II and TcR molecules. <b>2000</b> , 302, 527-37	47
1753	Crystal structure of <i>Mycobacterium tuberculosis</i> 7,8-dihydropteroate synthase in complex with pterin monophosphate: new insight into the enzymatic mechanism and sulfa-drug action. <b>2000</b> , 302, 1193-212	125
1752	Identification of an allosteric anion-binding site on O-acetylserine sulphydrylase: structure of the enzyme with chloride bound. <b>2000</b> , 303, 279-86	68
1751	Novel dimerization fold of RAP30/RAP74 in human TFIIIF at 1.7 Å resolution. <b>2000</b> , 302, 1119-27	75
1750	Carbohydrate specificity and salt-bridge mediated conformational change in acidic winged bean agglutinin. <b>2000</b> , 302, 1129-37	36
1749	Determination of a high precision structure of a novel protein, <i>Linum usitatissimum</i> trypsin inhibitor (LUTI), using computer-aided assignment of NOESY cross-peaks. <b>2000</b> , 302, 1179-92	24
1748	Structural identification of a key protective B-cell epitope in Lyme disease antigen OspA. <b>2000</b> , 302, 1153-64	47

1747	Structural analysis of the transcriptional activation region on Fis: crystal structures of six Fis mutants with different activation properties. <b>2000</b> , 302, 1139-51	36
1746	Structure of a mutant EF-G reveals domain III and possibly the fusidic acid binding site. <b>2000</b> , 303, 593-603	128
1745	Crystal structure of a cohesin module from <i>Clostridium cellulolyticum</i> : implications for dockerin recognition. <b>2000</b> , 304, 189-200	53
1744	A snapshot of a transition state analogue of a novel thermophilic esterase belonging to the subfamily of mammalian hormone-sensitive lipase. <b>2000</b> , 303, 761-71	117
1743	The N-terminal domain of betaB2-crystallin resembles the putative ancestral homodimer. <b>2000</b> , 304, 253-7	23
1742	Structural basis for the binding of an immunodominant peptide from myelin basic protein in different registers by two HLA-DR2 proteins. <b>2000</b> , 304, 177-88	117
1741	The crystal structure of UUCG tetraloop. <b>2000</b> , 304, 35-42	133
1740	Crystal structure of human GM2-activator protein with a novel beta-cup topology. <b>2000</b> , 304, 411-22	92
1739	Crystal structures of a Rab protein in its inactive and active conformations. <b>2000</b> , 304, 585-98	91
1738	Crystal structure of a truncated mutant of glucose-fructose oxidoreductase shows that an N-terminal arm controls tetramer formation. <b>2000</b> , 304, 575-84	13
1737	Crystal structure of the oligomerization domain of NSP4 from rotavirus reveals a core metal-binding site. <b>2000</b> , 304, 861-71	65
1736	Crystal structure of Hsc20, a J-type Co-chaperone from <i>Escherichia coli</i> . <b>2000</b> , 304, 835-45	59
1735	Viral escape at the molecular level explained by quantitative T-cell receptor/peptide/MHC interactions and the crystal structure of a peptide/MHC complex. <b>2000</b> , 302, 873-85	35
1734	Catalysis of decarboxylation by a preorganized heterogeneous microenvironment: crystal structures of abzyme 21D8. <b>2000</b> , 302, 1213-25	15
1733	Structure of the light-driven chloride pump halorhodopsin at 1.8 Å resolution. <b>2000</b> , 288, 1390-6	495
1732	Crystal structure determination of aristolochene synthase from the blue cheese mold, <i>Penicillium roqueforti</i> . <b>2000</b> , 275, 25533-9	142
1731	Use of a single glycine residue to determine the tilt and orientation of a transmembrane helix. A new structural label for infrared spectroscopy. <b>2000</b> , 79, 3139-43	49
1730	Properties and crystal structure of a beta-barrel folding mutant. <b>2000</b> , 78, 1551-60	7



1729	An intermediate step in the recognition of tRNA(Asp) by aspartyl-tRNA synthetase. <b>2000</b> , 299, 1051-60	43
1728	Structural basis for specificity switching of the Src SH2 domain. <b>2000</b> , 5, 1043-9	41
1727	Activation of Human Liver Glycogen Phosphorylase by Alteration of the Secondary Structure and Packing of the Catalytic Core. <b>2000</b> , 6, 139-148	82
1726	Crystal Structure of the DNA Binding Domain of the Replication Initiation Protein E1 from Papillomavirus. <b>2000</b> , 6, 149-158	76
1725	Crystal Structure of Human Survivin Reveals a Bow Tie Shaped Dimer with Two Unusual $\beta$ -Helical Extensions. <b>2000</b> , 6, 183-189	170
1724	Crystal Structure of a Flp Recombinase Holliday Junction Complex. <b>2000</b> , 6, 885-897	9
1723	Structural determinants of phosphoinositide 3-kinase inhibition by wortmannin, LY294002, quercetin, myricetin, and staurosporine. <b>2000</b> , 6, 909-19	978
1722	Structure of the human IgE-Fc C epsilon 3-C epsilon 4 reveals conformational flexibility in the antibody effector domains. <b>2000</b> , 13, 375-85	78
1721	Crystal structure and ligand binding properties of the D1D2 region of the inhibitory receptor LIR-1 (ILT2). <b>2000</b> , 13, 727-36	114
1720	A functional hot spot for antigen recognition in a superagonist TCR/MHC complex. <b>2000</b> , 12, 251-61	187
1719	RNA methylation under heat shock control. <b>2000</b> , 6, 349-60	211
1718	Structural basis for discrimination of 3-phosphoinositides by pleckstrin homology domains. <b>2000</b> , 6, 373-84	310
1717	Molecular basis for the dephosphorylation of the activation segment of the insulin receptor by protein tyrosine phosphatase 1B. <b>2000</b> , 6, 1401-12	384
1716	Modulation of host signaling by a bacterial mimic: structure of the Salmonella effector SptP bound to Rac1. <b>2000</b> , 6, 1449-60	146
1715	Crystal structure of the hexameric traffic ATPase of the Helicobacter pylori type IV secretion system. <b>2000</b> , 6, 1461-72	187
1714	Structure of the AAA ATPase p97. <b>2000</b> , 6, 1473-84	366
1713	Mammalian microsomal cytochrome P450 monooxygenase: structural adaptations for membrane binding and functional diversity. <b>2000</b> , 5, 121-31	691
1712	The crystal structure of the nuclear receptor for vitamin D bound to its natural ligand. <b>2000</b> , 5, 173-9	695

1711	The crystal structure of an unusual processivity factor, herpes simplex virus UL42, bound to the C terminus of its cognate polymerase. <b>2000</b> , 5, 267-78	132
1710	Structure of the dimerization and beta-catenin-binding region of alpha-catenin. <b>2000</b> , 5, 533-43	199
1709	Crystallographic location of two Zn(2+)-binding sites in the avian cytochrome bc(1) complex. <b>2000</b> , 1459, 440-8	55
1708	Structure of PAK1 in an autoinhibited conformation reveals a multistage activation switch. <b>2000</b> , 102, 387-97	440
1707	The 4 A X-ray structure of a tubulin:stathmin-like domain complex. <b>2000</b> , 102, 809-16	221
1706	Structure of functionally activated small ribosomal subunit at 3.3 angstroms resolution. <b>2000</b> , 102, 615-23	821
1705	Structural basis for relief of autoinhibition of the Dbl homology domain of proto-oncogene Vav by tyrosine phosphorylation. <b>2000</b> , 102, 625-33	318
1704	The polar T1 interface is linked to conformational changes that open the voltage-gated potassium channel. <b>2000</b> , 102, 657-70	159
1703	Structure of the molecular chaperone prefoldin: unique interaction of multiple coiled coil tentacles with unfolded proteins. <b>2000</b> , 103, 621-32	265
1702	Crystal and solution structures of an HslUV protease-chaperone complex. <b>2000</b> , 103, 633-43	266
1701	Structural basis for double-sieve discrimination of L-valine from L-isoleucine and L-threonine by the complex of tRNA(Val) and valyl-tRNA synthetase. <b>2000</b> , 103, 793-803	244
1700	Transfer RNA-mediated editing in threonyl-tRNA synthetase. The class II solution to the double discrimination problem. <b>2000</b> , 103, 877-84	157
1699	Crystal structure of a beta-catenin/Tcf complex. <b>2000</b> , 103, 885-96	347
1698	Crystal structure and functional analysis of Ras binding to its effector phosphoinositide 3-kinase gamma. <b>2000</b> , 103, 931-43	496
1697	The structural basis for the action of the antibiotics tetracycline, pactamycin, and hygromycin B on the 30S ribosomal subunit. <b>2000</b> , 103, 1143-54	709
1696	Structural basis of collagen recognition by integrin alpha2beta1. <b>2000</b> , 101, 47-56	821
1695	The crystal structure of human eukaryotic release factor eRF1--mechanism of stop codon recognition and peptidyl-tRNA hydrolysis. <b>2000</b> , 100, 311-21	396
1694	Crystal structure of the VHS and FYVE tandem domains of Hrs, a protein involved in membrane trafficking and signal transduction. <b>2000</b> , 100, 447-56	159

1693	The 1.7 Å crystal structure of human cell cycle checkpoint kinase Chk1: implications for Chk1 regulation. <b>2000</b> , 100, 681-92	174
1692	Crystal structures of two FGF-FGFR complexes reveal the determinants of ligand-receptor specificity. <b>2000</b> , 101, 413-24	329
1691	A novel mechanism of TRAF signaling revealed by structural and functional analyses of the TRADD-TRAF2 interaction. <b>2000</b> , 101, 777-87	154
1690	Structural biology of Rad50 ATPase: ATP-driven conformational control in DNA double-strand break repair and the ABC-ATPase superfamily. <b>2000</b> , 101, 789-800	820
1689	Crystal structure of the lambda repressor C-terminal domain provides a model for cooperative operator binding. <b>2000</b> , 101, 801-11	123
1688	Crystal structure of rat heme oxygenase-1 in complex with heme. <b>2000</b> , 471, 61-6	125
1687	Structure of the photosynthetic reaction centre from Rhodospirillum rubrum reconstituted with anthraquinone as primary quinone Q(A). <b>2000</b> , 472, 114-6	4
1686	Crystal structure of SULT2A3, human hydroxysteroid sulfotransferase. <b>2000</b> , 475, 61-4	86
1685	The three-dimensional structure of human transaldolase. <b>2000</b> , 475, 205-8	33
1684	Phenylethylthiazolylthiourea (PETT) non-nucleoside inhibitors of HIV-1 and HIV-2 reverse transcriptases. Structural and biochemical analyses. <b>2000</b> , 275, 5633-9	90
1683	Crystal structure of yeast initiation factor 4A, a DEAD-box RNA helicase. <b>2000</b> , 97, 13080-5	240
1682	Structure of Acinetobacter strain ADP1 protocatechuate 3, 4-dioxygenase at 2.2 Å resolution: implications for the mechanism of an intradiol dioxygenase. <b>2000</b> , 39, 7943-55	87
1681	The X-ray crystal structure of neuronal Sec1 from squid sheds new light on the role of this protein in exocytosis. <b>2000</b> , 8, 685-94	36
1680	Crystal structure of a gamma delta T cell receptor ligand T22: a truncated MHC-like fold. <b>2000</b> , 287, 310-4	56
1679	Convergent solutions to binding at a protein-protein interface. <b>2000</b> , 287, 1279-83	586
1678	The catalytic pathway of cytochrome p450cam at atomic resolution. <b>2000</b> , 287, 1615-22	1164
1677	Structure of the S15,S6,S18-rRNA complex: assembly of the 30S ribosome central domain. <b>2000</b> , 288, 107-13	176
1676	A structural framework for deciphering the link between I-Ag7 and autoimmune diabetes. <b>2000</b> , 288, 505-11	225

1675	Structure and function of a human TAFII250 double bromodomain module. <b>2000</b> , 288, 1422-5	704
1674	Three-dimensional structure of the Tn5 synaptic complex transposition intermediate. <b>2000</b> , 289, 77-85	329
1673	Crystal structure of rhodopsin: A G protein-coupled receptor. <b>2000</b> , 289, 739-45	5015
1672	Structure of yeast poly(A) polymerase alone and in complex with 3'-dATP. <b>2000</b> , 289, 1346-9	95
1671	The productive conformation of arachidonic acid bound to prostaglandin synthase. <b>2000</b> , 289, 1933-7	257
1670	Structural mechanism for STI-571 inhibition of abelson tyrosine kinase. <b>2000</b> , 289, 1938-42	1546
1669	Structure of the protease domain of memapsin 2 (beta-secretase) complexed with inhibitor. <b>2000</b> , 290, 150-3	668
1668	Crystal structure of the second domain of the human copper chaperone for superoxide dismutase. <b>2000</b> , 39, 1589-95	84
1667	Crystal structure of the BMP-2-BRIA ectodomain complex. <b>2000</b> , 7, 492-6	255
1666	Crystal structures of bovine milk xanthine dehydrogenase and xanthine oxidase: structure-based mechanism of conversion. <b>2000</b> , 97, 10723-8	542
1665	The structure of human beta-defensin-2 shows evidence of higher order oligomerization. <b>2000</b> , 275, 32911-8	253
1664	Crystal structure of pseudomonas aeruginosa lipase in the open conformation. The prototype for family I.1 of bacterial lipases. <b>2000</b> , 275, 31219-25	209
1663	Crystal structure of human CD69: a C-type lectin-like activation marker of hematopoietic cells. <b>2000</b> , 39, 14779-86	66
1662	Molecular basis for P-site inhibition of adenylyl cyclase. <b>2000</b> , 39, 14464-71	101
1661	Crystal structure of the haloalkane dehalogenase from Sphingomonas paucimobilis UT26. <b>2000</b> , 39, 14082-6	106
1660	Evolution of enzymatic activity in the enolase superfamily: structure of o-succinylbenzoate synthase from Escherichia coli in complex with Mg <sup>2+</sup> and o-succinylbenzoate. <b>2000</b> , 39, 10662-76	66
1659	Methyl groups of thymine bases are important for nucleic acid recognition by DtxR. <b>2000</b> , 39, 10397-407	54
1658	Role of SRP19 in assembly of the Archaeoglobus fulgidus signal recognition particle. <b>2000</b> , 39, 12862-74	61

1657	The Crystal Structure of a Pyrrolinone Peptide Hybrid Ligand Bound to the Human Class II MHC Protein HLA-DR1. <b>2000</b> , 122, 8370-8375	15
1656	Determining DNA Global Structure and DNA Bending by Application of NMR Residual Dipolar Couplings. <b>2000</b> , 122, 9638-9647	89
1655	Helical interactions in the HIV-1 gp41 core reveal structural basis for the inhibitory activity of gp41 peptides. <b>2000</b> , 39, 1634-42	71
1654	Halophilic adaptation: novel solvent protein interactions observed in the 2.9 and 2.6 Å resolution structures of the wild type and a mutant of malate dehydrogenase from <i>Haloarcula marismortui</i> . <b>2000</b> , 39, 992-1000	96
1653	Functional consequences of the Kaposi's sarcoma-associated herpesvirus protease structure: regulation of activity and dimerization by conserved structural elements. <b>2000</b> , 39, 12796-803	37
1652	Crystal structures of the cellulase Cel48F in complex with inhibitors and substrates give insights into its processive action. <b>2000</b> , 39, 11238-46	89
1651	Structural basis for the catalytic mechanism of a proficient enzyme: orotidine 5'-monophosphate decarboxylase. <b>2000</b> , 39, 4217-24	95
1650	Role for lysine 142 in the excision of adenine from A:G mispairs by MutY DNA glycosylase of <i>Escherichia coli</i> . <b>2000</b> , 39, 14768-78	30
1649	Role of the loop containing residue 115 in the induced-fit mechanism of the bacterial cell wall biosynthetic enzyme MurA. <b>2000</b> , 39, 2164-73	43
1648	Zinc ion mediated amino acid discrimination by threonyl-tRNA synthetase. <b>2000</b> , 7, 461-5	124
1647	The 2 Å crystal structure of leucyl-tRNA synthetase and its complex with a leucyl-adenylate analogue. <b>2000</b> , 19, 2351-61	223
1646	Crystal structure of mammalian poly(A) polymerase in complex with an analog of ATP. <b>2000</b> , 19, 4193-203	115
1645	Active and alkylated human AGT structures: a novel zinc site, inhibitor and extrahelical base binding. <b>2000</b> , 19, 1719-30	158
1644	Crystal structures of fructose 1,6-bisphosphatase: mechanism of catalysis and allosteric inhibition revealed in product complexes. <b>2000</b> , 39, 8565-74	63
1643	Reactions of <i>Pseudomonas</i> 7A glutaminase-asparaginase with diazo analogues of glutamine and asparagine result in unexpected covalent inhibitions and suggests an unusual catalytic triad Thr-Tyr-Glu. <b>2000</b> , 39, 1199-204	58
1642	Shedding light on disulfide bond formation: engineering a redox switch in green fluorescent protein. <b>2001</b> , 20, 5853-62	249
1641	Bovine alpha1,3-galactosyltransferase catalytic domain structure and its relationship with ABO histo-blood group and glycosphingolipid glycosyltransferases. <b>2001</b> , 20, 638-49	154
1640	Turning a disulfide isomerase into an oxidase: DsbC mutants that imitate DsbA. <b>2001</b> , 20, 1555-62	91

1639	The structural basis of acyl coenzyme A-dependent regulation of the transcription factor FadR. <b>2001</b> , 20, 2041-50	133
1638	An ancestral nuclear protein assembly: crystal structure of the Methanopyrus kandleri histone. <b>2001</b> , 10, 2002-7	38
1637	Crystal structure of an archaeal DNA sliding clamp: proliferating cell nuclear antigen from Pyrococcus furiosus. <b>2001</b> , 10, 17-23	126
1636	Structure of soybean seed coat peroxidase: a plant peroxidase with unusual stability and haem-apoprotein interactions. <b>2001</b> , 10, 108-15	114
1635	Crystal structure of human cyclin-dependent kinase 2 in complex with the adenine-derived inhibitor H717. <b>2001</b> , 44, 524-30	68
1634	NADPH-cytochrome P450 oxidoreductase. Structural basis for hydride and electron transfer. <b>2001</b> , 276, 29163-70	174
1633	Structural basis of transcription: an RNA polymerase II elongation complex at 3.3 Å resolution. <b>2001</b> , 292, 1876-82	743
1632	Crystal structure of ATP sulfurylase from the bacterial symbiont of the hydrothermal vent tubeworm Riftia pachytila. <b>2001</b> , 40, 14509-17	36
1631	The structural basis for substrate specificity and inhibition of human S-adenosylmethionine decarboxylase. <b>2001</b> , 40, 9484-94	57
1630	Mechanistic and metabolic inferences from the binding of substrate analogues and products to arginase. <b>2001</b> , 40, 2689-701	69
1629	Xenon and halogenated alkanes track putative substrate binding cavities in the soluble methane monooxygenase hydroxylase. <b>2001</b> , 40, 3476-82	85
1628	Automated assignment of ambiguous nuclear overhauser effects with ARIA. <b>2001</b> , 339, 71-90	300
1627	Human glutathione transferase P1-1 and nitric oxide carriers; a new role for an old enzyme. <b>2001</b> , 276, 42138-45	79
1626	Structural insights into the catalytic mechanism of a family 18 exo-chitinase. <b>2001</b> , 98, 8979-84	375
1625	Conformational change of elongation factor Tu (EF-Tu) induced by antibiotic binding. Crystal structure of the complex between EF-Tu.GDP and aurodox. <b>2001</b> , 276, 17149-55	95
1624	Overexpression, purification, and crystal structure of native ER alpha LBD. <b>2001</b> , 22, 165-73	73
1623	Structure of the unliganded cAMP-dependent protein kinase catalytic subunit from Saccharomyces cerevisiae. <b>2001</b> , 387, 11-9	11
1622	Identification and structure of the nerve growth factor binding site on TrkA. <b>2001</b> , 282, 131-41	33

1621	Crystal structure of a light-harvesting protein C-phycoyanin from <i>Spirulina platensis</i> . <b>2001</b> , 282, 893-8	78
1620	Crystal structure of cobalt-containing nitrile hydratase. <b>2001</b> , 288, 1169-74	206
1619	Three-dimensional structure of <i>Erwinia chrysanthemi</i> pectin methylesterase reveals a novel esterase active site. <b>2001</b> , 305, 951-60	95
1618	Structural basis for oligosaccharide recognition by <i>Pyrococcus furiosus</i> maltodextrin-binding protein. <b>2001</b> , 305, 891-904	55
1617	Structural basis for enantiomer binding and separation of a common beta-blocker: crystal structure of cellobiohydrolase Cel7A with bound (S)-propranolol at 1.9 Å resolution. <b>2001</b> , 305, 79-93	53
1616	Crystal structure and novel recognition motif of rho ADP-ribosylating C3 exoenzyme from <i>Clostridium botulinum</i> : structural insights for recognition specificity and catalysis. <b>2001</b> , 305, 95-107	129
1615	Crystal structures of <i>Streptococcus pneumoniae</i> N-acetylglucosamine-1-phosphate uridylyltransferase, GlmU, in apo form at 2.33 Å resolution and in complex with UDP-N-acetylglucosamine and Mg(2+) at 1.96 Å resolution. <b>2001</b> , 305, 279-89	83
1614	X-ray crystallographic analyses of complexes between bovine beta-trypsin and Schiff base copper(II) or iron(III) chelates. <b>2001</b> , 305, 471-9	34
1613	The molecular mechanism of sulfated carbohydrate recognition by the cysteine-rich domain of mannose receptor. <b>2001</b> , 305, 481-90	26
1612	Role of conserved nucleotides in building the 16 S rRNA binding site for ribosomal protein S15. <b>2001</b> , 305, 785-803	24
1611	A 2.1 Å resolution structure of an uncleaved alpha(1)-antitrypsin shows variability of the reactive center and other loops. <b>2001</b> , 306, 109-19	50
1610	Structural basis of diverse sequence-dependent target recognition by the 8 kDa dynein light chain. <b>2001</b> , 306, 97-108	126
1609	Crystal structure of the SMC head domain: an ABC ATPase with 900 residues antiparallel coiled-coil inserted. <b>2001</b> , 306, 25-35	132
1608	Crystal structure of the NADP(H)-dependent ketose reductase from <i>Bemisia argentifolii</i> at 2.3 Å resolution. <b>2001</b> , 306, 239-50	65
1607	Solution structure and dynamics of an open beta-sheet, glycolytic enzyme, monomeric 23.7 kDa phosphoglycerate mutase from <i>Schizosaccharomyces pombe</i> . <b>2001</b> , 306, 275-90	19
1606	Crystal structure of the hexameric replicative helicase RepA of plasmid RSF1010. <b>2001</b> , 306, 479-87	87
1605	Crystal structure of DNA polymerase from hyperthermophilic archaeon <i>Pyrococcus kodakaraensis</i> KOD1. <b>2001</b> , 306, 469-77	127
1604	X-ray structure analysis and crystallographic refinement of lumazine synthase from the hyperthermophile <i>Aquifex aeolicus</i> at 1.6 Å resolution: determinants of thermostability revealed from structural comparisons. <b>2001</b> , 306, 1099-114	137

1603	Crystal structure of the catalytic core component of the alkylhydroperoxide reductase AhpF from <i>Escherichia coli</i> . <b>2001</b> , 307, 1-8	17
1602	Structural and energetic analysis of RNA recognition by a universally conserved protein from the signal recognition particle. <b>2001</b> , 307, 229-46	80
1601	Refined structures of beta-ketoacyl-acyl carrier protein synthase III. <b>2001</b> , 307, 341-56	133
1600	The crystal structure of dTDP-D-Glucose 4,6-dehydratase (RmlB) from <i>Salmonella enterica</i> serovar Typhimurium, the second enzyme in the dTDP-l-rhamnose pathway. <b>2001</b> , 307, 283-95	103
1599	Crystal structure of the <i>Acidaminococcus fermentans</i> 2-hydroxyglutaryl-CoA dehydratase component A. <b>2001</b> , 307, 297-308	60
1598	Crystal structure of alginate lyase A1-III complexed with trisaccharide product at 2.0 Å resolution. <b>2001</b> , 307, 9-16	76
1597	Family 7 cellobiohydrolases from <i>Phanerochaete chrysosporium</i> : crystal structure of the catalytic module of Cel7D (CBH58) at 1.32 Å resolution and homology models of the isozymes. <b>2001</b> , 314, 1097-111	91
1596	Crystal structure of the N-terminal domain of <i>Oxytricha nova</i> telomere end-binding protein alpha subunit both uncomplexed and complexed with telomeric ssDNA. <b>2001</b> , 314, 1113-25	38
1595	Crystal structure of the lambda repressor C-terminal domain octamer. <b>2001</b> , 314, 1127-36	45
1594	Crystal structures of human serum albumin complexed with monounsaturated and polyunsaturated fatty acids. <b>2001</b> , 314, 955-60	390
1593	How methionyl-tRNA synthetase creates its amino acid recognition pocket upon L-methionine binding. <b>2001</b> , 306, 863-76	73
1592	Structural biochemistry of a type 2 RNase H: RNA primer recognition and removal during DNA replication. <b>2001</b> , 307, 541-56	72
1591	Solution structure, domain features, and structural implications of mutants of the chromo domain from the fission yeast histone methyltransferase Clr4. <b>2001</b> , 307, 861-70	16
1590	Crystal structure of the MJ0490 gene product of the hyperthermophilic archaeobacterium <i>Methanococcus jannaschii</i> , a novel member of the lactate/malate family of dehydrogenases. <b>2001</b> , 307, 1351-62	29
1589	Structural studies on the empty capsids of <i>Physalis mottle</i> virus. <b>2001</b> , 307, 1035-47	20
1588	Structure and function of a novel purine specific nucleoside hydrolase from <i>Trypanosoma vivax</i> . <b>2001</b> , 307, 1363-79	82
1587	Sequence and crystal structure determination of a basic phospholipase A2 from common krait ( <i>Bungarus caeruleus</i> ) at 2.4 Å resolution: identification and characterization of its pharmacological sites. <b>2001</b> , 307, 1049-59	45
1586	Formation of the single-layer beta-sheet of <i>Borrelia burgdorferi</i> OspA in the absence of the C-terminal capping globular domain. <b>2001</b> , 308, 367-75	8



1585	The X-ray crystal structure of the <i>Trichoderma reesei</i> family 12 endoglucanase 3, Cel12A, at 1.9 Å resolution. <b>2001</b> , 308, 295-310	111
1584	Conformational changes in <i>Leishmania mexicana</i> glyceraldehyde-3-phosphate dehydrogenase induced by designed inhibitors. <b>2001</b> , 309, 423-35	51
1583	What is the average conformation of bacteriophage T4 lysozyme in solution? A domain orientation study using dipolar couplings measured by solution NMR. <b>2001</b> , 308, 745-64	80
1582	Crystal structure of the PDZ1 domain of human Na(+)/H(+) exchanger regulatory factor provides insights into the mechanism of carboxyl-terminal leucine recognition by class I PDZ domains. <b>2001</b> , 308, 963-73	83
1581	Weak protein-protein interactions in lectins: the crystal structure of a vegetative lectin from the legume <i>Dolichos biflorus</i> . <b>2001</b> , 309, 193-201	36
1580	The N-terminal domain of Homer/Vesl is a new class II EVH1 domain. <b>2001</b> , 309, 155-69	46
1579	Structure and binding determinants of the recombinant kringle-2 domain of human plasminogen to an internal peptide from a group A Streptococcal surface protein. <b>2001</b> , 308, 705-19	53
1578	On the mechanism of biological methane formation: structural evidence for conformational changes in methyl-coenzyme M reductase upon substrate binding. <b>2001</b> , 309, 315-30	158
1577	Kinetic and crystallographic studies on deacetoxycephalosporin C synthase (DAOCS). <b>2001</b> , 308, 937-48	90
1576	The structure of <i>Escherichia coli</i> nitroreductase complexed with nicotinic acid: three crystal forms at 1.7 Å, 1.8 Å and 2.4 Å resolution. <b>2001</b> , 309, 203-13	89
1575	Mechanism of hydrolysis of phosphate esters by the dimetal center of 5'-nucleotidase based on crystal structures. <b>2001</b> , 309, 239-54	83
1574	<i>E. coli</i> 5'-nucleotidase undergoes a hinge-bending domain rotation resembling a ball-and-socket motion. <b>2001</b> , 309, 255-66	37
1573	The crystal structure of <i>Bacillus subtilis</i> lipase: a minimal alpha/beta hydrolase fold enzyme. <b>2001</b> , 309, 215-26	224
1572	Selection, characterization and x-ray structure of anti-ampicillin single-chain Fv fragments from phage-displayed murine antibody libraries. <b>2001</b> , 309, 671-85	34
1571	The importance of framework residues H6, H7 and H10 in antibody heavy chains: experimental evidence for a new structural subclassification of antibody V(H) domains. <b>2001</b> , 309, 701-16	53
1570	Molecular basis for immune complex recognition: a comparison of Fc-receptor structures. <b>2001</b> , 309, 737-49	115
1569	Solution-state NMR investigations of triosephosphate isomerase active site loop motion: ligand release in relation to active site loop dynamics. <b>2001</b> , 310, 271-80	154
1568	Crystal structure of a heptameric Sm-like protein complex from archaea: implications for the structure and evolution of snRNPs. <b>2001</b> , 309, 915-23	79

1567	Ligand-induced structural changes to maltodextrin-binding protein as studied by solution NMR spectroscopy. <b>2001</b> , 309, 961-74	114
1566	Incorporation of beta-selenolo[3,2-b]pyrrolyl-alanine into proteins for phase determination in protein X-ray crystallography. <b>2001</b> , 309, 925-36	45
1565	A succession of substrate induced conformational changes ensures the amino acid specificity of <i>Thermus thermophilus</i> prolyl-tRNA synthetase: comparison with histidyl-tRNA synthetase. <b>2001</b> , 309, 989-1002	93
1564	Biochemical characterization of the structure-specific DNA-binding protein Cmb1 from <i>Schizosaccharomyces pombe</i> . <b>2001</b> , 309, 1101-15	5
1563	Crystal structure of thiamin pyrophosphokinase. <b>2001</b> , 310, 195-204	36
1562	X-ray structure of <i>Escherichia coli</i> pyridoxine 5'-phosphate oxidase complexed with pyridoxal 5'-phosphate at 2.0 Å resolution. <b>2001</b> , 310, 817-26	36
1561	Calculation of ensembles of structures representing the unfolded state of an SH3 domain. <b>2001</b> , 308, 1011-32	184
1560	The role of ecotin dimerization in protease inhibition. <b>2001</b> , 308, 975-91	37
1559	Crystal structure of lactose synthase reveals a large conformational change in its catalytic component, the beta1,4-galactosyltransferase-I. <b>2001</b> , 310, 205-18	171
1558	Plasmid transcriptional repressor CopG oligomerises to render helical superstructures unbound and in complexes with oligonucleotides. <b>2001</b> , 310, 403-17	19
1557	Solution structure of interleukin-13 and insights into receptor engagement. <b>2001</b> , 310, 231-41	33
1556	DNA G-quartets in a 1.86 Å resolution structure of an <i>Oxytricha nova</i> telomeric protein-DNA complex. <b>2001</b> , 310, 367-77	151
1555	The crystal structure of <i>Escherichia coli</i> MoeA, a protein from the molybdopterin synthesis pathway. <b>2001</b> , 310, 419-31	45
1554	Crystal structure of the 30 S ribosomal subunit from <i>Thermus thermophilus</i> : purification, crystallization and structure determination. <b>2001</b> , 310, 827-43	116
1553	The dimerization domain of HNF-1alpha: structure and plasticity of an intertwined four-helix bundle with application to diabetes mellitus. <b>2001</b> , 310, 635-58	15
1552	Crystal structures of YBHB and YBCL from <i>Escherichia coli</i> , two bacterial homologues to a Raf kinase inhibitor protein. <b>2001</b> , 310, 617-34	67
1551	Crystal structure of a T cell receptor Valpha11 (AV11S5) domain: new canonical forms for the first and second complementarity determining regions. <b>2001</b> , 310, 689-98	12
1550	Crystal structure of native and Cd/Cd-substituted <i>Dioclea guianensis</i> seed lectin. A novel manganese-binding site and structural basis of dimer-tetramer association. <b>2001</b> , 310, 885-94	43

1549	Folate-binding triggers the activation of folylpolyglutamate synthetase. <b>2001</b> , 310, 1067-78	53
1548	High-resolution structure of HLA-A*0201 in complex with a tumour-specific antigenic peptide encoded by the MAGE-A4 gene. <b>2001</b> , 310, 1167-76	44
1547	Interplay between an AAA module and an integrin I domain may regulate the function of magnesium chelatase. <b>2001</b> , 311, 111-22	150
1546	Crystal structure of a cocaine-binding antibody. <b>2001</b> , 311, 9-15	46
1545	The crystal and molecular structure of a collagen-like peptide with a biologically relevant sequence. <b>2001</b> , 311, 131-47	167
1544	Structure and mechanism of the RuvB Holliday junction branch migration motor. <b>2001</b> , 311, 297-310	145
1543	Lateral recognition of a dye hapten by a llama VHH domain. <b>2001</b> , 311, 123-9	70
1542	Detailed analysis of RNA-protein interactions within the ribosomal protein S8-rRNA complex from the archaeon <i>Methanococcus jannaschii</i> . <b>2001</b> , 311, 311-24	43
1541	Crystal structure of histidinol phosphate aminotransferase (HisC) from <i>Escherichia coli</i> , and its covalent complex with pyridoxal-5'-phosphate and l-histidinol phosphate. <b>2001</b> , 311, 761-76	38
1540	Crystal structure of PTP-SL/PTPBR7 catalytic domain: implications for MAP kinase regulation. <b>2001</b> , 311, 557-68	18
1539	High resolution crystal structures of T4 phage beta-glucosyltransferase: induced fit and effect of substrate and metal binding. <b>2001</b> , 311, 569-77	59
1538	The X-ray structure of <i>Aspergillus aculeatus</i> polygalacturonase and a modeled structure of the polygalacturonase-octagalacturonate complex. <b>2001</b> , 311, 863-78	76
1537	The analysis of the human high affinity IgE receptor Fc epsilon Ri alpha from multiple crystal forms. <b>2001</b> , 311, 1049-62	47
1536	The crystal structure of <i>Thermotoga maritima</i> maltosyltransferase and its implications for the molecular basis of the novel transfer specificity. <b>2001</b> , 312, 119-31	13
1535	<i>Trichoderma reesei</i> alpha-1,2-mannosidase: structural basis for the cleavage of four consecutive mannose residues. <b>2001</b> , 312, 157-65	31
1534	Crystal structure of human macrophage elastase (MMP-12) in complex with a hydroxamic acid inhibitor. <b>2001</b> , 312, 743-51	68
1533	Substrate specificity determinants of human macrophage elastase (MMP-12) based on the 1.1 A crystal structure. <b>2001</b> , 312, 731-42	92
1532	Unusual molecular architecture of the <i>Yersinia pestis</i> cytotoxin YopM: a leucine-rich repeat protein with the shortest repeating unit. <b>2001</b> , 312, 807-21	138

1531	Structural and functional linkages between subunit interfaces in mammalian pyruvate kinase. <b>2001</b> , 312, 525-40	44
1530	Domain swing upon His to Ala mutation in nitrite reductase of <i>Pseudomonas aeruginosa</i> . <b>2001</b> , 312, 541-54	21
1529	Internalins from the human pathogen <i>Listeria monocytogenes</i> combine three distinct folds into a contiguous internalin domain. <b>2001</b> , 312, 783-94	100
1528	Genetic selection for and molecular dynamic modeling of a protein transmembrane domain multimerization motif from a random <i>Escherichia coli</i> genomic library. <b>2001</b> , 313, 181-95	23
1527	Crystal structure of rat GTP cyclohydrolase I feedback regulatory protein, GFRP. <b>2001</b> , 312, 1051-7	11
1526	Zooming in on the hydrophobic ridge of H-2D(b): implications for the conformational variability of bound peptides. <b>2001</b> , 312, 1059-71	16
1525	Crystallographic analysis of Lac repressor bound to natural operator O1. <b>2001</b> , 312, 921-6	73
1524	The 1.2 Å structure of a novel quorum-sensing protein, <i>Bacillus subtilis</i> LuxS. <b>2001</b> , 313, 111-22	67
1523	The crystal structure of bar-headed goose hemoglobin in deoxy form: the allosteric mechanism of a hemoglobin species with high oxygen affinity. <b>2001</b> , 313, 123-37	55
1522	Structure of c-phycocyanin from the thermophilic cyanobacterium <i>Synechococcus vulcanus</i> at 2.5 Å: structural implications for thermal stability in phycobilisome assembly. <b>2001</b> , 313, 71-81	56
1521	The 1.85 Å resolution crystal structures of tissue factor in complex with humanized Fab D3h44 and of free humanized Fab D3h44: revisiting the solvation of antigen combining sites. <b>2001</b> , 313, 83-97	35
1520	Structure of a variant of lac repressor with increased thermostability and decreased affinity for operator. <b>2001</b> , 313, 99-109	29
1519	Crystal structure of an RNA duplex r(gugucgac)(2) with uridine bulges. <b>2001</b> , 313, 573-82	16
1518	High resolution crystal structures of the catalytic domain of human phenylalanine hydroxylase in its catalytically active Fe(II) form and binary complex with tetrahydrobiopterin. <b>2001</b> , 314, 279-91	96
1517	Crystal structure of the <i>Escherichia coli</i> RNA degradosome component enolase. <b>2001</b> , 313, 583-92	77
1516	Crystal structure of the D85S mutant of bacteriorhodopsin: model of an O-like photocycle intermediate. <b>2001</b> , 313, 615-28	84
1515	The "open" and "closed" structures of the type-C inorganic pyrophosphatases from <i>Bacillus subtilis</i> and <i>Streptococcus gordonii</i> . <b>2001</b> , 313, 797-811	76
1514	Crystal structure of the liganded SCP-2-like domain of human peroxisomal multifunctional enzyme type 2 at 1.75 Å resolution. <b>2001</b> , 313, 1127-38	66

1513	Indirect readout of DNA sequence at the primary-kink site in the CAP-DNA complex: DNA binding specificity based on energetics of DNA kinking. <b>2001</b> , 314, 63-74	51
1512	Indirect readout of DNA sequence at the primary-kink site in the CAP-DNA complex: alteration of DNA binding specificity through alteration of DNA kinking. <b>2001</b> , 314, 75-82	50
1511	Crystal structure of the dimeric phosphoenolpyruvate carboxykinase (PEPCK) from <i>Trypanosoma cruzi</i> at 2 Å resolution. <b>2001</b> , 313, 1059-72	55
1510	Crystal structure of a protein repair methyltransferase from <i>Pyrococcus furiosus</i> with its L-isoaspartyl peptide substrate. <b>2001</b> , 313, 1103-16	50
1509	The complex structures of ATP sulfurylase with thiosulfate, ADP and chlorate reveal new insights in inhibitory effects and the catalytic cycle. <b>2001</b> , 313, 1117-25	29
1508	Structural basis for a disfavored elimination reaction in catalytic antibody 1D4. <b>2001</b> , 314, 93-102	10
1507	Crystal structure of an isolated V(alpha) domain of the 2C T-cell receptor. <b>2001</b> , 314, 1-8	7
1506	Protease C of <i>Erwinia chrysanthemi</i> : the crystal structure and role of amino acids Y228 and E189. <b>2001</b> , 314, 187-93	39
1505	The conserved methionine residue of the metzincins: a site-directed mutagenesis study. <b>2001</b> , 314, 181-6	26
1504	The 1.55 Å resolution structure of <i>Nicotiana glauca</i> S(F11)-RNase associated with gametophytic self-incompatibility. <b>2001</b> , 314, 103-12	54
1503	NTF2 monomer-dimer equilibrium. <b>2001</b> , 314, 465-77	27
1502	Crystal structure of a ternary SAP-1/SRF/c-fos SRE DNA complex. <b>2001</b> , 314, 495-506	56
1501	Solution structures of two FHA1-phosphothreonine peptide complexes provide insight into the structural basis of the ligand specificity of FHA1 from yeast Rad53. <b>2001</b> , 314, 563-75	34
1500	The crystal structure of a hyper-thermophilic carboxylesterase from the archaeon <i>Archaeoglobus fulgidus</i> . <b>2001</b> , 314, 507-18	137
1499	Recognition of cello-oligosaccharides by a family 17 carbohydrate-binding module: an X-ray crystallographic, thermodynamic and mutagenic study. <b>2001</b> , 314, 797-806	76
1498	Crystal structure of omega transcriptional repressor encoded by <i>Streptococcus pyogenes</i> plasmid pSM19035 at 1.5 Å resolution. <b>2001</b> , 314, 789-96	66
1497	Crystal structure of the non-regulatory A(4) isoform of spinach chloroplast glyceraldehyde-3-phosphate dehydrogenase complexed with NADP. <b>2001</b> , 314, 527-42	38
1496	Crystal structure of an antigen-binding fragment bound to single-stranded DNA. <b>2001</b> , 314, 807-22	50

1495	Structure and properties of a dimeric N-terminal fragment of human ubiquitin. <b>2001</b> , 314, 773-87	14
1494	Refined crystallographic structure of <i>Pseudomonas aeruginosa</i> exotoxin A and its implications for the molecular mechanism of toxicity. <b>2001</b> , 314, 823-37	86
1493	The contactin-related protein FAR-2 defines purkinje cell clusters and labels subpopulations of climbing fibers in the developing cerebellum. <b>2001</b> , 18, 91-107	20
1492	Construction of low-resolution x-ray crystallographic electron density maps of the ribosome. <b>2001</b> , 25, 303-8	4
1491	Crystal structure of a carbon monoxide dehydrogenase reveals a [Ni-4Fe-5S] cluster. <b>2001</b> , 293, 1281-5	409
1490	Recognition of cognate transfer RNA by the 30S ribosomal subunit. <b>2001</b> , 292, 897-902	959
1489	Structure of the gating domain of a Ca <sup>2+</sup> -activated K <sup>+</sup> channel complexed with Ca <sup>2+</sup> /calmodulin. <b>2001</b> , 410, 1120-4	495
1488	The structural basis of Arfaptin-mediated cross-talk between Rac and Arf signalling pathways. <b>2001</b> , 411, 215-9	209
1487	Structural analysis of BAG1 cochaperone and its interactions with Hsc70 heat shock protein. <b>2001</b> , 8, 349-52	123
1486	Crystal structure of an Xrcc4-DNA ligase IV complex. <b>2001</b> , 8, 1015-9	200
1485	Crystal structure of the ribosome at 5.5 Å resolution. <b>2001</b> , 292, 883-96	1606
1484	Mapping the energy surface of transmembrane helix-helix interactions. <b>2001</b> , 81, 2681-92	28
1483	Conformational disorder of proteins assessed by real-space molecular dynamics refinement. <b>2001</b> , 80, 1466-72	10
1482	Plasticity in protein-peptide recognition: crystal structures of two different peptides bound to concanavalin A. <b>2001</b> , 80, 2912-21	18
1481	Solution conformation of the Met 61 to His 61 mutant of <i>Pseudomonas stutzeri</i> ZoBell ferrocytochrome c-551. <b>2001</b> , 80, 2928-34	0
1480	Crystal structure and biophysical properties of a complex between the N-terminal SNARE region of SNAP25 and syntaxin 1a. <b>2001</b> , 276, 41301-9	41
1479	Adrenodoxin reductase-adrenodoxin complex structure suggests electron transfer path in steroid biosynthesis. <b>2001</b> , 276, 2786-9	130
1478	A structure-based design approach to the development of novel, reversible AChE inhibitors. <b>2001</b> , 44, 3203-15	49

1477	Crystal structure of an ephrin ectodomain. <b>2001</b> , 1, 83-92	83
1476	Structure of the RCK domain from the E. coli K <sup>+</sup> channel and demonstration of its presence in the human BK channel. <b>2001</b> , 29, 593-601	264
1475	Model for the structure of the HIV gp41 ectodomain: insight into the intermolecular interactions of the gp41 loop. <b>2001</b> , 1536, 116-22	63
1474	Two different, highly exposed, bulged structures for an unusually long peptide bound to rat MHC class I RT1-Aa. <b>2001</b> , 14, 81-92	103
1473	Crystal structure of a superantigen bound to the high-affinity, zinc-dependent site on MHC class II. <b>2001</b> , 14, 93-104	119
1472	The crystal structures of K(bm1) and K(bm8) reveal that subtle changes in the peptide environment impact thermostability and alloreactivity. <b>2001</b> , 14, 231-42	52
1471	Mutations changing the kinetics of class II MHC peptide exchange. <b>2001</b> , 14, 513-22	20
1470	Crystal structure of the IL-10/IL-10R1 complex reveals a shared receptor binding site. <b>2001</b> , 15, 35-46	166
1469	Conformational plasticity revealed by the cocrystal structure of NKG2D and its class I MHC-like ligand ULBP3. <b>2001</b> , 15, 1039-49	127
1468	Phosphoprotein-protein interactions revealed by the crystal structure of kinase-associated phosphatase in complex with phosphoCDK2. <b>2001</b> , 7, 615-26	152
1467	Crystal structure of a Pumilio homology domain. <b>2001</b> , 7, 855-65	192
1466	Crystal structure at 2.8 Å of an FcRn/heterodimeric Fc complex: mechanism of pH-dependent binding. <b>2001</b> , 7, 867-77	319
1465	An extended RNA binding surface through arrayed S1 and KH domains in transcription factor NusA. <b>2001</b> , 7, 1177-89	86
1464	Herpes simplex virus glycoprotein D bound to the human receptor HveA. <b>2001</b> , 8, 169-79	304
1463	Crystal structure of the human nuclear cap binding complex. <b>2001</b> , 8, 383-96	115
1462	Structure of the catalytic core of <i>S. cerevisiae</i> DNA polymerase $\epsilon$ : implications for translesion DNA synthesis. <b>2001</b> , 8, 417-26	309
1461	The Structure of calnexin, an ER chaperone involved in quality control of protein folding. <b>2001</b> , 8, 633-44	323
1460	Atomic structure of the clamp loader small subunit from <i>Pyrococcus furiosus</i> . <b>2001</b> , 8, 455-63	66

1459	The TGF beta receptor activation process: an inhibitor- to substrate-binding switch. <b>2001</b> , 8, 671-82	310
1458	A small domain of CBP/p300 binds diverse proteins: solution structure and functional studies. <b>2001</b> , 8, 581-90	87
1457	Differential dimer activities of the transcription factor Oct-1 by DNA-induced interface swapping. <b>2001</b> , 8, 569-80	100
1456	Structure and regulation of the CDK5-p25(nck5a) complex. <b>2001</b> , 8, 657-69	220
1455	Structural basis for the recognition of a nucleoporin FG repeat by the NTF2-like domain of the TAP/p15 mRNA nuclear export factor. <b>2001</b> , 8, 645-56	193
1454	The crystal structure of the PX domain from p40(phox) bound to phosphatidylinositol 3-phosphate. <b>2001</b> , 8, 829-39	248
1453	Crystal structure of colicin E3: implications for cell entry and ribosome inactivation. <b>2001</b> , 8, 1053-62	136
1452	Structural studies of Ets-1/Pax5 complex formation on DNA. <b>2001</b> , 8, 1267-76	159
1451	Structure of the SH3-guanylate kinase module from PSD-95 suggests a mechanism for regulated assembly of MAGUK scaffolding proteins. <b>2001</b> , 8, 1291-301	204
1450	Bacterial polypeptide release factor RF2 is structurally distinct from eukaryotic eRF1. <b>2001</b> , 8, 1375-82	177
1449	Structural basis of Smad1 activation by receptor kinase phosphorylation. <b>2001</b> , 8, 1303-12	84
1448	Structure of the ExoS GTPase activating domain. <b>2001</b> , 491, 26-9	28
1447	Crystal structure of the bacterial cell division regulator MinD. <b>2001</b> , 492, 160-5	68
1446	A refined structure of human aquaporin-1. <b>2001</b> , 504, 206-11	110
1445	Structural basis for the emission of violet bioluminescence from a W92F obelin mutant. <b>2001</b> , 506, 281-5	41
1444	Structure of the complete extracellular domain of the common beta subunit of the human GM-CSF, IL-3, and IL-5 receptors reveals a novel dimer configuration. <b>2001</b> , 104, 291-300	91
1443	A novel all helix fold of the AP180 amino-terminal domain for phosphoinositide binding and clathrin assembly in synaptic vesicle endocytosis. <b>2001</b> , 104, 433-40	81
1442	Crystal structure of a SIR2 homolog-NAD complex. <b>2001</b> , 105, 269-79	267



1441	Specificity determinants in phosphoinositide dephosphorylation: crystal structure of an archetypal inositol polyphosphate 5-phosphatase. <b>2001</b> , 105, 379-89	111
1440	Structural biochemistry and interaction architecture of the DNA double-strand break repair Mre11 nuclease and Rad50-ATPase. <b>2001</b> , 105, 473-85	397
1439	Structure of the replicating complex of a pol alpha family DNA polymerase. <b>2001</b> , 105, 657-67	507
1438	Molecular insights into polyubiquitin chain assembly: crystal structure of the Mms2/Ubc13 heterodimer. <b>2001</b> , 105, 711-20	257
1437	Crystal structure of negative cofactor 2 recognizing the TBP-DNA transcription complex. <b>2001</b> , 106, 71-81	128
1436	Mechanism of Processivity Clamp Opening by the Delta Subunit Wrench of the Clamp Loader Complex of E. coli DNA Polymerase III. <b>2001</b> , 106, 417-428	205
1435	Crystal structure of the processivity clamp loader gamma (gamma) complex of E. coli DNA polymerase III. <b>2001</b> , 106, 429-41	253
1434	Crystal structure of LexA: a conformational switch for regulation of self-cleavage. <b>2001</b> , 106, 585-94	169
1433	A novel peptide recognition mode revealed by the X-ray structure of a core U2AF35/U2AF65 heterodimer. <b>2001</b> , 106, 595-605	164
1432	Cocrystal structure of a tRNA Psi55 pseudouridine synthase: nucleotide flipping by an RNA-modifying enzyme. <b>2001</b> , 107, 929-39	234
1431	Site-directed mutagenesis and X-ray crystallography of the PQQ-containing quinoprotein methanol dehydrogenase and its electron acceptor, cytochrome c(L). <b>2001</b> , 40, 9799-809	62
1430	Crystal structure of an initiation factor bound to the 30S ribosomal subunit. <b>2001</b> , 291, 498-501	319
1429	Implications for isoform-selective inhibitor design derived from the binding mode of bulky isothioureas to the heme domain of endothelial nitric-oxide synthase. <b>2001</b> , 276, 26486-91	23
1428	Reducing the environmental sensitivity of yellow fluorescent protein. Mechanism and applications. <b>2001</b> , 276, 29188-94	821
1427	Co-crystal of Escherichia coli RNase HI with Mn <sup>2+</sup> ions reveals two divalent metals bound in the active site. <b>2001</b> , 276, 7266-71	78
1426	Crystal structure analysis of warfarin binding to human serum albumin: anatomy of drug site I. <b>2001</b> , 276, 22804-9	619
1425	The structure of the chloroplast F1-ATPase at 3.2 A resolution. <b>2001</b> , 276, 1345-52	100
1424	The structure of human beta-defensin-1: new insights into structural properties of beta-defensins. <b>2001</b> , 276, 39021-6	145

1423	Structures of the acyl-enzyme complexes of the <i>Staphylococcus aureus</i> beta-lactamase mutant Glu166Asp:Asn170Gln with benzylpenicillin and cephaloridine. <b>2001</b> , 40, 2351-8	35
1422	Structural basis for recognition of the intron branch site RNA by splicing factor 1. <b>2001</b> , 294, 1098-102	190
1421	Antigen specificity and high affinity binding provided by one single loop of a camel single-domain antibody. <b>2001</b> , 276, 26285-90	119
1420	Crystal structure of <i>Nitrosomonas europaea</i> cytochrome c peroxidase and the structural basis for ligand switching in bacterial di-heme peroxidases. <b>2001</b> , 40, 13483-90	72
1419	Crystal structure of a complex between <i>Pseudomonas aeruginosa</i> alkaline protease and its cognate inhibitor: inhibition by a zinc-NH <sub>2</sub> coordinative bond. <b>2001</b> , 276, 35087-92	45
1418	Ligand variation in the transferrin family: the crystal structure of the H249Q mutant of the human transferrin N-lobe as a model for iron binding in insect transferrins. <b>2001</b> , 40, 11670-5	26
1417	Crystal structures of the soluble methane monooxygenase hydroxylase from <i>Methylococcus capsulatus</i> (Bath) demonstrating geometrical variability at the dinuclear iron active site. <b>2001</b> , 123, 827-38	187
1416	Chemical rescue of phosphoryl transfer in a cavity mutant: a cautionary tale for site-directed mutagenesis. <b>2001</b> , 40, 403-13	25
1415	Structures of cytochrome c-549 and cytochrome c6 from the cyanobacterium <i>Arthrospira maxima</i> . <b>2001</b> , 40, 9215-25	61
1414	Structural and kinetic analysis of the chemical rescue of the proton transfer function of carbonic anhydrase II. <b>2001</b> , 40, 1741-8	90
1413	Enhanced binding of a rationally designed peptide ligand of concanavalin A arises from improved geometrical complementarity. <b>2001</b> , 40, 12059-66	9
1412	Probing erectile function: S-(2-boronoethyl)-L-cysteine binds to arginase as a transition state analogue and enhances smooth muscle relaxation in human penile corpus cavernosum. <b>2001</b> , 40, 2678-88	150
1411	Human thymidylate synthase is in the closed conformation when complexed with dUMP and raltitrexed, an antifolate drug. <b>2001</b> , 40, 1897-902	88
1410	Crystal structure of ATP sulfurylase from <i>Penicillium chrysogenum</i> : insights into the allosteric regulation of sulfate assimilation. <b>2001</b> , 40, 6795-804	55
1409	Crystal structures of the yeast prion Ure2p functional region in complex with glutathione and related compounds. <b>2001</b> , 40, 13564-73	61
1408	Structural basis for the activity and substrate specificity of <i>Erwinia chrysanthemi</i> L-asparaginase. <b>2001</b> , 40, 5655-64	133
1407	Structures of <i>Saccharomyces cerevisiae</i> N-myristoyltransferase with bound myristoylCoA and peptide provide insights about substrate recognition and catalysis. <b>2001</b> , 40, 6335-43	66
1406	Crystal structures and iron release properties of mutants (K206A and K296A) that abolish the dilysine interaction in the N-lobe of human transferrin. <b>2001</b> , 40, 1616-23	33

1405	Solution structure of the carboxyl-terminal cysteine-rich domain of the VHv1.1 polydnviral gene product: comparison with other cystine knot structural folds. <b>2001</b> , 40, 14404-12	15
1404	Advances in determination of a high-resolution three-dimensional structure of rhodopsin, a model of G-protein-coupled receptors (GPCRs). <b>2001</b> , 40, 7761-72	597
1403	Phosphorylation mutants elucidate the mechanism of annexin IV-mediated membrane aggregation. <b>2001</b> , 40, 4192-9	73
1402	Crystal structure of rabbit phosphoglucose isomerase complexed with 5-phospho-D-arabinonate identifies the role of Glu357 in catalysis. <b>2001</b> , 40, 1560-6	56
1401	Structural basis for the catalysis and substrate specificity of homoserine kinase. <b>2001</b> , 40, 10810-8	71
1400	Crystal structure of thrombin-ecotin reveals conformational changes and extended interactions. <b>2001</b> , 40, 10038-46	17
1399	High-resolution NMR structure of the chemically-synthesized melanocortin receptor binding domain AGRP(87-132) of the agouti-related protein. <b>2001</b> , 40, 15520-7	75
1398	Insights into the molecular basis for the carbenicillinase activity of PSE-4 beta-lactamase from crystallographic and kinetic studies. <b>2001</b> , 40, 395-402	40
1397	Evolution of enzymatic activities in the enolase superfamily: identification of the general acid catalyst in the active site of D-glucarate dehydratase from Escherichia coli. <b>2001</b> , 40, 10054-62	25
1396	Solution structure of HI0257, a bacterial ribosome binding protein. <b>2001</b> , 40, 10979-86	11
1395	Crystal structure of nitric oxide synthase bound to nitro indazole reveals a novel inactivation mechanism. <b>2001</b> , 40, 13448-55	74
1394	Crystal structure of maleylacetoacetate isomerase/glutathione transferase zeta reveals the molecular basis for its remarkable catalytic promiscuity. <b>2001</b> , 40, 1567-76	108
1393	Crystal structure of heme oxygenase from the gram-negative pathogen Neisseria meningitidis and a comparison with mammalian heme oxygenase-1. <b>2001</b> , 40, 11552-8	127
1392	Structures of tetrahydrobiopterin binding-site mutants of inducible nitric oxide synthase oxygenase dimer and implicated roles of Trp457. <b>2001</b> , 40, 12826-32	31
1391	The human nuclear xenobiotic receptor PXR: structural determinants of directed promiscuity. <b>2001</b> , 292, 2329-33	675
1390	The role of cation-pi interactions in biomolecular association. Design of peptides favoring interactions between cationic and aromatic amino acid side chains. <b>2001</b> , 123, 6232-45	117
1389	Crystal structure of an early protein-RNA assembly complex of the signal recognition particle. <b>2001</b> , 294, 598-601	69
1388	Contributions of valine-292 in the nicotinamide binding site of liver alcohol dehydrogenase and dynamics to catalysis. <b>2001</b> , 40, 12686-94	48

1387	Crystal structure of a model branchpoint-U2 snRNA duplex containing bulged adenosines. <b>2001</b> , 7, 682-91	41
1386	Ribosomal protein L5 has a highly twisted concave surface and flexible arms responsible for rRNA binding. <b>2001</b> , 7, 692-701	16
1385	Structure of UDP complex of UDP-galactose:beta-galactoside-alpha -1,3-galactosyltransferase at 1.53-A resolution reveals a conformational change in the catalytically important C terminus. <b>2001</b> , 276, 48608-14	75
1384	The location of the ligand-binding site of carbohydrate-binding modules that have evolved from a common sequence is not conserved. <b>2001</b> , 276, 48580-7	93
1383	Crystal structure of a monocotyledon (maize ZMGlu1) beta-glucosidase and a model of its complex with p-nitrophenyl beta-D-thioglucoside. <b>2001</b> , 354, 37-46	70
1382	Macrophage migration inhibitory factor of the parasitic nematode <i>Trichinella spiralis</i> . <b>2001</b> , 357, 373-83	42
1381	Crystal structure of the wild-type and D30A mutant thioredoxin h of <i>Chlamydomonas reinhardtii</i> and implications for the catalytic mechanism. <b>2001</b> , 359, 65-75	39
1380	Structure of a factor VIII C2 domain-immunoglobulin G4kappa Fab complex: identification of an inhibitory antibody epitope on the surface of factor VIII. <b>2001</b> , 98, 13-9	119
1379	Identification of receptor and heparin binding sites in fibroblast growth factor 4 by structure-based mutagenesis. <b>2001</b> , 21, 5946-57	59
1378	Solution structure of the ribosome recycling factor from <i>Aquifex aeolicus</i> . <b>2001</b> , 40, 2387-96	53
1377	Insights into the Functional Architecture of the Catalytic Center of a Maize $\beta$ -Glucosidase Zm-p60.1. <b>2001</b> , 127, 973-985	47
1376	Using surface-bound rubidium ions for protein phasing. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2001</b> , 57, 1008-12	7
1375	The xenograft antigen in complex with GS-1-B4 lectin: crystallization and preliminary X-ray analysis. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2001</b> , 57, 1639-42	2
1374	<i>Streptococcus pneumoniae</i> YlxR at 1.35 Å shows a putative new fold. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2001</b> , 57, 1747-51	16
1373	Crystal structure of the global regulator FlhD from <i>Escherichia coli</i> at 1.8 Å resolution. <b>2001</b> , 39, 567-80	13
1372	Le calcul du déplacement chimique, un outil de validation des structures d'acides nucléiques. <b>2001</b> , 4, 779-782	
1371	Energetic, structural, and antimicrobial analyses of beta-lactam side chain recognition by beta-lactamases. <b>2001</b> , 8, 17-31	67
1370	Structure-based design and in-parallel synthesis of inhibitors of AmpC beta-lactamase. <b>2001</b> , 8, 593-611	39

1369	Predicting and harnessing protein flexibility in the design of species-specific inhibitors of thymidylate synthase. <b>2001</b> , 8, 981-95	25
1368	Structure of cephalosporin acylase in complex with glutaryl-7-aminocephalosporanic acid and glutarate: insight into the basis of its substrate specificity. <b>2001</b> , 8, 1253-64	48
1367	Structural basis for chloramphenicol tolerance in <i>Streptomyces venezuelae</i> by chloramphenicol phosphotransferase activity. <b>2001</b> , 10, 1508-13	13
1366	Crystal structure of YecO from <i>Haemophilus influenzae</i> (HI0319) reveals a methyltransferase fold and a bound S-adenosylhomocysteine. <b>2001</b> , 45, 397-407	25
1365	The crystal structure of chorismate lyase shows a new fold and a tightly retained product. <b>2001</b> , 44, 304-11	30
1364	A new method to model membrane protein structure based on silent amino acid substitutions. <b>2001</b> , 44, 370-5	45
1363	Interactions of <i>Streptomyces griseus</i> aminopeptidase with amino acid reaction products and their implications toward a catalytic mechanism. <b>2001</b> , 44, 490-504	45
1362	Structure of an anti-HIV monoclonal Fab antibody fragment specific to a gp120 C-4 region peptide. <b>2001</b> , 45, 281-2	2
1361	Computation and mutagenesis suggest a right-handed structure for the synaptobrevin transmembrane dimer. <b>2001</b> , 45, 313-7	50
1360	Structure determination of membrane-associated proteins from nuclear magnetic resonance data. <b>2001</b> , 288, 1-15	19
1359	The VMD-XPLOR visualization package for NMR structure refinement. <b>2001</b> , 149, 239-44	107
1358	A maximum likelihood method for determining D(a)(PQ) and R for sets of dipolar coupling data. <b>2001</b> , 149, 271-5	58
1357	X-ray Crystal Structure of a Bisubstrate Inhibitor Bound to the Enzyme Catechol-O-methyltransferase: A Dramatic Effect of Inhibitor Preorganization on Binding Affinity. <b>2001</b> , 113, 4164-4166	16
1356	Cytotoxic T lymphocytes recognize structurally diverse, clade-specific and cross-reactive peptides in human immunodeficiency virus type-1 gag through HLA-B53. <b>2001</b> , 31, 1747-1756	41
1355	Sampling of conformation space in torsion angle dynamics calculations. <b>2001</b> , 138, 155-169	7
1354	Role of Phe286 in the recognition mechanism of cyclomaltooligosaccharides (cyclodextrins) by <i>Thermoactinomyces vulgaris</i> R-47 alpha-amylase 2 (TVAII). X-ray structures of the mutant TVAII, F286A and F286Y, and kinetic analyses of the Phe286-replaced mutant TVAII. <b>2001</b> , 334, 309-13	15
1353	Packing contacts in orthorhombic and monoclinic crystals of a thermophilic aspartyl-tRNA synthetase favor the hydrophobic regions of the protein. <b>2001</b> , 232, 376-386	10
1352	Effect of a mutation at arginine 301 on the stability, crystal quality and the preliminary crystallographic analysis of recombinant canavalin from <i>Canavalia ensiformis</i> . <b>2001</b> , 232, 387-398	3

1351	Protein packing interactions and polymorphy of chorismate lyase from E. Coli. <b>2001</b> , 232, 215-220	
1350	Structures of ceftazidime and its transition-state analogue in complex with AmpC beta-lactamase: implications for resistance mutations and inhibitor design. <b>2001</b> , 40, 9207-14	101
1349	Rational design of diflunisal analogues with reduced affinity for human serum albumin. <b>2001</b> , 123, 10429-35	82
1348	Mammalian reovirus L2 gene and lambda2 core spike protein sequences and whole-genome comparisons of reoviruses type 1 Lang, type 2 Jones, and type 3 Dearing. <b>2001</b> , 287, 333-48	48
1347	The crystal structure of the influenza matrix protein M1 at neutral pH: M1-M1 protein interfaces can rotate in the oligomeric structures of M1. <b>2001</b> , 289, 34-44	98
1346	Application of dipolar coupling data to the refinement of the solution structure of the sarcin-ricin loop RNA. <b>2001</b> , 20, 311-23	38
1345	NMR-based structure of the conserved protein MTH865 from the archaeon Methanobacterium thermoautotrophicum. <b>2001</b> , 21, 63-6	1
1344	Direct structure refinement of high molecular weight proteins against residual dipolar couplings and carbonyl chemical shift changes upon alignment: an application to maltose binding protein. <b>2001</b> , 21, 31-40	46
1343	Rapid protein fold determination using secondary chemical shifts and cross-hydrogen bond <sup>15</sup> N- <sup>13</sup> C' scalar couplings (3hbJNC'). <b>2001</b> , 21, 221-33	22
1342	Structural mechanism for statin inhibition of HMG-CoA reductase. <b>2001</b> , 292, 1160-4	1042
1341	Structure of beta-ketoacyl-[acyl carrier protein] reductase from Escherichia coli: negative cooperativity and its structural basis. <b>2001</b> , 40, 12772-81	126
1340	Structural mechanisms of QacR induction and multidrug recognition. <b>2001</b> , 294, 2158-63	325
1339	High-resolution crystal structure of apolipoprotein(a) kringle IV type 7: insights into ligand binding. <b>2001</b> , 10, 1124-9	28
1338	Specific protein dynamics near the solvent glass transition assayed by radiation-induced structural changes. <b>2001</b> , 10, 1953-61	58
1337	The structure of apo protein-tyrosine phosphatase 1B C215S mutant: more than just an S --> O change. <b>2001</b> , 10, 1596-605	36
1336	Oligomerization and ligand binding in a homotetrameric hemoglobin: two high-resolution crystal structures of hemoglobin Bart's (gamma(4)), a marker for alpha-thalassemia. <b>2001</b> , 10, 1739-49	21
1335	Binding of phosphate and pyrophosphate ions at the active site of human angiogenin as revealed by X-ray crystallography. <b>2001</b> , 10, 1669-76	22
1334	The roles of turn formation and cross-strand interactions in fibrillization of peptides derived from the OspA single-layer beta-sheet. <b>2001</b> , 10, 2083-92	18

1333	Crystal structure of <i>Staphylococcus aureus</i> tyrosyl-tRNA synthetase in complex with a class of potent and specific inhibitors. <b>2001</b> , 10, 2008-16	89
1332	Crystal structure of an anti-interleukin-2 monoclonal antibody Fab complexed with an antigenic nonapeptide. <b>2001</b> , 10, 1514-21	5
1331	Structural features of a zinc binding site in the superantigen streptococcal pyrogenic exotoxin A (SpeA1): implications for MHC class II recognition. <b>2001</b> , 10, 1268-73	29
1330	HMG-D complexed to a bulge DNA: an NMR model. <b>2001</b> , 10, 504-18	18
1329	Overcoming the problems associated with poor spectra quality of the protein kinase Byr2 using residual dipolar couplings. <b>2001</b> , 10, 1260-3	1
1328	Crystal structure of threonine synthase from <i>Arabidopsis thaliana</i> . <b>2001</b> , 10, 638-48	35
1327	Crystal structure of <i>E. coli</i> beta-carbonic anhydrase, an enzyme with an unusual pH-dependent activity. <b>2001</b> , 10, 911-22	131
1326	Crystal structure of a deletion mutant of human thymidylate synthase Delta (7-29) and its ternary complex with Tomudex and dUMP. <b>2001</b> , 10, 988-96	56
1325	Catalytic center of an archaeal type 2 ribonuclease H as revealed by X-ray crystallographic and mutational analyses. <b>2001</b> , 10, 707-14	66
1324	Effect of pH and salt bridges on structural assembly: molecular structures of the monomer and intertwined dimer of the Eps8 SH3 domain. <b>2001</b> , 10, 1046-55	37
1323	Structural basis of pheromone binding to mouse major urinary protein (MUP-I). <b>2001</b> , 10, 997-1004	86
1322	Molecular mimicry of substrate oxygen atoms by water molecules in the beta-amylase active site. <b>2001</b> , 10, 1645-57	12
1321	The crystal structure of the ttCsaA protein: an export-related chaperone from <i>Thermus thermophilus</i> . <b>2001</b> , 20, 562-9	23
1320	Structural investigations of the active-site mutant Asn156Ala of outer membrane phospholipase A: function of the Asn-His interaction in the catalytic triad. <b>2001</b> , 10, 1962-9	13
1319	The structural GDP/GTP cycle of human Arf6. <b>2001</b> , 2, 234-8	102
1318	The solution structure of PapGII from uropathogenic <i>Escherichia coli</i> and its recognition of glycolipid receptors. <b>2001</b> , 2, 621-7	42
1317	CD81 extracellular domain 3D structure: insight into the tetraspanin superfamily structural motifs. <b>2001</b> , 20, 12-8	214
1316	Structural basis for the inactivation of retinoblastoma tumor suppressor by SV40 large T antigen. <b>2001</b> , 20, 295-304	129

1315	Structure of a genetically engineered molecular motor. <b>2001</b> , 20, 40-6	55
1314	Crystal structure of the bacterial cell division inhibitor MinC. <b>2001</b> , 20, 2454-61	73
1313	Structure and mechanism of the RNA triphosphatase component of mammalian mRNA capping enzyme. <b>2001</b> , 20, 2575-86	74
1312	Structure of Golgi alpha-mannosidase II: a target for inhibition of growth and metastasis of cancer cells. <b>2001</b> , 20, 3008-17	167
1311	The B-box dominates SAP-1-SRF interactions in the structure of the ternary complex. <b>2001</b> , 20, 3018-28	82
1310	Crystal structure of a superantigen bound to MHC class II displays zinc and peptide dependence. <b>2001</b> , 20, 3306-12	90
1309	Proximity of the invariant loop of U5 snRNA to the second intron residue during pre-mRNA splicing. <b>2001</b> , 20, 3577-86	21
1308	Intertwined structure of the DNA-binding domain of intron endonuclease I-TevI with its substrate. <b>2001</b> , 20, 3631-7	61
1307	The interaction of insulin-like growth factor-I with the N-terminal domain of IGFBP-5. <b>2001</b> , 20, 3638-44	80
1306	Crystal structure of the M-fragment of alpha-catenin: implications for modulation of cell adhesion. <b>2001</b> , 20, 3645-56	65
1305	Crystal structure of an activated form of the PTS regulation domain from the LicT transcriptional antiterminator. <b>2001</b> , 20, 3789-99	55
1304	Mycobacterium tuberculosis hemoglobin N displays a protein tunnel suited for O <sub>2</sub> diffusion to the heme. <b>2001</b> , 20, 3902-9	180
1303	Structure of human cystathionine beta-synthase: a unique pyridoxal 5'-phosphate-dependent heme protein. <b>2001</b> , 20, 3910-6	248
1302	X-ray structure of HPr kinase: a bacterial protein kinase with a P-loop nucleotide-binding domain. <b>2001</b> , 20, 3917-27	75
1301	Polymerization of the SAM domain of TEL in leukemogenesis and transcriptional repression. <b>2001</b> , 20, 4173-82	190
1300	The kink-turn: a new RNA secondary structure motif. <b>2001</b> , 20, 4214-21	617
1299	Structure of the ABC ATPase domain of human TAP1, the transporter associated with antigen processing. <b>2001</b> , 20, 4964-72	209
1298	Crystal structure of the outer membrane protease OmpT from Escherichia coli suggests a novel catalytic site. <b>2001</b> , 20, 5033-9	223



1297	The structure of an AspRS-tRNA(Asp) complex reveals a tRNA-dependent control mechanism. <b>2001</b> , 20, 5290-301	88
1296	Crystal structure of human protein kinase CK2: insights into basic properties of the CK2 holoenzyme. <b>2001</b> , 20, 5320-31	308
1295	Structural basis for the high-affinity interaction of nidogen-1 with immunoglobulin-like domain 3 of perlecan. <b>2001</b> , 20, 5342-6	39
1294	Structure and function of the N-terminal 40 kDa fragment of human PMS2: a monomeric GHL ATPase. <b>2001</b> , 20, 5521-31	94
1293	Crystal structures of NK1-heparin complexes reveal the basis for NK1 activity and enable engineering of potent agonists of the MET receptor. <b>2001</b> , 20, 5543-55	93
1292	Crystal structure of a dynamin GTPase domain in both nucleotide-free and GDP-bound forms. <b>2001</b> , 20, 5813-21	96
1291	X-ray structure of the orphan nuclear receptor RORbeta ligand-binding domain in the active conformation. <b>2001</b> , 20, 5822-31	99
1290	Crystal structures of two human pyrophosphorylase isoforms in complexes with UDPGlc(Gal)NAc: role of the alternatively spliced insert in the enzyme oligomeric assembly and active site architecture. <b>2001</b> , 20, 6191-202	116
1289	Molecular mechanisms of beta-catenin recognition by adenomatous polyposis coli revealed by the structure of an APC-beta-catenin complex. <b>2001</b> , 20, 6203-12	102
1288	Structure of a fast kinesin: implications for ATPase mechanism and interactions with microtubules. <b>2001</b> , 20, 6213-25	68
1287	Structures of F420H2:NADP+ oxidoreductase with and without its substrates bound. <b>2001</b> , 20, 6561-9	50
1286	V-shaped structure of glutamyl-tRNA reductase, the first enzyme of tRNA-dependent tetrapyrrole biosynthesis. <b>2001</b> , 20, 6583-90	101
1285	Specific roles of protein-phospholipid interactions in the yeast cytochrome bc1 complex structure. <b>2001</b> , 20, 6591-600	352
1284	Crystal structure of the fission yeast mitochondrial Holliday junction resolvase Ydc2. <b>2001</b> , 20, 6601-11	54
1283	Crystal structure of the CENP-B protein-DNA complex: the DNA-binding domains of CENP-B induce kinks in the CENP-B box DNA. <b>2001</b> , 20, 6612-8	72
1282	The structure of the negative transcriptional regulator NmrA reveals a structural superfamily which includes the short-chain dehydrogenase/reductases. <b>2001</b> , 20, 6619-26	80
1281	The structure of bovine IF(1), the regulatory subunit of mitochondrial F-ATPase. <b>2001</b> , 20, 6990-6	108
1280	Translocation portals for the substrates and products of a viral transcription complex: the bluetongue virus core. <b>2001</b> , 20, 7229-39	67

1279	Structure of a two-domain fragment of HIV-1 integrase: implications for domain organization in the intact protein. <b>2001</b> , 20, 7333-43	278
1278	Crystal structure of ATP sulfurylase from <i>Saccharomyces cerevisiae</i> , a key enzyme in sulfate activation. <b>2001</b> , 20, 316-29	85
1277	Structure of the EMAPII domain of human aminoacyl-tRNA synthetase complex reveals evolutionary dimer mimicry. <b>2001</b> , 20, 570-8	56
1276	Structure of the major single-stranded DNA-binding domain of replication protein A suggests a dynamic mechanism for DNA binding. <b>2001</b> , 20, 612-8	128
1275	Crystal structure of dihydropyrimidine dehydrogenase, a major determinant of the pharmacokinetics of the anti-cancer drug 5-fluorouracil. <b>2001</b> , 20, 650-60	91
1274	Crystal structure of outer surface protein C (OspC) from the Lyme disease spirochete, <i>Borrelia burgdorferi</i> . <b>2001</b> , 20, 971-8	86
1273	Structure of the reovirus outer capsid and dsRNA-binding protein sigma3 at 1.8 Å resolution. <b>2001</b> , 20, 979-89	68
1272	The hairpin structure of the (6)F1(1)F2(2)F2 fragment from human fibronectin enhances gelatin binding. <b>2001</b> , 20, 1519-29	66
1271	Crystal structure of isopentenyl diphosphate:dimethylallyl diphosphate isomerase. <b>2001</b> , 20, 1530-7	72
1270	Structural and functional studies of MinD ATPase: implications for the molecular recognition of the bacterial cell division apparatus. <b>2001</b> , 20, 1819-28	110
1269	Crystal structures of complexes of the small ribosomal subunit with tetracycline, edeine and IF3. <b>2001</b> , 20, 1829-39	391
1268	RNA binding in an Sm core domain: X-ray structure and functional analysis of an archaeal Sm protein complex. <b>2001</b> , 20, 2293-303	135
1267	Toward rational design of species-specific inhibitors of <i>Pneumocystis carinii</i> thymidylate synthase and <i>Toxoplasma gondii</i> dihydrofolate reductase-thymidylate synthase. <b>2001</b> , Suppl, 174S-175S	
1266	The three-dimensional structure of human granzyme B compared to caspase-3, key mediators of cell death with cleavage specificity for aspartic acid in P1. <b>2001</b> , 8, 357-68	64
1265	Approaches to solving the rigid receptor problem by identifying a minimal set of flexible residues during ligand docking. <b>2001</b> , 8, 445-57	63
1264	Crystal structure of the anthrax lethal factor. <b>2001</b> , 414, 229-33	330
1263	Structural basis of water-specific transport through the AQP1 water channel. <b>2001</b> , 414, 872-8	938
1262	How the <i>Pseudomonas aeruginosa</i> ExoS toxin downregulates Rac. <b>2001</b> , 8, 23-6	92

1261	SMN tudor domain structure and its interaction with the Sm proteins. <b>2001</b> , 8, 27-31	247
1260	Mechanism-based design of a protein kinase inhibitor. <b>2001</b> , 8, 37-41	160
1259	Crystal structure of an activated response regulator bound to its target. <b>2001</b> , 8, 52-6	119
1258	Crystal structure of the Holliday junction resolving enzyme T7 endonuclease I. <b>2001</b> , 8, 62-7	79
1257	Structure of the electron transfer complex between ferredoxin and ferredoxin-NADP(+) reductase. <b>2001</b> , 8, 117-21	256
1256	Structure of the N6-adenine DNA methyltransferase M.TaqI in complex with DNA and a cofactor analog. <b>2001</b> , 8, 121-5	182
1255	Structural basis for recognition of AU-rich element RNA by the HuD protein. <b>2001</b> , 8, 141-5	193
1254	The 2.0 Å structure of human ferrochelatase, the terminal enzyme of heme biosynthesis. <b>2001</b> , 8, 156-60	179
1253	Crystal structure of the retaining galactosyltransferase LgtC from <i>Neisseria meningitidis</i> in complex with donor and acceptor sugar analogs. <b>2001</b> , 8, 166-75	286
1252	The structure of Sky1p reveals a novel mechanism for constitutive activity. <b>2001</b> , 8, 176-83	67
1251	Structure of the RTP-DNA complex and the mechanism of polar replication fork arrest. <b>2001</b> , 8, 206-10	31
1250	A domain-swapped RNase A dimer with implications for amyloid formation. <b>2001</b> , 8, 211-4	216
1249	Structure of human biliverdin IXbeta reductase, an early fetal bilirubin IXbeta producing enzyme. <b>2001</b> , 8, 215-20	85
1248	Predicting the emergence of antibiotic resistance by directed evolution and structural analysis. <b>2001</b> , 8, 238-42	184
1247	Structure of the cooperative allosteric anthranilate synthase from <i>Salmonella typhimurium</i> . <b>2001</b> , 8, 243-7	69
1246	The L3 loop and C-terminal phosphorylation jointly define Smad protein trimerization. <b>2001</b> , 8, 248-53	119
1245	Vam3p structure reveals conserved and divergent properties of syntaxins. <b>2001</b> , 8, 258-64	120
1244	Structures of two natural product methyltransferases reveal the basis for substrate specificity in plant O-methyltransferases. <b>2001</b> , 8, 271-9	253

1243	The homing endonuclease I-CreI uses three metals, one of which is shared between the two active sites. <b>2001</b> , 8, 312-6	95
1242	Human cystatin C, an amyloidogenic protein, dimerizes through three-dimensional domain swapping. <b>2001</b> , 8, 316-20	318
1241	A universal mode of helix packing in RNA. <b>2001</b> , 8, 339-43	204
1240	Nucleotide binding by the histidine kinase CheA. <b>2001</b> , 8, 353-60	131
1239	The leukemia-associated AML1 (Runx1)--CBF beta complex functions as a DNA-induced molecular clamp. <b>2001</b> , 8, 371-8	130
1238	Crystal structure of a bifunctional transformylase and cyclohydrolase enzyme in purine biosynthesis. <b>2001</b> , 8, 402-6	67
1237	Solution structure of a Nedd4 WW domain-ENaC peptide complex. <b>2001</b> , 8, 407-12	181
1236	Crystal structure of proteolytic fragments of the redox-sensitive Hsp33 with constitutive chaperone activity. <b>2001</b> , 8, 459-66	42
1235	The structure of ADP-ribose pyrophosphatase reveals the structural basis for the versatility of the Nudix family. <b>2001</b> , 8, 467-72	100
1234	Complex structure of the activating immunoreceptor NKG2D and its MHC class I-like ligand MICA. <b>2001</b> , 2, 443-51	305
1233	Crystal structure of the human natural killer cell inhibitory receptor KIR2DL1-HLA-Cw4 complex. <b>2001</b> , 2, 452-60	220
1232	Implications for familial hypercholesterolemia from the structure of the LDL receptor YWTD-EGF domain pair. <b>2001</b> , 8, 499-504	180
1231	Supramolecular assembly and acid resistance of Helicobacter pylori urease. <b>2001</b> , 8, 505-9	347
1230	Aminoglycoside binding displaces a divalent metal ion in a tRNA-neomycin B complex. <b>2001</b> , 8, 510-4	72
1229	Pteridine reductase mechanism correlates pterin metabolism with drug resistance in trypanosomatid parasites. <b>2001</b> , 8, 521-5	99
1228	Crystal structures of nucleotide exchange intermediates in the eEF1A-eEF1Balpha complex. <b>2001</b> , 8, 531-4	98
1227	Structure of a human insulin peptide-HLA-DQ8 complex and susceptibility to type 1 diabetes. <b>2001</b> , 2, 501-7	305
1226	Structure of the Rho-activating domain of Escherichia coli cytotoxic necrotizing factor 1. <b>2001</b> , 8, 584-8	84

1225	Structural basis for substrate specificities of cellular deoxyribonucleoside kinases. <b>2001</b> , 8, 616-20	106
1224	Structure of the histone deacetylase SIRT2. <b>2001</b> , 8, 621-5	304
1223	The SAND domain structure defines a novel DNA-binding fold in transcriptional regulation. <b>2001</b> , 8, 626-33	167
1222	Crystal structure and mutational analysis of a perlecan-binding fragment of nidogen-1. <b>2001</b> , 8, 634-40	58
1221	Structure of 4-diphosphocytidyl-2-C- methylerythritol synthetase involved in mevalonate-independent isoprenoid biosynthesis. <b>2001</b> , 8, 641-8	88
1220	Questions about the structure of the botulinum neurotoxin B light chain in complex with a target peptide. <b>2001</b> , 8, 663-4	29
1219	Structure of NaeI-DNA complex reveals dual-mode DNA recognition and complete dimer rearrangement. <b>2001</b> , 8, 665-9	48
1218	Crystal structure of the human ubiquitin conjugating enzyme complex, hMms2-hUbc13. <b>2001</b> , 8, 669-73	130
1217	Structure of beta-lactam synthetase reveals how to synthesize antibiotics instead of asparagine. <b>2001</b> , 8, 684-9	55
1216	X-ray snapshots of serine protease catalysis reveal a tetrahedral intermediate. <b>2001</b> , 8, 689-94	89
1215	The laminin-binding domain of agrin is structurally related to N-TIMP-1. <b>2001</b> , 8, 705-9	38
1214	The crystal structure of MarR, a regulator of multiple antibiotic resistance, at 2.3 Å resolution. <b>2001</b> , 8, 710-4	314
1213	Heterodimeric structure of superoxide dismutase in complex with its metallochaperone. <b>2001</b> , 8, 751-5	231
1212	Structure of the DLM-1-Z-DNA complex reveals a conserved family of Z-DNA-binding proteins. <b>2001</b> , 8, 761-5	203
1211	Crystal structure of the human prion protein reveals a mechanism for oligomerization. <b>2001</b> , 8, 770-4	411
1210	Crystal structure of Mip, a prolyl isomerase from <i>Legionella pneumophila</i> . <b>2001</b> , 8, 779-83	95
1209	Crystal structure of the APC10/DOC1 subunit of the human anaphase-promoting complex. <b>2001</b> , 8, 784-8	72
1208	Crystal structure and functional analysis of the SurE protein identify a novel phosphatase family. <b>2001</b> , 8, 789-94	177

1207	Structure of the rgRGS domain of p115RhoGEF. <b>2001</b> , 8, 805-9	51
1206	Molecular mechanism for dimerization to regulate the catalytic activity of human cytomegalovirus protease. <b>2001</b> , 8, 810-7	42
1205	Structure of a BRCA1-BARD1 heterodimeric RING-RING complex. <b>2001</b> , 8, 833-7	381
1204	Crystal structure of the BRCT repeat region from the breast cancer-associated protein BRCA1. <b>2001</b> , 8, 838-42	201
1203	Arsenate reductase from <i>S. aureus</i> plasmid p1258 is a phosphatase drafted for redox duty. <b>2001</b> , 8, 843-7	80
1202	Crystal structure and kinetic analysis of beta-lactamase inhibitor protein-II in complex with TEM-1 beta-lactamase. <b>2001</b> , 8, 848-52	67
1201	UDP-galactopyranose mutase has a novel structure and mechanism. <b>2001</b> , 8, 858-63	127
1200	Structural insight into Parkinson's disease treatment from drug-inhibited DOPA decarboxylase. <b>2001</b> , 8, 963-7	164
1199	Crystal structures of restrictocin-inhibitor complexes with implications for RNA recognition and base flipping. <b>2001</b> , 8, 968-73	88
1198	Structure of the <i>Yersinia</i> type III secretory system chaperone SycE. <b>2001</b> , 8, 974-8	62
1197	The structure of a Michaelis serpin-protease complex. <b>2001</b> , 8, 979-83	125
1196	Crystal structure of a DinB family error-prone DNA polymerase from <i>Sulfolobus solfataricus</i> . <b>2001</b> , 8, 984-9	148
1195	Structural and biochemical characterization of the type III secretion chaperones CesT and SigE. <b>2001</b> , 8, 1031-6	112
1194	Tcf4 can specifically recognize beta-catenin using alternative conformations. <b>2001</b> , 8, 1048-52	152
1193	Structure of a human Tcf4-beta-catenin complex. <b>2001</b> , 8, 1053-7	158
1192	Structure and autoregulation of the insulin-like growth factor 1 receptor kinase. <b>2001</b> , 8, 1058-63	271
1191	Crystal structure and assembly of a eukaryotic small heat shock protein. <b>2001</b> , 8, 1025-30	579
1190	A novel solenoid fold in the cell wall anchoring domain of the pneumococcal virulence factor LytA. <b>2001</b> , 8, 1020-4	145

1189	Crystal structures of coaxially stacked kissing complexes of the HIV-1 RNA dimerization initiation site. <b>2001</b> , 8, 1064-8	158
1188	Identification of the transmembrane dimer interface of the bovine papillomavirus E5 protein. <b>2001</b> , 20, 3824-34	39
1187	The bacterial conjugation protein TrwB resembles ring helicases and F1-ATPase. <b>2001</b> , 409, 637-41	279
1186	Structural determinants for regulation of phosphodiesterase by a G protein at 2.0 Å. <b>2001</b> , 409, 1071-7	228
1185	A mechanism for initiating RNA-dependent RNA polymerization. <b>2001</b> , 410, 235-40	432
1184	Covalent inhibition revealed by the crystal structure of the caspase-8/p35 complex. <b>2001</b> , 410, 494-7	157
1183	Structural basis for co-stimulation by the human CTLA-4/B7-2 complex. <b>2001</b> , 410, 604-8	266
1182	Crystal structure of the B7-1/CTLA-4 complex that inhibits human immune responses. <b>2001</b> , 410, 608-11	371
1181	Crystal structure of a hairpin ribozyme-inhibitor complex with implications for catalysis. <b>2001</b> , 410, 780-6	402
1180	Crystal structure of an ACh-binding protein reveals the ligand-binding domain of nicotinic receptors. <b>2001</b> , 411, 269-76	1558
1179	Switch-based mechanism of kinesin motors. <b>2001</b> , 411, 439-45	281
1178	Structure of a human gammadelta T-cell antigen receptor. <b>2001</b> , 411, 820-4	204
1177	Crystal structure of a complex of a type IA DNA topoisomerase with a single-stranded DNA molecule. <b>2001</b> , 411, 1077-81	90
1176	Insights into Wnt binding and signalling from the structures of two Frizzled cysteine-rich domains. <b>2001</b> , 412, 86-90	361
1175	Structure of the Ku heterodimer bound to DNA and its implications for double-strand break repair. <b>2001</b> , 412, 607-14	858
1174	Catalysis by hen egg-white lysozyme proceeds via a covalent intermediate. <b>2001</b> , 412, 835-8	520
1173	Prokaryotic origin of the actin cytoskeleton. <b>2001</b> , 413, 39-44	646
1172	Structural basis for the interaction of antibiotics with the peptidyl transferase centre in eubacteria. <b>2001</b> , 413, 814-21	829

1171	Energetic optimization of ion conduction rate by the K <sup>+</sup> selectivity filter. <b>2001</b> , 414, 37-42	660
1170	Chemistry of ion coordination and hydration revealed by a K <sup>+</sup> channel-Fab complex at 2.0 Å resolution. <b>2001</b> , 414, 43-8	1713
1169	Maintenance of an unfolded polypeptide by a cognate chaperone in bacterial type III secretion. <b>2001</b> , 414, 77-81	252
1168	Crystal structure of the tricorn protease reveals a protein disassembly line. <b>2001</b> , 414, 466-70	79
1167	Heterogeneous DNA binding modes of berenil. <b>2001</b> , 1519, 175-84	23
1166	Do bacterial L-asparaginases utilize a catalytic triad Thr-Tyr-Glu?. <b>2001</b> , 1550, 117-28	36
1165	Annexin V--heparin oligosaccharide complex suggests heparan sulfate--mediated assembly on cell surfaces. <b>2001</b> , 9, 57-64	98
1164	Structural basis for inhibition promiscuity of dual specific thrombin and factor Xa blood coagulation inhibitors. <b>2001</b> , 9, 29-37	76
1163	Structure of the globular region of the prion protein Ure2 from the yeast <i>Saccharomyces cerevisiae</i> . <b>2001</b> , 9, 39-46	113
1162	Directed evolution of a new catalytic site in 2-keto-3-deoxy-6-phosphogluconate aldolase from <i>Escherichia coli</i> . <b>2001</b> , 9, 1-9	67
1161	Molecular basis for regulatory subunit diversity in cAMP-dependent protein kinase: crystal structure of the type II beta regulatory subunit. <b>2001</b> , 9, 73-82	122
1160	Crystal structure of phosphoserine phosphatase from <i>Methanococcus jannaschii</i> , a hyperthermophile, at 1.8 Å resolution. <b>2001</b> , 9, 65-71	122
1159	The hydrophobin EAS is largely unstructured in solution and functions by forming amyloid-like structures. <b>2001</b> , 9, 83-91	126
1158	Crystal structure of the 100 kDa arsenite oxidase from <i>Alcaligenes faecalis</i> in two crystal forms at 1.64 Å and 2.03 Å. <b>2001</b> , 9, 125-32	242
1157	Crystal structures of the HslVU peptidase-ATPase complex reveal an ATP-dependent proteolysis mechanism. <b>2001</b> , 9, 177-84	210
1156	Crystal structure of the calcium-loaded spherulin 3a dimer sheds light on the evolution of the eye lens beta-gamma-crystallin domain fold. <b>2001</b> , 9, 115-24	49
1155	Crystal structure of the archaeal holliday junction resolvase Hjc and implications for DNA recognition. <b>2001</b> , 9, 197-204	84
1154	Structural basis of the enhanced stability of a mutant ribozyme domain and a detailed view of RNA--solvent interactions. <b>2001</b> , 9, 221-31	146



1153	Structures of beta-ketoacyl-acyl carrier protein synthase I complexed with fatty acids elucidate its catalytic machinery. <b>2001</b> , 9, 233-43	88
1152	Structure of apoptosis-linked protein ALG-2: insights into Ca <sup>2+</sup> -induced changes in penta-EF-hand proteins. <b>2001</b> , 9, 267-75	65
1151	Crystal structure of <i>Streptococcus mutans</i> pyrophosphatase: a new fold for an old mechanism. <b>2001</b> , 9, 289-97	66
1150	Crystal structures of a novel ferric reductase from the hyperthermophilic archaeon <i>Archaeoglobus fulgidus</i> and its complex with NADP <sup>+</sup> . <b>2001</b> , 9, 311-9	60
1149	The 2.2 Å crystal structure of Hsp33: a heat shock protein with redox-regulated chaperone activity. <b>2001</b> , 9, 367-75	52
1148	X-ray structure of 12-oxophytodienoate reductase 1 provides structural insight into substrate binding and specificity within the family of OYE. <b>2001</b> , 9, 419-29	93
1147	Crystal structure of a novel-type archaeal rubisco with pentagonal symmetry. <b>2001</b> , 9, 473-81	67
1146	Crystal structure of diisopropylfluorophosphatase from <i>Loligo vulgaris</i> . <b>2001</b> , 9, 493-502	99
1145	The kappa-carrageenase of <i>P. carrageenovora</i> features a tunnel-shaped active site: a novel insight in the evolution of Clan-B glycoside hydrolases. <b>2001</b> , 9, 513-25	167
1144	A structural genomics approach to the study of quorum sensing: crystal structures of three LuxS orthologs. <b>2001</b> , 9, 527-37	82
1143	Crystal structure of precorrin-8x methyl mutase. <b>2001</b> , 9, 587-96	30
1142	Crystal structure of the alpha-actinin rod reveals an extensive torsional twist. <b>2001</b> , 9, 597-604	146
1141	Structure of the RGS-like domain from PDZ-RhoGEF: linking heterotrimeric G protein-coupled signaling to Rho GTPases. <b>2001</b> , 9, 559-69	69
1140	Crystal structures of mitochondrial processing peptidase reveal the mode for specific cleavage of import signal sequences. <b>2001</b> , 9, 615-25	183
1139	Crystal structure of methylmalonyl-coenzyme A epimerase from <i>P. shermanii</i> : a novel enzymatic function on an ancient metal binding scaffold. <b>2001</b> , 9, 637-46	53
1138	Crystal structure of maltose phosphorylase from <i>Lactobacillus brevis</i> : unexpected evolutionary relationship with glucoamylases. <b>2001</b> , 9, 689-97	106
1137	Structural basis for allosteric substrate specificity regulation in anaerobic ribonucleotide reductases. <b>2001</b> , 9, 739-50	42
1136	Crystal structure of paromomycin docked into the eubacterial ribosomal decoding A site. <b>2001</b> , 9, 647-58	336

1135	Complex between Peptostreptococcus magnus protein L and a human antibody reveals structural convergence in the interaction modes of Fab binding proteins. <b>2001</b> , 9, 679-87	104
1134	Active transport of an antibiotic rifamycin derivative by the outer-membrane protein FhuA. <b>2001</b> , 9, 707-16	83
1133	Structure of the PPARalpha and -gamma ligand binding domain in complex with AZ 242; ligand selectivity and agonist activation in the PPAR family. <b>2001</b> , 9, 699-706	273
1132	Structure-based development of anticancer drugs: complexes of NAD(P)H:quinone oxidoreductase 1 with chemotherapeutic quinones. <b>2001</b> , 9, 659-67	74
1131	Enzyme mechanism and catalytic property of beta propeller phytase. <b>2001</b> , 9, 851-8	92
1130	The hydroxynitrile lyase from almond: a lyase that looks like an oxidoreductase. <b>2001</b> , 9, 803-15	81
1129	Combined EM/X-ray imaging yields a quasi-atomic model of the adenovirus-related bacteriophage PRD1 and shows key capsid and membrane interactions. <b>2001</b> , 9, 917-30	63
1128	Two polymorphic forms of human histamine methyltransferase: structural, thermal, and kinetic comparisons. <b>2001</b> , 9, 837-49	80
1127	Crystal structure of beta-arrestin at 1.9 A: possible mechanism of receptor binding and membrane Translocation. <b>2001</b> , 9, 869-80	309
1126	Glycerol dehydrogenase. structure, specificity, and mechanism of a family III polyol dehydrogenase. <b>2001</b> , 9, 789-802	90
1125	Crystal structure of bisphosphorylated IGF-1 receptor kinase: insight into domain movements upon kinase activation. <b>2001</b> , 9, 955-65	72
1124	Structure of a conjugating enzyme-ubiquitin thiolester intermediate reveals a novel role for the ubiquitin tail. <b>2001</b> , 9, 897-904	144
1123	The structure of an engineered domain-swapped ribonuclease dimer and its implications for the evolution of proteins toward oligomerization. <b>2001</b> , 9, 967-76	43
1122	Crystal Structure of Imidazole Glycerol Phosphate Synthase. <b>2001</b> , 9, 987-997	91
1121	Getting the adrenaline going: crystal structure of the adrenaline-synthesizing enzyme PNMT. <b>2001</b> , 9, 977-85	54
1120	Crystal structure of transcription factor MalT domain III: a novel helix repeat fold implicated in regulated oligomerization. <b>2001</b> , 9, 1051-60	35
1119	Single-site mutations induce 3D domain swapping in the B1 domain of protein L from Peptostreptococcus magnus. <b>2001</b> , 9, 1017-27	50
1118	Solution structure of the Ras binding domain of the protein kinase Byr2 from Schizosaccharomyces pombe. <b>2001</b> , 9, 1029-41	48

1117	Catalytic mechanisms and reaction intermediates along the hydrolytic pathway of a plant beta-D-glucan glucohydrolase. <b>2001</b> , 9, 1005-16	65
1116	The Ras-Byr2RBD complex: structural basis for Ras effector recognition in yeast. <b>2001</b> , 9, 1043-50	51
1115	Structure of <i>Thermotoga maritima</i> stationary phase survival protein SurE: a novel acid phosphatase. <b>2001</b> , 9, 1095-106	99
1114	The structure of phosphorylated GSK-3beta complexed with a peptide, FRATtide, that inhibits beta-catenin phosphorylation. <b>2001</b> , 9, 1143-52	163
1113	Structure of the universal stress protein of <i>Haemophilus influenzae</i> . <b>2001</b> , 9, 1135-41	80
1112	Specificity in Trk receptor:neurotrophin interactions: the crystal structure of TrkB-d5 in complex with neurotrophin-4/5. <b>2001</b> , 9, 1191-9	79
1111	The 1.6 A crystal structure of <i>E. coli</i> argininosuccinate synthetase suggests a conformational change during catalysis. <b>2001</b> , 9, 1153-64	30
1110	Crystallographic and modeling studies of RNase III suggest a mechanism for double-stranded RNA cleavage. <b>2001</b> , 9, 1225-36	188
1109	Crystal structure of human AUH protein, a single-stranded RNA binding homolog of enoyl-CoA hydratase. <b>2001</b> , 9, 1253-63	27
1108	Promiscuous antigen presentation by the nonclassical MHC Ib Qa-2 is enabled by a shallow, hydrophobic groove and self-stabilized peptide conformation. <b>2001</b> , 9, 1213-24	47
1107	Crystallographic studies on damaged DNAs IV. N(4)-methoxycytosine shows a second face for Watson-Crick base-pairing, leading to purine transition mutagenesis. <b>2001</b> , 29, 3949-54	11
1106	Crystal structure of the macrocycle-forming thioesterase domain of the erythromycin polyketide synthase: versatility from a unique substrate channel. <b>2001</b> , 98, 14808-13	193
1105	The nitrite reductase from <i>Pseudomonas aeruginosa</i> : essential role of two active-site histidines in the catalytic and structural properties. <b>2001</b> , 98, 2232-7	66
1104	Toward a quantum-mechanical description of metal-assisted phosphoryl transfer in pyrophosphatase. <b>2001</b> , 98, 3121-6	89
1103	Structure and function of the C-terminal PABC domain of human poly(A)-binding protein. <b>2001</b> , 98, 4409-13	166
1102	Covalent intermediate trapped in 2-keto-3-deoxy-6-phosphogluconate (KDPG) aldolase structure at 1.95-A resolution. <b>2001</b> , 98, 3679-84	54
1101	X-ray structure of the human hyperplastic discs protein: an ortholog of the C-terminal domain of poly(A)-binding protein. <b>2001</b> , 98, 4414-9	70
1100	Crystal structure of the dimeric extracellular domain of human carbonic anhydrase XII, a bitopic membrane protein overexpressed in certain cancer tumor cells. <b>2001</b> , 98, 9545-50	229

1099	Structural features of an influenza virus promoter and their implications for viral RNA synthesis. <b>2001</b> , 98, 10602-7	72
1098	Identification of the collagen-binding site of the von Willebrand factor A3-domain. <b>2001</b> , 276, 9985-91	70
1097	Substrate and metal complexes of 3-deoxy-D-manno-octulosonate-8-phosphate synthase from <i>Aquifex aeolicus</i> at 1.9-Å resolution. Implications for the condensation mechanism. <b>2001</b> , 276, 8393-402	58
1096	The crystal structure of human placenta growth factor-1 (PlGF-1), an angiogenic protein, at 2.0 Å resolution. <b>2001</b> , 276, 12153-61	84
1095	Crystal structure of a mutant hERα ligand-binding domain reveals key structural features for the mechanism of partial agonism. <b>2001</b> , 276, 15059-65	106
1094	Crystallographic and solution studies of an activation loop mutant of the insulin receptor tyrosine kinase: insights into kinase mechanism. <b>2001</b> , 276, 10049-55	63
1093	Amylosucrase, a glucan-synthesizing enzyme from the alpha-amylase family. <b>2001</b> , 276, 25273-8	121
1092	Crystal structure of <i>Streptococcus pneumoniae</i> N-acetylglucosamine-1-phosphate uridylyltransferase bound to acetyl-coenzyme A reveals a novel active site architecture. <b>2001</b> , 276, 11844-51	79
1091	Alteration of the co-substrate selectivity of deacetoxycephalosporin C synthase. The role of arginine 258. <b>2001</b> , 276, 18290-5	32
1090	Crystal structure of the eosinophil major basic protein at 1.8 Å. An atypical lectin with a paradigm shift in specificity. <b>2001</b> , 276, 26197-203	44
1089	Crystal structure of activated CheY. Comparison with other activated receiver domains. <b>2001</b> , 276, 16425-31	129
1088	Crystalline ligand transitions in lamprey hemoglobin. Structural evidence for the regulation of oxygen affinity. <b>2001</b> , 276, 26230-6	10
1087	The solution structure of the complex formed between alpha-bungarotoxin and an 18-mer cognate peptide derived from the alpha 1 subunit of the nicotinic acetylcholine receptor from <i>Torpedo californica</i> . <b>2001</b> , 276, 22930-40	42
1086	Recombinant mouse muscle adenylosuccinate synthetase: overexpression, kinetics, and crystal structure. <b>2001</b> , 276, 42146-52	16
1085	Structure of crystalline D-Tyr-tRNA(Tyr) deacylase. A representative of a new class of tRNA-dependent hydrolases. <b>2001</b> , 276, 47285-90	47
1084	Mechanism of product chain length determination and the role of a flexible loop in <i>Escherichia coli</i> undecaprenyl-pyrophosphate synthase catalysis. <b>2001</b> , 276, 47474-82	70
1083	Crystal structure of the tumor-promoter okadaic acid bound to protein phosphatase-1. <b>2001</b> , 276, 44078-82	132
1082	Allosteric activation of a spring-loaded natriuretic peptide receptor dimer by hormone. <b>2001</b> , 293, 1657-62	142

1081	Structural and functional analysis of interhelical interactions in the human immunodeficiency virus type 1 gp41 envelope glycoprotein by alanine-scanning mutagenesis. <b>2001</b> , 75, 11146-56	69
1080	An autoinhibitory mechanism for nonsyntaxin SNARE proteins revealed by the structure of Ykt6p. <b>2001</b> , 293, 698-702	110
1079	The crystal structure of the inhibitor-complexed carboxypeptidase D domain II and the modeling of regulatory carboxypeptidases. <b>2001</b> , 276, 16177-84	67
1078	The iota-carrageenase of <i>Alteromonas fortis</i> . A beta-helix fold-containing enzyme for the degradation of a highly polyanionic polysaccharide. <b>2001</b> , 276, 40202-9	62
1077	Crystal structure of a DEAD box protein from the hyperthermophile <i>Methanococcus jannaschii</i> . <b>2001</b> , 98, 1465-70	128
1076	The trimer-of-hairpins motif in membrane fusion: <i>Visna virus</i> . <b>2001</b> , 98, 8502-6	47
1075	Structures of yeast ARF2 and ARL1: distinct roles for the N terminus in the structure and function of ARF family GTPases. <b>2001</b> , 276, 42477-84	51
1074	Structural and functional consequences of altering a peptide MHC anchor residue. <b>2001</b> , 166, 3345-54	95
1073	Urkinase: structure of acetate kinase, a member of the ASKHA superfamily of phosphotransferases. <b>2001</b> , 183, 680-6	90
1072	A new lysozyme fold. Crystal structure of the muramidase from <i>Streptomyces coelicolor</i> at 1.65 Å resolution. <b>2001</b> , 276, 31994-9	55
1071	<i>Bacillus subtilis</i> arsenate reductase is structurally and functionally similar to low molecular weight protein tyrosine phosphatases. <b>2001</b> , 98, 13577-82	70
1070	Anion-mediated Fe <sup>3+</sup> release mechanism in ovotransferrin C-lobe: a structurally identified SO <sub>4</sub> ( <sup>2-</sup> ) binding site and its implications for the kinetic pathway. <b>2001</b> , 276, 35940-6	17
1069	Crystal structures of two closely related but antigenically distinct HLA-A2/melanocyte-melanoma tumor-antigen peptide complexes. <b>2001</b> , 167, 3276-84	73
1068	Structures of trypanothione revealing interaction with trypanothione. <b>2001</b> , 382, 459-71	52
1067	The active N-terminal region of p67phox. Structure at 1.8 Å resolution and biochemical characterizations of the A128V mutant implicated in chronic granulomatous disease. <b>2001</b> , 276, 21627-31	61
1066	The crystallographic structure of the mannitol 2-dehydrogenase NADP <sup>+</sup> binary complex from <i>Agaricus bisporus</i> . <b>2001</b> , 276, 27555-61	49
1065	Biochemical and structural assessment of the 1-N-azasugar GalNAc-isofagomine as a potent family 20 beta-N-acetylhexosaminidase inhibitor. <b>2001</b> , 276, 42131-7	36
1064	Structure of human thymidylate synthase suggests advantages of chemotherapy with noncompetitive inhibitors. <b>2001</b> , 276, 14170-7	62

1063	Subunit-subunit interactions in trimeric arginase. Generation of active monomers by mutation of a single amino acid. <b>2001</b> , 276, 14242-8	41
1062	Biophysical characterization of interactions involving importin-alpha during nuclear import. <b>2001</b> , 276, 34189-98	129
1061	Crystal structures of 1-aminocyclopropane-1-carboxylate (ACC) synthase in complex with aminoethoxyvinylglycine and pyridoxal-5'-phosphate provide new insight into catalytic mechanisms. <b>2001</b> , 276, 38210-6	49
1060	Structure of eicosapentaenoic and linoleic acids in the cyclooxygenase site of prostaglandin endoperoxide H synthase-1. <b>2001</b> , 276, 37547-55	103
1059	Crystal structures of the vitamin D receptor complexed to superagonist 20-epi ligands. <b>2001</b> , 98, 5491-6	211
1058	The 2.0-A crystal structure of tachylectin 5A provides evidence for the common origin of the innate immunity and the blood coagulation systems. <b>2001</b> , 98, 13519-24	124
1057	Interaction of the herbicide glyphosate with its target enzyme 5-enolpyruvylshikimate 3-phosphate synthase in atomic detail. <b>2001</b> , 98, 1376-80	361
1056	Three-dimensional structure of a mammalian thioredoxin reductase: implications for mechanism and evolution of a selenocysteine-dependent enzyme. <b>2001</b> , 98, 9533-8	282
1055	Structural genomics of enzymes involved in sterol/isoprenoid biosynthesis. <b>2001</b> , 98, 12896-901	108
1054	X-ray structures of H5 avian and H9 swine influenza virus hemagglutinins bound to avian and human receptor analogs. <b>2001</b> , 98, 11181-6	371
1053	Structural and mutational studies of the recognition of the arginine tRNA-specific major identity element, A20, by arginyl-tRNA synthetase. <b>2001</b> , 98, 13537-42	41
1052	Crystallographic structures of the ligand-binding domains of the androgen receptor and its T877A mutant complexed with the natural agonist dihydrotestosterone. <b>2001</b> , 98, 4904-9	402
1051	Structure of a multifunctional protein. Mammalian phosphatidylinositol transfer protein complexed with phosphatidylcholine. <b>2001</b> , 276, 9246-52	110
1050	Dimer formation drives the activation of the cell death protease caspase 9. <b>2001</b> , 98, 14250-5	362
1049	Identification, retinoid binding, and x-ray analysis of a human retinol-binding protein. <b>2001</b> , 98, 3710-5	81
1048	Catalytic mechanism of quinoprotein methanol dehydrogenase: A theoretical and x-ray crystallographic investigation. <b>2001</b> , 98, 432-434	64
1047	Structure of trichodiene synthase from <i>Fusarium sporotrichioides</i> provides mechanistic inferences on the terpene cyclization cascade. <b>2001</b> , 98, 13543-8	218
1046	Crystal structure of the SarR protein from <i>Staphylococcus aureus</i> . <b>2001</b> , 98, 6877-82	92

1045	Unusual conformational changes in 6-hydroxymethyl-7,8-dihydropterin pyrophosphokinase as revealed by X-ray crystallography and NMR. <b>2001</b> , 276, 40274-81	32
1044	Structure of the gene 2.5 protein, a single-stranded DNA binding protein encoded by bacteriophage T7. <b>2001</b> , 98, 9557-62	79
1043	Structure of a sialic acid-activating synthetase, CMP-acylneuraminate synthetase in the presence and absence of CDP. <b>2001</b> , 276, 8190-6	48
1042	RNA tertiary interactions in the large ribosomal subunit: the A-minor motif. <b>2001</b> , 98, 4899-903	564
1041	Recruitment of the transcriptional machinery through GAL11P: structure and interactions of the GAL4 dimerization domain. <b>2001</b> , 15, 1007-20	36
1040	Glycosaminoglycan binding properties of the myxoma virus CC-chemokine inhibitor, M-T1. <b>2001</b> , 276, 30504-13	41
1039	Crystal structure at 1.5-Å resolution of <i>Pyrus pyrifolia</i> pistil ribonuclease responsible for gametophytic self-incompatibility. <b>2001</b> , 276, 45261-9	50
1038	Dynamic properties of the Ras switch I region and its importance for binding to effectors. <b>2001</b> , 98, 4944-9	245
1037	The FadR-DNA complex. Transcriptional control of fatty acid metabolism in <i>Escherichia coli</i> . <b>2001</b> , 276, 17373-9	102
1036	Crystal structure of the CCAAT box/enhancer-binding protein beta activating transcription factor-4 basic leucine zipper heterodimer in the absence of DNA. <b>2001</b> , 276, 505-13	61
1035	A novel snare N-terminal domain revealed by the crystal structure of Sec22b. <b>2001</b> , 276, 24203-11	68
1034	X-ray structure of sensory rhodopsin II at 2.1-Å resolution. <b>2001</b> , 98, 10131-6	263
1033	Crystal structure of the Holliday junction migration motor protein RuvB from <i>Thermus thermophilus</i> HB8. <b>2001</b> , 98, 1442-1447	73
1032	X-ray analysis of an RNA tetraplex (UGGGU) <sub>4</sub> with divalent Sr <sup>2+</sup> ions at subatomic resolution (0.61 Å). <b>2001</b> , 98, 13665-70	135
1031	X-ray crystal structure of the trimeric N-terminal domain of gephyrin. <b>2001</b> , 276, 25294-301	70
1030	Structural basis for fibroblast growth factor receptor 2 activation in Apert syndrome. <b>2001</b> , 98, 7182-7	168
1029	Structure of rat BCKD kinase: nucleotide-induced domain communication in a mitochondrial protein kinase. <b>2001</b> , 98, 11218-23	68
1028	Crystallographic evidence for substrate-assisted catalysis in a bacterial beta-hexosaminidase. <b>2001</b> , 276, 10330-7	211

1027	Structural basis for the thioredoxin-like activity profile of the glutaredoxin-like NrdH-redoxin from <i>Escherichia coli</i> . <b>2001</b> , 276, 35836-41	39
1026	Structure of the yeast ribonucleotide reductase Y2Y4 heterodimer. <b>2001</b> , 98, 10073-8	49
1025	Crystal structure of the human CD4 N-terminal two-domain fragment complexed to a class II MHC molecule. <b>2001</b> , 98, 10799-804	193
1024	Crystal structure of the <i>Mycobacterium tuberculosis</i> beta-ketoacyl-acyl carrier protein synthase III. <b>2001</b> , 276, 20516-22	88
1023	Structural analyses of a malate dehydrogenase with a variable active site. <b>2001</b> , 276, 31156-62	24
1022	Structure of the bound dioxygen species in the cytochrome oxidase reaction of cytochrome cd1 nitrite reductase. <b>2001</b> , 276, 13072-6	33
1021	Life on carbon monoxide: X-ray structure of <i>Rhodospirillum rubrum</i> Ni-Fe-S carbon monoxide dehydrogenase. <b>2001</b> , 98, 11973-8	249
1020	Crystal structure of the ectodomain of Methuselah, a <i>Drosophila</i> G protein-coupled receptor associated with extended lifespan. <b>2001</b> , 98, 3744-9	57
1019	Structure of the induced antibacterial protein from tasar silkworm, <i>Antheraea mylitta</i> . Implications to molecular evolution. <b>2001</b> , 276, 41377-82	24
1018	Crystal structure of the ligand-binding domain of the ultraspiracle protein USP, the ortholog of retinoid X receptors in insects. <b>2001</b> , 276, 7465-74	143
1017	Structural basis for Ni(2+) transport and assembly of the urease active site by the metallochaperone UreE from <i>Bacillus pasteurii</i> . <b>2001</b> , 276, 49365-70	68
1016	Crystal structure of an anticoagulant protein in complex with the Gla domain of factor X. <b>2001</b> , 98, 7230-4	125
1015	Structural basis for the activation of human procaspase-7. <b>2001</b> , 98, 14790-5	188
1014	Crystal structure of MtaN, a global multidrug transporter gene activator. <b>2001</b> , 276, 47178-84	58
1013	Three molecules of ubiquinone bind specifically to mitochondrial cytochrome bc1 complex. <b>2001</b> , 276, 35231-4	54
1012	Crystal structure of the complex of plasminogen activator inhibitor 2 with a peptide mimicking the reactive center loop. <b>2001</b> , 276, 43374-82	20
1011	Probing the open state of cytochrome P450cam with ruthenium-linker substrates. <b>2001</b> , 98, 12420-5	93
1010	The crystal structures of Apo and complexed <i>Saccharomyces cerevisiae</i> GNA1 shed light on the catalytic mechanism of an amino-sugar N-acetyltransferase. <b>2001</b> , 276, 16328-34	65



1009	Structural basis for the recognition of isoleucyl-adenylate and an antibiotic, mupirocin, by isoleucyl-tRNA synthetase. <b>2001</b> , 276, 47387-93	137
1008	Electron tunneling in protein crystals. <b>2001</b> , 98, 5002-6	114
1007	Side-chain repacking calculations for predicting structures and stabilities of heterodimeric coiled coils. <b>2001</b> , 98, 14825-30	73
1006	Crystal structure and substrate binding modeling of the uroporphyrinogen-III decarboxylase from <i>Nicotiana tabacum</i> . Implications for the catalytic mechanism. <b>2001</b> , 276, 44108-16	42
1005	alpha-Lactalbumin (LA) stimulates milk beta-1,4-galactosyltransferase I (beta 4Gal-T1) to transfer glucose from UDP-glucose to N-acetylglucosamine. Crystal structure of beta 4Gal-T1 x LA complex with UDP-Glc. <b>2001</b> , 276, 37665-71	97
1004	The NMR structure of the 47-kDa dimeric enzyme 3,4-dihydroxy-2-butanone-4-phosphate synthase and ligand binding studies reveal the location of the active site. <b>2001</b> , 98, 13025-30	29
1003	Crystal structure of human PEDF, a potent anti-angiogenic and neurite growth-promoting factor. <b>2001</b> , 98, 11131-5	100
1002	Insights into ligand binding and catalysis of a central step in NAD <sup>+</sup> synthesis: structures of <i>Methanobacterium thermoautotrophicum</i> NMN adenylyltransferase complexes. <b>2001</b> , 276, 7225-32	39
1001	Structure of pyruvate dehydrogenase kinase. Novel folding pattern for a serine protein kinase. <b>2001</b> , 276, 37443-50	72
1000	Glutamate 170 of human l-3-hydroxyacyl-CoA dehydrogenase is required for proper orientation of the catalytic histidine and structural integrity of the enzyme. <b>2001</b> , 276, 36718-26	30
999	Structure of a quinoxinoprotein amine dehydrogenase with an uncommon redox cofactor and highly unusual crosslinking. <b>2001</b> , 98, 14268-73	121
998	The crystal structure of a heptameric archaeal Sm protein: Implications for the eukaryotic snRNP core. <b>2001</b> , 98, 5532-7	91
997	Crystal structure of thermostable DNA photolyase: pyrimidine-dimer recognition mechanism. <b>2001</b> , 98, 13560-5	100
996	Structure of a flavin-binding plant photoreceptor domain: insights into light-mediated signal transduction. <b>2001</b> , 98, 2995-3000	430
995	Crystal structure of the quorum-sensing protein LuxS reveals a catalytic metal site. <b>2001</b> , 98, 11169-74	91
994	Chicken avidin exhibits pseudo-catalytic properties. Biochemical, structural, and electrostatic consequences. <b>2001</b> , 276, 32031-9	22
993	Crystal structure of paprika ferredoxin-NADP <sup>+</sup> reductase. Implications for the electron transfer pathway. <b>2001</b> , 276, 9253-63	30
992	The role of Asn14 in the stability and conformation of the reactive-site loop of winged bean chymotrypsin inhibitor: crystal structures of two point mutants Asn14-->Lys and Asn14-->Asp. <b>2001</b> , 14, 349-57	13

991	Crystal structure of fibroblast growth factor 9 reveals regions implicated in dimerization and autoinhibition. <b>2001</b> , 276, 4322-9	53
990	A 1.2-A snapshot of the final step of bacterial cell wall biosynthesis. <b>2001</b> , 98, 1427-31	105
989	Structure of the human 3alpha-hydroxysteroid dehydrogenase type 3 in complex with testosterone and NADP at 1.25-A resolution. <b>2001</b> , 276, 42091-8	45
988	The structure of a human type III Fcgamma receptor in complex with Fc. <b>2001</b> , 276, 16469-77	286
987	A beta -hairpin structure in a 13-mer peptide that binds alpha -bungarotoxin with high affinity and neutralizes its toxicity. <b>2001</b> , 98, 6629-34	60
986	Crystal structure of PBP2x from a highly penicillin-resistant <i>Streptococcus pneumoniae</i> clinical isolate: a mosaic framework containing 83 mutations. <b>2001</b> , 276, 45106-12	99
985	The three-dimensional structure of cystathionine beta-lyase from <i>Arabidopsis</i> and its substrate specificity. <b>2001</b> , 126, 631-42	43
984	Oxygen access to the active site of cholesterol oxidase through a narrow channel is gated by an Arg-Glu pair. <b>2001</b> , 276, 30435-41	86
983	Structural and mutational analysis of the PhoQ histidine kinase catalytic domain. Insight into the reaction mechanism. <b>2001</b> , 276, 41182-90	98
982	Self-association of the H3 region of syntaxin 1A. Implications for intermediates in SNARE complex assembly. <b>2001</b> , 276, 13273-82	48
981	Mutational and X-ray crystallographic analysis of the interaction of dihomo-gamma -linolenic acid with prostaglandin endoperoxide H synthases. <b>2001</b> , 276, 10358-65	42
980	Crystal structure of Sar1-GDP at 1.7 A resolution and the role of the NH2 terminus in ER export. <b>2001</b> , 155, 937-48	133
979	Calpain mutants with increased Ca <sup>2+</sup> sensitivity and implications for the role of the C(2)-like domain. <b>2001</b> , 276, 7404-7	43
978	Dissection of a nuclear localization signal. <b>2001</b> , 276, 1317-25	251
977	The Structure of an alternative form of <i>Paracoccus pantotrophus</i> cytochrome cd(1) nitrite reductase. <b>2001</b> , 276, 29450-5	25
976	Crystal structure of sensory rhodopsin II at 2.4 angstroms: insights into color tuning and transducer interaction. <b>2001</b> , 293, 1499-503	34 <sup>o</sup>
975	Crystal structure of Lyme disease antigen outer surface protein C from <i>Borrelia burgdorferi</i> . <b>2001</b> , 276, 10010-5	71
974	Conversion of monomeric protein L to an obligate dimer by computational protein design. <b>2001</b> , 98, 10687-91	62

973	Crystal structure of the precursor of galactose oxidase: an unusual self-processing enzyme. <b>2001</b> , 98, 12932-7	97
972	Preparation and crystal structure of the recombinant alpha(1)/alpha(2) catalytic heterodimer of bovine brain platelet-activating factor acetylhydrolase Ib. <b>2001</b> , 14, 513-9	16
971	Structure and site-directed mutagenesis of a flavoprotein from <i>Escherichia coli</i> that reduces nitrocompounds: alteration of pyridine nucleotide binding by a single amino acid substitution. <b>2001</b> , 276, 2816-23	76
970	The potency and specificity of the interaction between the IA3 inhibitor and its target aspartic proteinase from <i>Saccharomyces cerevisiae</i> . <b>2001</b> , 276, 2023-30	30
969	Three-dimensional structure of human follicle-stimulating hormone. <b>2001</b> , 15, 378-89	205
968	Interaction between Ran and Mog1 is required for efficient nuclear protein import. <b>2001</b> , 276, 41255-62	23
967	T cell activity correlates with oligomeric peptide-major histocompatibility complex binding on T cell surface. <b>2001</b> , 276, 47320-8	16
966	Conformational changes in four regions of the <i>Escherichia coli</i> ArsA ATPase link ATP hydrolysis to ion translocation. <b>2001</b> , 276, 30414-22	34
965	Functional equality in the absence of structural similarity: an added dimension to molecular mimicry. <b>2001</b> , 276, 39277-81	35
964	Structure of neurolysin reveals a deep channel that limits substrate access. <b>2001</b> , 98, 3127-32	109
963	Crystal structure of the C-type lectin-like domain from the human hematopoietic cell receptor CD69. <b>2001</b> , 276, 7312-9	63
962	The structure of the ultraspiracle ligand-binding domain reveals a nuclear receptor locked in an inactive conformation. <b>2001</b> , 98, 1549-1554	135
961	Crystal structure of a recombinant anti-estradiol Fab fragment in complex with 17beta -estradiol. <b>2001</b> , 276, 36687-94	25
960	Crystal structure of the mouse p53 core DNA-binding domain at 2.7 A resolution. <b>2001</b> , 276, 12120-7	70
959	Structural determinants of ligand binding selectivity between the peroxisome proliferator-activated receptors. <b>2001</b> , 98, 13919-24	461
958	Crystal structure of <i>Klebsiella aerogenes</i> UreE, a nickel-binding metallochaperone for urease activation. <b>2001</b> , 276, 49359-64	77
957	Crystal structure of the CheA histidine phosphotransfer domain that mediates response regulator phosphorylation in bacterial chemotaxis. <b>2001</b> , 276, 31074-82	71
956	The structure of the T127L/S128A mutant of cAMP receptor protein facilitates promoter site binding. <b>2001</b> , 276, 11230-6	18

955	Immunocytochemical localization and crystal structure of human frequenin (neuronal calcium sensor 1). <b>2001</b> , 276, 11949-55	154
954	A crystallographic map of the transition from B-DNA to A-DNA. <b>2001</b> , 98, 7265-70	99
953	Dissection of the regional roles of the archaeal Holliday junction resolvase Hjc by structural and mutational analyses. <b>2001</b> , 276, 35735-40	17
952	Antigen presentation subverted: Structure of the human cytomegalovirus protein US2 bound to the class I molecule HLA-A2. <b>2001</b> , 98, 6794-9	129
951	Active site of chondroitin AC lyase revealed by the structure of enzyme-oligosaccharide complexes and mutagenesis. <b>2001</b> , 40, 2359-72	70
950	Porcine carbonyl reductase. structural basis for a functional monomer in short chain dehydrogenases/reductases. <b>2001</b> , 276, 18457-63	76
949	Hormone selectivity in thyroid hormone receptors. <b>2001</b> , 15, 398-410	137
948	BeF(3)(-) acts as a phosphate analog in proteins phosphorylated on aspartate: structure of a BeF(3)(-) complex with phosphoserine phosphatase. <b>2001</b> , 98, 8525-30	117
947	NMR study of a heterochiral DNA hairpin: impact of L-enantiomery in the loop. <b>2001</b> , 19, 459-70	3
946	Crystal structure of the extracellular segment of integrin alpha Vbeta3. <b>2001</b> , 294, 339-45	1086
945	Crystal structure of cytochrome P450 14alpha -sterol demethylase (CYP51) from Mycobacterium tuberculosis in complex with azole inhibitors. <b>2001</b> , 98, 3068-73	456
944	Observation of covalent intermediates in an enzyme mechanism at atomic resolution. <b>2001</b> , 294, 369-74	251
943	Enzyme-substrate interactions in the purine-specific nucleoside hydrolase from Trypanosoma vivax. <b>2002</b> , 277, 15938-46	44
942	Effects of deletion of streptokinase residues 48-59 on plasminogen activation. <b>2002</b> , 15, 753-61	27
941	The atomic structure of adeno-associated virus (AAV-2), a vector for human gene therapy. <b>2002</b> , 99, 10405-10	443
940	The mechanism of topoisomerase I poisoning by a camptothecin analog. <b>2002</b> , 99, 15387-92	618
939	Subunit association and conformational flexibility in the head subdomain of human CD81 large extracellular loop. <b>2002</b> , 383, 1447-52	42
938	Structural basis for the modulation of lignin monomer methylation by caffeic acid/5-hydroxyferulic acid 3/5-O-methyltransferase. <b>2002</b> , 14, 1265-77	183

937	Crystal structure of the Bse634I restriction endonuclease: comparison of two enzymes recognizing the same DNA sequence. <b>2002</b> , 30, 876-85	52
936	The xenograft antigen bound to Griffonia simplicifolia lectin 1-B(4). X-ray crystal structure of the complex and molecular dynamics characterization of the binding site. <b>2002</b> , 277, 6615-21	52
935	The solution structures of the human beta-defensins lead to a better understanding of the potent bactericidal activity of HBD3 against Staphylococcus aureus. <b>2002</b> , 277, 8279-89	282
934	Ligand exchange between proteins. Exchange of biotin and biotin derivatives between avidin and streptavidin. <b>2002</b> , 277, 30892-900	60
933	The two GAF domains in phosphodiesterase 2A have distinct roles in dimerization and in cGMP binding. <b>2002</b> , 99, 13260-5	219
932	Crystal structures of the semireduced and inhibitor-bound forms of cyclic nucleotide phosphodiesterase from Arabidopsis thaliana. <b>2002</b> , 277, 1419-25	23
931	IMP, GTP, and 6-phosphoryl-IMP complexes of recombinant mouse muscle adenylosuccinate synthetase. <b>2002</b> , 277, 26779-87	23
930	Smad3 allostery links TGF-beta receptor kinase activation to transcriptional control. <b>2002</b> , 16, 1950-63	108
929	X-ray crystallographic structures of the Escherichia coli periplasmic protein FhuD bound to hydroxamate-type siderophores and the antibiotic albomycin. <b>2002</b> , 277, 13966-72	114
928	Twists and turns of the cation-dependent mannose 6-phosphate receptor. Ligand-bound versus ligand-free receptor. <b>2002</b> , 277, 10156-61	39
927	Crystallographic and biochemical studies of DivK reveal novel features of an essential response regulator in Caulobacter crescentus. <b>2002</b> , 277, 42003-10	22
926	Evidence for plasticity and structural mimicry at the immunoglobulin light chain-protein L interface. <b>2002</b> , 277, 47500-6	33
925	Structural conservation between the actin monomer-binding sites of twinfilin and actin-depolymerizing factor (ADF)/cofilin. <b>2002</b> , 277, 43089-95	41
924	The structure of human prokallikrein 6 reveals a novel activation mechanism for the kallikrein family. <b>2002</b> , 277, 27273-81	64
923	PDZ7 of glutamate receptor interacting protein binds to its target via a novel hydrophobic surface area. <b>2002</b> , 277, 41140-6	28
922	NAD binding induces conformational changes in Rho ADP-ribosylating clostridium botulinum C3 exoenzyme. <b>2002</b> , 277, 30950-7	57
921	The crystal structure of Helicobacter pylori cysteine-rich protein B reveals a novel fold for a penicillin-binding protein. <b>2002</b> , 277, 10187-93	33
920	Solution structure of peptide toxins that block mechanosensitive ion channels. <b>2002</b> , 277, 34443-50	82

919	Crystal structure of the anticoagulant slow form of thrombin. <b>2002</b> , 277, 40177-80	44
918	Structures of nitroreductase in three states: effects of inhibitor binding and reduction. <b>2002</b> , 277, 11513-20	109
917	Crystal structure of ClpA, an Hsp100 chaperone and regulator of ClpAP protease. <b>2002</b> , 277, 46743-52	172
916	Structure of equine infectious anemia virus matrix protein. <b>2002</b> , 76, 1876-83	37
915	Three-dimensional structure of the amino-terminal domain of syntaxin 6, a SNAP-25 C homolog. <b>2002</b> , 99, 9184-9	50
914	Improving nucleoside diphosphate kinase for antiviral nucleotide analogs activation. <b>2002</b> , 277, 39953-9	23
913	Precursor structure of cephalosporin acylase. Insights into autoproteolytic activation in a new N-terminal hydrolase family. <b>2002</b> , 277, 2823-9	47
912	Structural studies of allelic diversity of the MHC class I homolog MIC-B, a stress-inducible ligand for the activating immunoreceptor NKG2D. <b>2002</b> , 169, 1395-400	47
911	An approach to membrane protein structure without crystals. <b>2002</b> , 99, 14037-40	88
910	Crystal structure of quinohemoprotein alcohol dehydrogenase from <i>Comamonas testosteroni</i> : structural basis for substrate oxidation and electron transfer. <b>2002</b> , 277, 3727-32	63
909	The crystal structure of the allosteric non-phosphorylating glyceraldehyde-3-phosphate dehydrogenase from the hyperthermophilic archaeum <i>Thermoproteus tenax</i> . <b>2002</b> , 277, 19938-45	28
908	Structural basis for activation of fibroblast growth factor signaling by sucrose octasulfate. <b>2002</b> , 22, 7184-92	46
907	The crystal structure of <i>Mycobacterium tuberculosis</i> alkylhydroperoxidase AhpD, a potential target for antitubercular drug design. <b>2002</b> , 277, 20033-40	36
906	Structural and functional role of threonine 112 in a superantigen <i>Staphylococcus aureus</i> enterotoxin B. <b>2002</b> , 277, 2756-62	12
905	The crystal structure of the C-terminal fragment of striated-muscle alpha-tropomyosin reveals a key troponin T recognition site. <b>2002</b> , 99, 7378-83	84
904	BAG4/SODD protein contains a short BAG domain. <b>2002</b> , 277, 31172-8	43
903	Structural features of cytochrome c' folding intermediates revealed by fluorescence energy-transfer kinetics. <b>2002</b> , 99, 14778-82	43
902	A structural basis for the activity of retro-Diels-Alder catalytic antibodies: evidence for a catalytic aromatic residue. <b>2002</b> , 99, 9674-8	31

8901	The crystal structure of exonuclease RecJ bound to Mn <sup>2+</sup> ion suggests how its characteristic motifs are involved in exonuclease activity. <b>2002</b> , 99, 5908-12	69
8900	The molecular mechanism of multidrug resistance by the Q151M human immunodeficiency virus type 1 reverse transcriptase and its suppression using alpha-boranophosphate nucleotide analogues. <b>2002</b> , 277, 42097-104	81
899	Alternate interactions define the binding of peptides to the MHC molecule IA(b). <b>2002</b> , 99, 8820-5	67
898	Orientation of bound ligands in mannose-binding proteins. Implications for multivalent ligand recognition. <b>2002</b> , 277, 16088-95	77
897	Crystal structure of human L-isopartyl methyltransferase. <b>2002</b> , 277, 10642-6	20
896	The structure and evolution of the major capsid protein of a large, lipid-containing DNA virus. <b>2002</b> , 99, 14758-63	207
895	Structural views of the ligand-binding cores of a metabotropic glutamate receptor complexed with an antagonist and both glutamate and Gd <sup>3+</sup> . <b>2002</b> , 99, 2660-5	304
894	Functional role of internal water molecules in rhodopsin revealed by X-ray crystallography. <b>2002</b> , 99, 5982-7	650
893	A clogged gutter mechanism for protease inhibitors. <b>2002</b> , 99, 10316-21	116
892	Solution structure of human GABA(A) receptor-associated protein GABARAP: implications for biological function and its regulation. <b>2002</b> , 277, 13363-6	56
891	Three-dimensional structure of human gamma -glutamyl hydrolase. A class I glutamine amidotransferase adapted for a complex substrate. <b>2002</b> , 277, 24522-9	21
890	Structure of the GCN5 histone acetyltransferase bound to a bisubstrate inhibitor. <b>2002</b> , 99, 14065-70	95
889	Determination of the structure of a decay accelerating factor-binding clinical isolate of echovirus 11 allows mapping of mutants with altered receptor requirements for infection. <b>2002</b> , 76, 7694-704	44
888	Crystal structure of Lyme disease variable surface antigen VlsE of <i>Borrelia burgdorferi</i> . <b>2002</b> , 277, 21691-6	104
887	Structure of the globular tail of nuclear lamin. <b>2002</b> , 277, 17381-4	194
886	The X-ray crystal structure and putative ligand-derived peptide binding properties of gamma-aminobutyric acid receptor type A receptor-associated protein. <b>2002</b> , 277, 5556-61	57
885	Structure of the full-length HPr kinase/phosphatase from <i>Staphylococcus xylosum</i> at 1.95 Å resolution: Mimicking the product/substrate of the phospho transfer reactions. <b>2002</b> , 99, 3458-63	41
884	Protein and ligand dynamics in 4-hydroxybenzoate hydroxylase. <b>2002</b> , 99, 608-13	90

883	Isolectins I-A and I-B of <i>Griffonia (Bandeiraea) simplicifolia</i> . Crystal structure of metal-free GS I-B(4) and molecular basis for metal binding and monosaccharide specificity. <b>2002</b> , 277, 6608-14	44
882	Hinge-bending motion of D-allose-binding protein from <i>Escherichia coli</i> : three open conformations. <b>2002</b> , 277, 14077-84	61
881	Structure of the single-strand annealing domain of human RAD52 protein. <b>2002</b> , 99, 13492-7	175
880	Crystal structure of OxyB, a cytochrome P450 implicated in an oxidative phenol coupling reaction during vancomycin biosynthesis. <b>2002</b> , 277, 47476-85	111
879	Structure of HIV-2 reverse transcriptase at 2.35-Å resolution and the mechanism of resistance to non-nucleoside inhibitors. <b>2002</b> , 99, 14410-5	146
878	The crystal structure of metal-free human EF-hand protein S100A3 at 1.7-Å resolution. <b>2002</b> , 277, 33092-8	39
877	Leukotriene A4 hydrolase: selective abrogation of leukotriene B4 formation by mutation of aspartic acid 375. <b>2002</b> , 99, 4215-20	37
876	Structural basis for the NAD-dependent deacetylase mechanism of Sir2. <b>2002</b> , 277, 34489-98	77
875	Crystal structure of NC1 domains. Structural basis for type IV collagen assembly in basement membranes. <b>2002</b> , 277, 31142-53	125
874	X-ray structure of a neuronal complexin-SNARE complex from squid. <b>2002</b> , 277, 26517-23	93
873	Protein structure elucidation from NMR proton densities. <b>2002</b> , 99, 6713-8	34
872	Aspartate 313 in the <i>Streptomyces plicatus</i> hexosaminidase plays a critical role in substrate-assisted catalysis by orienting the 2-acetamido group and stabilizing the transition state. <b>2002</b> , 277, 40055-65	108
871	Distinct dimer interaction and regulation in nitric-oxide synthase types I, II, and III. <b>2002</b> , 277, 31020-30	101
870	Interactions causing the kinetic trap in serpin protein folding. <b>2002</b> , 277, 46347-54	54
869	Structure of spinach chloroplast F1-ATPase complexed with the phytopathogenic inhibitor tentoxin. <b>2002</b> , 99, 3464-8	52
868	Crystal structure of calcineurin-cyclophilin-cyclosporin shows common but distinct recognition of immunophilin-drug complexes. <b>2002</b> , 99, 12037-42	221
867	Subcloning, expression, purification, and characterization of recombinant human leptin-binding domain. <b>2002</b> , 277, 46304-9	49
866	Structure and flexibility of <i>Streptococcus agalactiae</i> hyaluronate lyase complex with its substrate. Insights into the mechanism of processive degradation of hyaluronan. <b>2002</b> , 277, 36678-88	63



865	Comparison of the crystal structures of the human manganese superoxide dismutase and the homologous <i>Aspergillus fumigatus</i> allergen at 2-A resolution. <b>2002</b> , 168, 1267-72	67
864	High resolution crystal structures of the wild type and Cys-55-->Ser and Cys-59-->Ser variants of the thioredoxin-like [2Fe-2S] ferredoxin from <i>Aquifex aeolicus</i> . <b>2002</b> , 277, 34499-507	28
863	Cosolvent-induced transformation of a death domain tertiary structure. <b>2002</b> , 99, 11151-6	10
862	Crystal structure of human sex hormone-binding globulin in complex with 2-methoxyestradiol reveals the molecular basis for high affinity interactions with C-2 derivatives of estradiol. <b>2002</b> , 277, 45219-25	28
861	X-ray structure of a bifunctional protein kinase in complex with its protein substrate HPr. <b>2002</b> , 99, 13437-41	69
860	Closed site complexes of adenine phosphoribosyltransferase from <i>Giardia lamblia</i> reveal a mechanism of ribosyl migration. <b>2002</b> , 277, 39981-8	31
859	Structure of <i>Penicillium citrinum</i> alpha 1,2-mannosidase reveals the basis for differences in specificity of the endoplasmic reticulum and Golgi class I enzymes. <b>2002</b> , 277, 5620-30	41
858	Crystal structure of the DNA-binding domain from Ndt80, a transcriptional activator required for meiosis in yeast. <b>2002</b> , 99, 14041-6	37
857	Specificity of RNA-RNA helix recognition. <b>2002</b> , 99, 11676-81	83
856	Cyclomaltodextrinase, neopullulanase, and maltogenic amylase are nearly indistinguishable from each other. <b>2002</b> , 277, 21891-7	120
855	Structural genomics of the <i>Thermotoga maritima</i> proteome implemented in a high-throughput structure determination pipeline. <b>2002</b> , 99, 11664-9	381
854	Structure of human chitotriosidase. Implications for specific inhibitor design and function of mammalian chitinase-like lectins. <b>2002</b> , 277, 25537-44	163
853	Prediction of novel Bag-1 homologs based on structure/function analysis identifies Snl1p as an Hsp70 co-chaperone in <i>Saccharomyces cerevisiae</i> . <b>2002</b> , 277, 33220-7	65
852	Structural basis for the guanine nucleotide-binding activity of tissue transglutaminase and its regulation of transamidation activity. <b>2002</b> , 99, 2743-7	277
851	Structural basis of transcription activation: the CAP-alpha CTD-DNA complex. <b>2002</b> , 297, 1562-6	197
850	GLFG and FxFG nucleoporins bind to overlapping sites on importin-beta. <b>2002</b> , 277, 50597-606	173
849	Epitope recognition by diverse antibodies suggests conformational convergence in an antibody response. <b>2002</b> , 168, 2371-82	72
848	Structure of the 53BP1 BRCT region bound to p53 and its comparison to the Brca1 BRCT structure. <b>2002</b> , 16, 583-93	171

847	Mechanism of action and NAD <sup>+</sup> -binding mode revealed by the crystal structure of L-histidinol dehydrogenase. <b>2002</b> , 99, 1859-64	45
846	The crystal structure and mutational analysis of a novel RNA-binding domain found in the human Tap nuclear mRNA export factor. <b>2002</b> , 99, 1888-93	25
845	Crystal structure of the yeast cytochrome bc <sub>1</sub> complex with its bound substrate cytochrome c. <b>2002</b> , 99, 2800-5	316
844	Solution structures of the cytoplasmic tail complex from platelet integrin alpha IIb- and beta 3-subunits. <b>2002</b> , 99, 5878-83	91
843	All intermediates of the arsenate reductase mechanism, including an intramolecular dynamic disulfide cascade. <b>2002</b> , 99, 8506-11	65
842	Crystal structure of conserved hypothetical protein Aq1575 from Aquifex aeolicus. <b>2002</b> , 99, 7980-5	28
841	Using deeply trapped intermediates to map the cytochrome c folding landscape. <b>2002</b> , 99, 8626-30	40
840	Crystal structure of DhbE, an archetype for aryl acid activating domains of modular nonribosomal peptide synthetases. <b>2002</b> , 99, 12120-5	231
839	Structure of factor-inhibiting hypoxia-inducible factor 1: An asparaginyl hydroxylase involved in the hypoxic response pathway. <b>2002</b> , 99, 15351-6	162
838	Solution structure and dynamics of the outer membrane enzyme PagP by NMR. <b>2002</b> , 99, 13560-5	282
837	Short constrained peptides that inhibit HIV-1 entry. <b>2002</b> , 99, 14664-9	176
836	Bornyl diphosphate synthase: structure and strategy for carbocation manipulation by a terpenoid cyclase. <b>2002</b> , 99, 15375-80	232
835	A helical region in the C terminus of small-conductance Ca <sup>2+</sup> -activated K <sup>+</sup> channels controls assembly with apo-calmodulin. <b>2002</b> , 277, 4558-64	34
834	The crystal structure and mechanism of 1-L-myo-inositol- 1-phosphate synthase. <b>2002</b> , 277, 9484-91	47
833	Conjugative plasmid protein TrwB, an integral membrane type IV secretion system coupling protein. Detailed structural features and mapping of the active site cleft. <b>2002</b> , 277, 7556-66	63
832	Solution structure and dynamics of the lipoic acid-bearing domain of human mitochondrial branched-chain alpha-keto acid dehydrogenase complex. <b>2002</b> , 277, 15865-73	24
831	Crystal structure of beta 1,3-glucuronyltransferase I in complex with active donor substrate UDP-GlcUA. <b>2002</b> , 277, 21869-73	63
830	Investigation of the roles of catalytic residues in serotonin N-acetyltransferase. <b>2002</b> , 277, 18118-26	55

829	X-ray structure of a serine protease acyl-enzyme complex at 0.95-Å resolution. <b>2002</b> , 277, 21962-70	53
828	Crystal structure of Haemophilus influenzae NadR protein. A bifunctional enzyme endowed with NMN adenylyltransferase and ribosylnicotinamide kinase activities. <b>2002</b> , 277, 33291-9	39
827	Characterization of the conserved interaction between GATA and FOG family proteins. <b>2002</b> , 277, 35720-9	20
826	Molecular basis for the local conformational rearrangement of human phosphoserine phosphatase. <b>2002</b> , 277, 46651-8	31
825	Feedback inhibition and product complexes of recombinant mouse muscle adenylosuccinate synthetase. <b>2002</b> , 277, 40536-43	10
824	Crystal structure of SEDL and its implications for a genetic disease spondyloepiphyseal dysplasia tarda. <b>2002</b> , 277, 49863-9	64
823	Acyl-intermediate structures of the extended-spectrum class A beta-lactamase, Toho-1, in complex with cefotaxime, cephalothin, and benzylpenicillin. <b>2002</b> , 277, 46601-8	88
822	Crystal structure of the heterodimeric complex of the adaptor, ClpS, with the N-domain of the AAA+ chaperone, ClpA. <b>2002</b> , 277, 46753-62	83
821	An alanine-zipper structure determined by long range intermolecular interactions. <b>2002</b> , 277, 48708-13	14
820	Crystal structure of venus, a yellow fluorescent protein with improved maturation and reduced environmental sensitivity. <b>2002</b> , 277, 50573-8	142
819	Crystal structure of argininosuccinate synthetase from Thermus thermophilus HB8. Structural basis for the catalytic action. <b>2002</b> , 277, 15890-6	11
818	Crystal structure of the 47-kDa lipoprotein of Treponema pallidum reveals a novel penicillin-binding protein. <b>2002</b> , 277, 41857-64	42
817	Crystal structure of the cytoskeleton-associated protein glycine-rich (CAP-Gly) domain. <b>2002</b> , 277, 48596-601	67
816	Photoexcited structure of a plant photoreceptor domain reveals a light-driven molecular switch. <b>2002</b> , 14, 1067-75	328
815	Structure of the Methanococcus jannaschii mevalonate kinase, a member of the GHMP kinase superfamily. <b>2002</b> , 277, 9462-7	72
814	Correlated alternative side chain conformations in the RNA-recognition motif of heterogeneous nuclear ribonucleoprotein A1. <b>2002</b> , 30, 1531-8	26
813	The 2.2-Å crystal structure of human pro-granzyme K reveals a rigid zymogen with unusual features. <b>2002</b> , 277, 50923-33	51
812	The PDZ1 domain of SAP90. Characterization of structure and binding. <b>2002</b> , 277, 6967-73	38

811	Crystal structure of <i>Thermotoga maritima</i> 0065, a member of the IclR transcriptional factor family. <b>2002</b> , 277, 19183-90	58
810	Asymmetric conductivity of engineered porins. <b>2002</b> , 15, 799-804	7
809	Reaction mechanism of chalcone isomerase. pH dependence, diffusion control, and product binding differences. <b>2002</b> , 277, 1361-9	112
808	The cystine knot promotes folding and not thermodynamic stability in vascular endothelial growth factor. <b>2002</b> , 277, 43410-6	38
807	Crystal structure of actinomycin D bound to the CTG triplet repeat sequences linked to neurological diseases. <b>2002</b> , 30, 4910-7	48
806	A Hoogsteen base pair embedded in undistorted B-DNA. <b>2002</b> , 30, 5244-52	59
805	The catalytic cycle of beta -lactam synthetase observed by x-ray crystallographic snapshots. <b>2002</b> , 99, 14752-7	64
804	Structure of the carboxyl-terminal Src kinase, Csk. <b>2002</b> , 277, 14351-4	112
803	Structure of mitogen-activated protein kinase-activated protein (MAPKAP) kinase 2 suggests a bifunctional switch that couples kinase activation with nuclear export. <b>2002</b> , 277, 37401-5	93
802	The remote substrate binding subsite -6 in cyclodextrin-glycosyltransferase controls the transferase activity of the enzyme via an induced-fit mechanism. <b>2002</b> , 277, 1113-9	39
801	Structural and functional analysis of the human mitotic-specific ubiquitin-conjugating enzyme, UbcH10. <b>2002</b> , 277, 21913-21	50
800	Mutations that destabilize the gp41 core are determinants for stabilizing the simian immunodeficiency virus-CPmac envelope glycoprotein complex. <b>2002</b> , 277, 12891-900	15
799	Crystal structure of imaginal disc growth factor-2. A member of a new family of growth-promoting glycoproteins from <i>Drosophila melanogaster</i> . <b>2002</b> , 277, 13229-36	64
798	Structure-based design of beta 1,4-galactosyltransferase I (beta 4Gal-T1) with equally efficient N-acetylgalactosaminyltransferase activity: point mutation broadens beta 4Gal-T1 donor specificity. <b>2002</b> , 277, 20833-9	181
797	Crystal structure of the MexR repressor of the mexRAB-oprM multidrug efflux operon of <i>Pseudomonas aeruginosa</i> . <b>2002</b> , 277, 29253-9	107
796	Crystal structure of the N-terminal segment of human eukaryotic translation initiation factor 2alpha. <b>2002</b> , 277, 17057-61	47
795	Crystal structure of the productive ternary complex of dihydropyrimidine dehydrogenase with NADPH and 5-iodouracil. Implications for mechanism of inhibition and electron transfer. <b>2002</b> , 277, 13155-66	42
794	Structure of two iron-binding proteins from <i>Bacillus anthracis</i> . <b>2002</b> , 277, 15093-8	97

793	Substrate induced conformational changes in argininosuccinate synthetase. <b>2002</b> , 277, 13074-81	17
792	Novel zinc-binding center and a temperature switch in the <i>Bacillus stearotherophilus</i> L1 lipase. <b>2002</b> , 277, 17041-7	84
791	Passive acquisition of ligand by the MopII molbindin from <i>Clostridium pasteurianum</i> : structures of apo and oxyanion-bound forms. <b>2002</b> , 277, 15013-20	18
790	Polylysine induces an antiparallel actin dimer that nucleates filament assembly: crystal structure at 3.5-Å resolution. <b>2002</b> , 277, 20999-1006	59
789	The X-ray structure of ferric <i>Escherichia coli</i> flavohemoglobin reveals an unexpected geometry of the distal heme pocket. <b>2002</b> , 277, 23725-32	103
788	Three camelid VHH domains in complex with porcine pancreatic alpha-amylase. Inhibition and versatility of binding topology. <b>2002</b> , 277, 23645-50	129
787	Crystal structures of inhibitor complexes reveal an alternate binding mode in orotidine-5'-monophosphate decarboxylase. <b>2002</b> , 277, 28080-7	32
786	Sequential and Environmental Dependence of Conformation in a Small Opioid Peptide. <b>2019</b> , 84, 13299-13312	0
785	Catalytic Plasticity of Germacrene A Oxidase Underlies Sesquiterpene Lactone Diversification. <b>2019</b> , 181, 945-960	11
784	MS-Based Approaches Enable the Structural Characterization of Transcription Factor/DNA Response Element Complex. <b>2019</b> , 9,	7
783	Structural characterization of PPTI, a kunitz-type protein from the venom of <i>Pseudocerastes persicus</i> . <b>2019</b> , 14, e0214657	3
782	Selectivity of the CUBAN domain in the recognition of ubiquitin and NEDD8. <b>2019</b> , 286, 653-677	11
781	Structural and Molecular Basis for Katanin-Mediated Severing of Glutamylated Microtubules. <b>2019</b> , 26, 1357-1367.e5	22
780	Cys.sqlite: A Structured-Information Approach to the Comprehensive Analysis of Cysteine Disulfide Bonds in the Protein Databank. <b>2019</b> , 59, 931-943	2
779	Crystallographic Snapshots of the Zika Virus NS3 Helicase Help Visualize the Reactant Water Replenishment. <b>2019</b> , 5, 177-183	3
778	Structures of the antibody 64M-5 Fab and its complex with dT(6-4)T indicate induced-fit and high-affinity mechanisms. <b>2019</b> , 75, 80-88	1
777	Crystal structure of the multidrug resistance regulator RamR complexed with bile acids. <b>2019</b> , 9, 177	19
776	Structure of the SLy1 SAM homodimer reveals a new interface for SAM domain self-association. <b>2019</b> , 9, 54	6

775	Structural analysis of proteins using X-ray diffraction technique. <b>2019</b> , 69-84	1
774	Structural insights to heterodimeric cis-prenyltransferases through yeast dehydrodolichyl diphosphate synthase subunit Nus1. <b>2019</b> , 515, 621-626	9
773	Molecular basis for enantioselective herbicide degradation imparted by aryloxyalkanoate dioxygenases in transgenic plants. <b>2019</b> , 116, 13299-13304	7
772	Cn29, a novel orphan peptide found in the venom of the scorpion <i>Centruroides noxius</i> : Structure and function. <b>2019</b> , 167, 184-191	3
771	Periplasmic Expression of 4/7 $\beta$ -Conotoxin TxIA Analogs in Favors Ribbon Isomer Formation - Suggestion of a Binding Mode at the $\beta$ nAChR. <b>2019</b> , 10, 577	8
770	Solution NMR Spectroscopy for the Determination of Structures of Membrane Proteins in a Lipid Environment. <b>2019</b> , 2003, 599-643	
769	Experimental characterization of the dynamics of IDPs and IDRs by NMR. <b>2019</b> , 65-92	1
768	Functional and structural investigations of fibronectin-binding protein Apa from <i>Mycobacterium tuberculosis</i> . <b>2019</b> , 1863, 1351-1359	3
767	Solution structure of the N-terminal domain of the <i>Staphylococcus aureus</i> hibernation promoting factor. <b>2019</b> , 73, 223-227	2
766	De novo protein design by citizen scientists. <b>2019</b> , 570, 390-394	63
765	I-PINE web server: an integrative probabilistic NMR assignment system for proteins. <b>2019</b> , 73, 213-222	26
764	AlphaFold at CASP13. <b>2019</b> , 35, 4862-4865	106
763	An integrative protocol for the structure determination of the mouse ASC-PYD filament. <b>2019</b> , 625, 205-222	
762	Alternative $\beta$ /anti- $\beta$ factors represent a unique form of bacterial $\beta$ /anti- $\beta$ complex. <b>2019</b> , 47, 5988-5997	9
761	Covalent binding of uracil DNA glycosylase UdgX to abasic DNA upon uracil excision. <b>2019</b> , 15, 607-614	18
760	Integrative biology of native cell extracts: a new era for structural characterization of life processes. <b>2019</b> , 400, 831-846	13
759	An Overview of Methods for Reconstructing 3-D Chromosome and Genome Structures from Hi-C Data. <b>2019</b> , 21, 7	38
758	Maximizing accuracy of RNA structure in refinement against residual dipolar couplings. <b>2019</b> , 73, 117-139	3

757	Direct Activation of Human MLKL by a Select Repertoire of Inositol Phosphate Metabolites. <b>2019</b> , 26, 863-877.e7	26
756	Dynamics of Zika Virus Capsid Protein in Solution: The Properties and Exposure of the Hydrophobic Cleft Are Controlled by the $\beta$ -Helix 1 Sequence. <b>2019</b> , 58, 2488-2498	11
755	NMR structure of CmPI-II, a non-classical Kazal protease inhibitor: Understanding its conformational dynamics and subtilisin A inhibition. <b>2019</b> , 206, 280-294	3
754	Quiet Outer Membrane Protein G (OmpG) Nanopore for Biosensing. <b>2019</b> , 4, 1230-1235	15
753	Structural and Functional Relevance of the Conserved Residue V13 in the Triheme Cytochrome PpcA from <i>Geobacter sulfurreducens</i> . <b>2019</b> , 123, 3050-3060	2
752	LARP4A recognizes polyA RNA via a novel binding mechanism mediated by disordered regions and involving the PAM2w motif, revealing interplay between PABP, LARP4A and mRNA. <b>2019</b> , 47, 4272-4291	12
751	Assembly and disassembly of conidial rodlets. <b>2019</b> , 5, 100023	12
750	The yeast C/D box snoRNA U14 adopts a "weak" K-turn like conformation recognized by the Snu13 core protein in solution. <b>2019</b> , 164, 70-82	5
749	Exploration of the Structure and Recognition of a G-quadruplex in the her2 Proto-oncogene Promoter and Its Transcriptional Regulation. <b>2019</b> , 9, 3966	6
748	Structure of McsB, a protein kinase for regulated arginine phosphorylation. <b>2019</b> , 15, 510-518	18
747	Arabidopsis DXO1 links RNA turnover and chloroplast function independently of its enzymatic activity. <b>2019</b> , 47, 4751-4764	13
746	The structure of an iron-containing alcohol dehydrogenase from a hyperthermophilic archaeon in two chemical states. <b>2019</b> , 75, 217-226	2
745	Structural basis for efonidipine block of a voltage-gated Ca channel. <b>2019</b> , 513, 631-634	1
744	An Ancient Peptide Family Buried within Vicilin Precursors. <b>2019</b> , 14, 979-993	12
743	High Skp2 expression is associated with a mesenchymal phenotype and increased tumorigenic potential of prostate cancer cells. <b>2019</b> , 9, 5695	14
742	Structure of SPH (self-incompatibility protein homologue) proteins: a widespread family of small, highly stable, secreted proteins. <b>2019</b> , 476, 809-826	1
741	NMR structures and mutational analysis of the two peptides constituting the bacteriocin plantaricin S. <b>2019</b> , 9, 2333	6
740	Solution structure of a unicellular microalgae-derived translationally controlled tumor protein revealed both conserved features and structural diversity. <b>2019</b> , 665, 23-29	2

739	Biochemical characterization of Mycobacterium tuberculosis LexA and structural studies of its C-terminal segment. <b>2019</b> , 75, 41-55	0
738	Crystal structure of substrate-bound bifunctional proline racemase/hydroxyproline epimerase from a hyperthermophilic archaeon. <b>2019</b> , 511, 135-140	4
737	Structural Investigation into the Threading Intercalation of a Chiral Dinuclear Ruthenium(II) Polypyridyl Complex through a B-DNA Oligonucleotide. <b>2019</b> , 141, 4644-4652	20
736	Conformational exchange in the potassium channel blocker ShK. <b>2019</b> , 9, 19307	1
735	The Ancestral N-Terminal Domain of Big Defensins Drives Bacterially Triggered Assembly into Antimicrobial Nanonets. <b>2019</b> , 10,	18
734	Differential modulation of energy landscapes of cyclic AMP receptor protein (CRP) as a regulatory mechanism for class II CRP-dependent promoters. <b>2019</b> , 294, 15544-15556	4
733	Roseltide rT7 is a disulfide-rich, anionic, and cell-penetrating peptide that inhibits proteasomal degradation. <b>2019</b> , 294, 19604-19615	7
732	Tuning the matrix metalloproteinase-1 degradability of peptide amphiphile nanofibers through supramolecular engineering. <b>2019</b> , 7, 5132-5142	13
731	Crystal Structure Of Photorespiratory Alanine:Glyoxylate Aminotransferase 1 (AGT1) From. <b>2019</b> , 10, 1229	2
730	Federating Structural Models and Data: Outcomes from A Workshop on Archiving Integrative Structures. <b>2019</b> , 27, 1745-1759	22
729	Intermediate-resolution crystal structure of the human adenovirus B serotype 3 fibre knob in complex with the EC2-EC3 fragment of desmoglein 2. <b>2019</b> , 75, 750-757	1
728	Structural and biochemical basis of the formation of isoaspartate in the complementarity-determining region of antibody 64M-5 Fab. <b>2019</b> , 9, 18494	5
727	Crystal structure of GAPDH of Streptococcus agalactiae and characterization of its interaction with extracellular matrix molecules. <b>2019</b> , 127, 359-367	2
726	Membrane-anchored carbonic anhydrase IV interacts with monocarboxylate transporters via their chaperones CD147 and GP70. <b>2019</b> , 294, 593-607	20
725	X-ray structure and characterization of a thermostable lipase from Geobacillus thermoleovorans. <b>2019</b> , 508, 145-151	11
724	Secreted amyloid- $\beta$ precursor protein functions as a GABAR1a ligand to modulate synaptic transmission. <b>2019</b> , 363,	134
723	Structural Studies of Autophagy-Related Proteins. <b>2019</b> , 1880, 17-56	2
722	Structural Studies of Selective Autophagy in Yeast. <b>2019</b> , 1880, 77-90	



721	The operon protects from copper toxicity: CopL is an extracellular membrane-associated copper-binding protein. <b>2019</b> , 294, 4027-4044	23
720	Co-option of the PRDM14-CBFA2T complex from motor neurons to pluripotent cells during vertebrate evolution. <b>2019</b> , 146,	3
719	Application of the immunoregulatory receptor LILRB1 as a crystallisation chaperone for human class I MHC complexes. <b>2019</b> , 464, 47-56	1
718	Expression of novel proteins by polyomaviruses and recent advances in the structural and functional features of agnoprotein of JC virus, BK virus, and simian virus 40. <b>2019</b> , 234, 8295-8315	17
717	Structural and functional analysis of single-nucleotide polymorphic variants of purine-rich element-binding protein B. <b>2019</b> , 120, 5835-5851	2
716	Exploring structural properties of potent human carbonic anhydrase inhibitors bearing a 4-(cycloalkylamino-1-carbonyl)benzenesulfonamide moiety. <b>2019</b> , 163, 443-452	16
715	Crystal structure of <i>Bacillus thuringiensis</i> Cry7Ca1 toxin active against <i>Locusta migratoria manilensis</i> . <b>2019</b> , 28, 609-619	5
714	Solid-State NMR Spectroscopy of RNA. <b>2019</b> , 615, 333-371	9
713	Peptide-Membrane Interactions Affect the Inhibitory Potency and Selectivity of Spider Toxins ProTx-II and GpTx-1. <b>2019</b> , 14, 118-130	6
712	The N-terminal RNA Recognition Motif of PFSR1 Confers Semi-specificity for Pyrimidines during RNA Recognition. <b>2019</b> , 431, 498-510	2
711	Construction and structure studies of DNA-bipyridine complexes as versatile scaffolds for site-specific incorporation of metal ions into DNA. <b>2019</b> , 37, 551-561	3
710	Identification of a molecular locus for normalizing dysregulated GABA release from interneurons in the Fragile X brain. <b>2020</b> , 25, 2017-2035	35
709	Lebetin Peptides, A New Class of Potent Platelet Aggregation Inhibitors: Chemical Synthesis, Biological Activity and NMR Spectroscopic Study. <b>2020</b> , 26, 21-31	1
708	Solution Structure and Dynamics of the Small Protein HVO_2922 from <i>Haloferax volcanii</i> . <b>2020</b> , 21, 149-156	6
707	Conjugation of NMR and SAXS for flexible and multidomain protein structure determination: From sample preparation to model refinement. <b>2020</b> , 150, 140-144	3
706	iScore: a novel graph kernel-based function for scoring protein-protein docking models. <b>2020</b> , 36, 112-121	27
705	Crystal and solution structures of human oncoprotein Musashi-2 N-terminal RNA recognition motif 1. <b>2020</b> , 88, 573-583	5
704	Biochemical and biophysical comparison of human and mouse beta-2 microglobulin reveals the molecular determinants of low amyloid propensity. <b>2020</b> , 287, 546-560	6

703	Characterization of perdeuterated high-potential iron-sulfur protein with high-resolution X-ray crystallography. <b>2020</b> , 88, 251-259	2
702	Analysis of several key factors influencing deep learning-based inter-residue contact prediction. <b>2020</b> , 36, 1091-1098	11
701	CAIX forms a transport metabolon with monocarboxylate transporters in human breast cancer cells. <b>2020</b> , 39, 1710-1723	26
700	Structural Bases for the Fitness Cost of the Antibiotic-Resistance and Lethal Mutations at Position 1408 of 16S rRNA. <b>2019</b> , 25,	2
699	Different ways to transport ammonia in human and Mycobacterium tuberculosis NAD synthetases. <b>2020</b> , 11, 16	6
698	Glutathione facilitates enterovirus assembly by binding at a druggable pocket. <b>2020</b> , 3, 9	6
697	Improved protein structure prediction using predicted interresidue orientations. <b>2020</b> , 117, 1496-1503	496
696	Weaponisation 'on the fly': Convergent recruitment of knottin and defensin peptide scaffolds into the venom of predatory assassin flies. <b>2020</b> , 118, 103310	7
695	The Structural Basis for Low Conductance in the Membrane Protein VDAC upon $\text{NADH}$ Binding and Voltage Gating. <b>2020</b> , 28, 206-214.e4	12
694	A nucleobase-binding pocket in a viral RNA-dependent RNA polymerase contributes to elongation complex stability. <b>2020</b> , 48, 1392-1405	15
693	Computational reconstruction of atomistic protein structures from coarse-grained models. <b>2020</b> , 18, 162-176	24
692	Structural insights into the lipid transfer mechanism of a non-specific lipid transfer protein. <b>2020</b> , 102, 340-352	7
691	Structural insights into the mechanism of c-di-GMP-bound YcgR regulating flagellar motility in. <b>2020</b> , 295, 808-821	10
690	SPOT-Fold: Fragment-Free Protein Structure Prediction Guided by Predicted Backbone Structure and Contact Map. <b>2020</b> , 41, 745-750	6
689	Integrative Structural Biology of Protein-RNA Complexes. <b>2020</b> , 28, 6-28	16
688	Single amino acid mutation altered substrate specificity for L-glucose and inositol in -inositol dehydrogenase isolated from. <b>2020</b> , 84, 734-742	1
687	Cyclization mechanism catalyzed by an ATP-grasp enzyme essential for d-cycloserine biosynthesis. <b>2020</b> , 287, 2763-2778	3
686	Quantitative Structural Interpretation of Protein Crosslinks. <b>2020</b> , 28, 75-82.e4	4

685	ARIAweb: a server for automated NMR structure calculation. <b>2020</b> , 48, W41-W47	3
684	Structural and biochemical characterization of an extremely thermostable FMN-dependent NADH-indigo reductase from <i>Bacillus smithii</i> . <b>2020</b> , 164, 3259-3267	4
683	Co-crystal structures of HIV TAR RNA bound to lab-evolved proteins show key roles for arginine relevant to the design of cyclic peptide TAR inhibitors. <b>2020</b> , 295, 16470-16486	11
682	Adeno-Associated Virus (AAV-DJ)-Cryo-EM Structure at 1.56 Å Resolution. <b>2020</b> , 12,	7
681	Defining the Familial Fold of the Vicilin-Buried Peptide Family. <b>2020</b> , 83, 3030-3040	3
680	Discovery and mechanism of a pH-dependent dual-binding-site switch in the interaction of a pair of protein modules. <b>2020</b> , 6,	4
679	Caffeine inhibits Notum activity by binding at the catalytic pocket. <b>2020</b> , 3, 555	6
678	Crystal structure of <i>Thermobifida fusca</i> cis-prenyltransferase reveals the dynamic nature of its RXG motif-mediated inter-subunit interactions critical for its catalytic activity. <b>2020</b> , 532, 459-465	2
677	Theoretical insights into mutation-mediated conformational changes of the GNP-bound H-RAS. <b>2020</b> , 759, 138042	6
676	The HIV-1 maturation inhibitor, EP39, interferes with the dynamic helix-coil equilibrium of the CA-SP1 junction of Gag. <b>2020</b> , 204, 112634	2
675	Structural Basis of AZD9291 Selectivity for EGFR T790M. <b>2020</b> , 63, 8502-8511	27
674	What ATP binding does to the Ca pump and how nonproductive phosphoryl transfer is prevented in the absence of Ca. <b>2020</b> , 117, 18448-18458	7
673	Exploration of Structure-Activity Relationship of Aromatic Aldehydes Bearing Pyridinylmethoxy-Methyl Esters as Novel Antisickling Agents. <b>2020</b> , 63, 14724-14739	2
672	The RNA Polymerase $\beta$ Subunit Recognizes the DNA Shape of the Upstream Promoter Element. <b>2020</b> , 59, 4523-4532	7
671	The Structure of an AAV5-AAVR Complex at 2.5 Å Resolution: Implications for Cellular Entry and Immune Neutralization of AAV Gene Therapy Vectors. <b>2020</b> , 12,	4
670	Recifin A, Initial Example of the Tyr-Lock Peptide Structural Family, Is a Selective Allosteric Inhibitor of Tyrosyl-DNA Phosphodiesterase I. <b>2020</b> , 142, 21178-21188	5
669	NMR Spectroscopic Characterization of the C-Mannose Conformation in a Thrombospondin Repeat Using a Selective Labeling Approach. <b>2020</b> , 59, 20659-20665	5
668	Predicting the Real-Valued Inter-Residue Distances for Proteins. <b>2020</b> , 7, 2001314	20

667	Structural basis of DNA binding to human YB-1 cold shock domain regulated by phosphorylation. <b>2020</b> , 48, 9361-9371	13
666	Characterization of the structure-function relationship of a novel salt-resistant antimicrobial peptide, RR12.. <b>2020</b> , 10, 23624-23631	2
665	Three-Dimensional Structures of Carbohydrates and Where to Find Them. <b>2020</b> , 21,	8
664	Calmodulin Directly Interacts with the Cx43 Carboxyl-Terminus and Cytoplasmic Loop Containing Three ODDD-Linked Mutants (M147T, R148Q, and T154A) that Retain $\alpha$ -Helical Structure, but Exhibit Loss-of-Function and Cellular Trafficking Defects. <b>2020</b> , 10,	1
663	Topological Regulation of the Bioactive Conformation of a Disulfide-Rich Peptide, Heat-Stable Enterotoxin. <b>2020</b> , 25,	4
662	MG1113, a specific anti-tissue factor pathway inhibitor antibody, rebalances the coagulation system and promotes hemostasis in hemophilia. <b>2020</b> , 4, 1301-1312	5
661	Crystal structure and site-directed mutagenesis of circular bacteriocin plantacyclin B21AG reveals cationic and aromatic residues important for antimicrobial activity. <b>2020</b> , 10, 17398	3
660	Structural Determinants within the Adenovirus Early Region 1A Protein Spacer Region Necessary for Tumorigenesis. <b>2020</b> , 94,	
659	Catalytic properties and crystal structure of UDP-galactose 4-epimerase-like l-threonine 3-dehydrogenase from <i>Phytophthora infestans</i> . <b>2020</b> , 140, 109627	3
658	Catechols: a new class of carbonic anhydrase inhibitors. <b>2020</b> , 56, 13033-13036	13
657	Biochemical and biophysical analyses of hypoxia sensing prolyl hydroxylases from and. <b>2020</b> , 295, 16545-165613	
656	Structural analysis and reaction mechanism of the disproportionating enzyme (D-enzyme) from potato. <b>2020</b> , 29, 2085-2100	4
655	Does the crystal structure of vanadium nitrogenase contain a reaction intermediate? Evidence from quantum refinement. <b>2020</b> , 25, 847-861	9
654	The dynamics of free and phosphopeptide-bound Grb2-SH2 reveals two dynamically independent subdomains and an encounter complex with fuzzy interactions. <b>2020</b> , 10, 13040	4
653	Structure and function of a malaria transmission blocking vaccine targeting Pfs230 and Pfs230-Pfs48/45 proteins. <b>2020</b> , 3, 395	14
652	NMR Spectroscopic Characterization of the C-Mannose Conformation in a Thrombospondin Repeat Using a Selective Labeling Approach. <b>2020</b> , 132, 20840-20846	0
651	Biophysical Investigation of Sodium Channel Interaction with $\beta$ Subunit Variants Associated with Arrhythmias. <b>2020</b> , 2, 269-278	0
650	Flexible NAD Binding in Deoxyhypusine Synthase Reflects the Dynamic Hypusine Modification of Translation Factor IF5A. <b>2020</b> , 21,	1

649	Expanding the space of protein geometries by computational design of de novo fold families. <b>2020</b> , 369, 1132-1136	28
648	Neurotoxic peptides from the venom of the giant Australian stinging tree. <b>2020</b> , 6,	6
647	GSDB: a database of 3D chromosome and genome structures reconstructed from Hi-C data. <b>2020</b> , 21, 60	3
646	Chemical shifts-based similarity restraints improve accuracy of RNA structures determined via NMR. <b>2020</b> , 26, 2051-2061	2
645	The genetic origin of evolidine, the first cyclopeptide discovered in plants, and related orbitides. <b>2020</b> , 295, 14510-14521	7
644	Taf14 recognizes a common motif in transcriptional machineries and facilitates their clustering by phase separation. <b>2020</b> , 11, 4206	6
643	Structural Basis for Design of New Purine-Based Inhibitors Targeting the Hydrophobic Binding Pocket of Hsp90. <b>2020</b> , 21,	1
642	Structural basis for inhibitory effects of Smad7 on TGF- $\beta$ family signaling. <b>2020</b> , 212, 107661	6
641	VZHE-039, a novel antisickling agent that prevents erythrocyte sickling under both hypoxic and anoxic conditions. <b>2020</b> , 10, 20277	4
640	A Novel N-Substituted Valine Derivative with Unique Peroxisome Proliferator-Activated Receptor $\alpha$ Binding Properties and Biological Activities. <b>2020</b> , 63, 13124-13139	1
639	Structural basis for distinct quality control mechanisms of GABA receptor during evolution. <b>2020</b> , 34, 16348-16363	2
638	A Global Ramachandran Score Identifies Protein Structures with Unlikely Stereochemistry. <b>2020</b> , 28, 1249-1258.e2	23
637	A conformation-based intra-molecular initiation factor identified in the flavivirus RNA-dependent RNA polymerase. <b>2020</b> , 16, e1008484	16
636	Targeted Delivery of Adamantylated Peptidoglycan Immunomodulators in Lipid Nanocarriers: NMR Shows That Cargo Fragments Are Available on the Surface. <b>2020</b> , 124, 4132-4145	3
635	Structural Basis for the Binding Selectivity of Human CDY Chromodomains. <b>2020</b> , 27, 827-838.e7	4
634	Coarse-grained (hybrid) integrative modeling of biomolecular interactions. <b>2020</b> , 18, 1182-1190	9
633	Crystal structure of adenylate kinase from an extremophilic archaeon <i>Aeropyrum pernix</i> with ATP and AMP. <b>2020</b> , 168, 223-229	2
632	Lysophosphatidic Acid Receptor Agonism: Discovery of Potent Nonlipid Benzofuran Ethanolamine Structures. <b>2020</b> , 374, 283-294	3

631	Structural and dynamic studies of TAPBPR and Tapasin reveal the mechanism of peptide loading of MHC-I molecules. <b>2020</b> , 64, 71-79	10
630	Stringent control of the RNA-dependent RNA polymerase translocation revealed by multiple intermediate structures. <b>2020</b> , 11, 2605	14
629	Structure of two G-quadruplexes in equilibrium in the KRAS promoter. <b>2020</b> , 48, 9336-9345	24
628	Interplay of Pyrrolidine Units with Homo/Hetero Chirality and CF-Aryl Substituents on Secondary Structures of $\beta$ -Proline Tripeptides in Solution. <b>2020</b> , 85, 8865-8871	1
627	Strict Assembly Restriction of Peptides from Rabbit Hemorrhagic Disease Virus Presented by Rabbit Major Histocompatibility Complex Class I Molecule RLA-A1. <b>2020</b> , 94,	4
626	Rapid Elaboration of Fragments into Leads by X-ray Crystallographic Screening of Parallel Chemical Libraries (REFIL). <b>2020</b> , 63, 6863-6875	9
625	Cryo-EM structure of islet amyloid polypeptide fibrils reveals similarities with amyloid- $\beta$ fibrils. <b>2020</b> , 27, 660-667	59
624	Structural basis for the catalytic activities of the multifunctional enzyme quinolinate synthase. <b>2020</b> , 417, 213370	2
623	Extended Experimental Inferential Structure Determination Method in Determining the Structural Ensembles of Disordered Protein States. <b>2020</b> , 3,	21
622	Structural basis for effector protein recognition by the Dot/Icm Type IVB coupling protein complex. <b>2020</b> , 11, 2623	14
621	Numerous severely twisted N-acetylglucosamine conformations found in the protein databank. <b>2020</b> , 88, 1376-1383	2
620	Biochemical and structural characterisation of a protozoan beta-carbonic anhydrase from. <b>2020</b> , 35, 1292-1299	18
619	An autoinhibitory intramolecular interaction proof-reads RNA recognition by the essential splicing factor U2AF2. <b>2020</b> , 117, 7140-7149	6
618	Structural basis of cell-surface signaling by a conserved sigma regulator in Gram-negative bacteria. <b>2020</b> , 295, 5795-5806	1
617	Crystal structure of an Escherichia coli Hfq Core (residues 2-69)-DNA complex reveals multifunctional nucleic acid binding sites. <b>2020</b> , 48, 3987-3997	11
616	The lipoprotein Pal stabilises the bacterial outer membrane during constriction by a mobilisation-and-capture mechanism. <b>2020</b> , 11, 1305	23
615	Structural Analysis Reveals that the Cytokine IL-17F Forms a Homodimeric Complex with Receptor IL-17RC to Drive IL-17RA-Independent Signaling. <b>2020</b> , 52, 499-512.e5	25
614	NMR and crystallographic structural studies of the Elongation factor P from Staphylococcus aureus. <b>2020</b> , 49, 223-230	1

613	Impaired O-Glycosylation at Consecutive Threonine TTX Motifs in Mucins Generates Conformationally Restricted Cancer Neopeptides. <b>2020</b> , 59, 1221-1241	4
612	Structural basis of substrate recognition by the substrate binding protein (SBP) of a hydrazide transporter, obtained from <i>Microbacterium hydrocarbonoxydans</i> . <b>2020</b> , 525, 720-725	2
611	Structure guided maturation of a novel humanized anti-HBV antibody and its preclinical development. <b>2020</b> , 180, 104757	3
610	Affinity maturation, humanization, and co-crystallization of a rabbit anti-human ROR2 monoclonal antibody for therapeutic applications. <b>2020</b> , 295, 5995-6006	14
609	Current approaches for integrating solution NMR spectroscopy and small-angle scattering to study the structure and dynamics of biomolecular complexes. <b>2020</b> , 432, 2890-2912	11
608	Structure and function of LCI1: a plasma membrane CO channel in the <i>Chlamydomonas</i> CO concentrating mechanism. <b>2020</b> , 102, 1107-1126	9
607	Pharmacological activity and NMR solution structure of the leech peptide HSTX-I. <b>2020</b> , 181, 114082	
606	Alternative splicing and allosteric regulation modulate the chromatin binding of UHRF1. <b>2020</b> , 48, 7728-7747	6
605	Parallel motif triplex formation a new, bi-directional hydrogen bonding pattern incorporating a synthetic cyanuril nucleoside into the sense chain.. <b>2020</b> , 10, 22766-22774	
604	Structure and Role of BCOR PUF1 in Noncanonical PRC1 Assembly and Disease. <b>2020</b> , 59, 2718-2728	5
603	Effect of Site-Specific O-Glycosylation on the Structural Behavior of NOTCH1 Receptor Extracellular EGF-like Domains 11 and 10. <b>2020</b> , 26, 12363-12372	3
602	Insights into the structure and function of Est3 from the <i>Hansenula polymorpha</i> telomerase. <b>2020</b> , 10, 11109	0
601	A Disorder-to-Order Transition Mediates RNA Binding of the <i>Caenorhabditis elegans</i> Protein MEX-5. <b>2020</b> , 118, 2001-2014	2
600	Structural insights into Fe-S protein biogenesis by the CIA targeting complex. <b>2020</b> , 27, 735-742	10
599	Crystal structure of the catalytic subunit of bovine pyruvate dehydrogenase phosphatase. <b>2020</b> , 76, 292-301	1
598	<i>Aedes aegypti</i> Odorant Binding Protein 22 selectively binds fatty acids through a conformational change in its C-terminal tail. <b>2020</b> , 10, 3300	11
597	Structural insights into TAZ2 domain-mediated CBP/p300 recruitment by transactivation domain 1 of the lymphopoietic transcription factor E2A. <b>2020</b> , 295, 4303-4315	2
596	The motif EEL in the cytosolic tail of the secretory human proprotein convertase PC7 regulates its trafficking and cleavage activity. <b>2020</b> , 295, 2068-2083	3

595	GloBody Technology: Detecting Anti-Drug Antibody against VH/VL domains. <b>2020</b> , 10, 1860	6
594	Protein Footprinting: Auxiliary Engine to Power the Structural Biology Revolution. <b>2020</b> , 432, 2973-2984	15
593	Structure of the agonist 12-HHT in its BLT2 receptor-bound state. <b>2020</b> , 10, 2630	4
592	The discovery and maturation of peptide biologics targeting the small G-protein Cdc42: A bioblockade for Ras-driven signaling. <b>2020</b> , 295, 2866-2884	10
591	Advanced approaches for elucidating structures of large RNAs using NMR spectroscopy and complementary methods. <b>2020</b> , 183, 93-107	9
590	Methionine sulfoxide reductase B from catalyzes sulfoxide reduction via an intramolecular disulfide cascade. <b>2020</b> , 295, 3664-3677	3
589	The SrrAB two-component system regulates pathogenicity through redox sensitive cysteines. <b>2020</b> , 117, 10989-10999	21
588	Steering Molecular Dynamics Simulations of Membrane-Associated Proteins with Neutron Reflection Results. <b>2020</b> , 16, 3408-3419	5
587	-Glutathionylation of human inducible Hsp70 reveals a regulatory mechanism involving the C-terminal helical lid. <b>2020</b> , 295, 8302-8324	7
586	OPUS-Fold: An Open-Source Protein Folding Framework Based on Torsion-Angle Sampling. <b>2020</b> , 16, 3970-3976	4
585	Methylation of Salmonella Typhimurium flagella promotes bacterial adhesion and host cell invasion. <b>2020</b> , 11, 2013	27
584	Structural and kinetic evidence of aging after organophosphate inhibition of human Cathepsin A. <b>2020</b> , 177, 113980	0
583	Skp1 Dimerization Conceals Its F-Box Protein Binding Site. <b>2020</b> , 59, 1527-1536	4
582	Unique hexameric structure of copper-containing nitrite reductase of an anammox bacterium KSU-1. <b>2020</b> , 526, 654-660	6
581	Insights into PPAR $\beta$ Phosphorylation and Its Inhibition Mechanism. <b>2020</b> , 63, 4811-4823	11
580	NMR Structure and Dynamics Studies of Yeast Respiratory Supercomplex Factor 2. <b>2021</b> , 29, 275-283.e4	5
579	Experimentally based structural model of Yih1 provides insight into its function in controlling the key translational regulator Gcn2. <b>2021</b> , 595, 324-340	0
578	Met-Glu residues in human PrP $^{\text{Sc}}$ loop account for evolutionary resistance to prion infection. <b>2021</b> , 47, 506-518	3



577	Ultrafast structural changes within a photosynthetic reaction centre. <b>2021</b> , 589, 310-314	13
576	Structural basis of human monocarboxylate transporter 1 inhibition by anti-cancer drug candidates. <b>2021</b> , 184, 370-383.e13	37
575	Motif orientation matters: Structural characterization of TEAD1 recognition of genomic DNA. <b>2021</b> , 29, 345-356.e8	1
574	Binding of cardiotonic steroids to Na,K-ATPase in the E2P state. <b>2021</b> , 118,	13
573	Atomic structure of, and valine binding to the regulatory ACT domain of the Mycobacterium tuberculosis Rel protein. <b>2021</b> , 288, 2377-2397	1
572	Structural interaction between DISC1 and ATF4 underlying transcriptional and synaptic dysregulation in an iPSC model of mental disorders. <b>2021</b> , 26, 1346-1360	13
571	Application of NMR Spectroscopy to Determine the 3D Structure of Small Non-Coding RNAs. <b>2021</b> , 2300, 251-266	
570	Lipid contact probability: an essential and predictive character for the structural and functional studies of membrane proteins.	1
569	Zeta-carbonic anhydrases show CS hydrolase activity: A new metabolic carbon acquisition pathway in diatoms?. <b>2021</b> , 19, 3427-3436	4
568	DeepDist: real-value inter-residue distance prediction with deep residual convolutional network. <b>2021</b> , 22, 30	20
567	Chemical Synthesis and NMR Solution Structure of Conotoxin GXIA from. <b>2021</b> , 19,	3
566	Structural basis for the DNA-binding activity of human ARID4B Tudor domain. <b>2021</b> , 296, 100506	2
565	Staphylococcus aureus N-terminus formylated $\beta$ -toxin tends to form amyloid fibrils, while the deformylated $\beta$ -toxin tends to form functional oligomer complexes. <b>2021</b> , 12, 1418-1437	1
564	Crystal structure of a tick-borne flavivirus RNA-dependent RNA polymerase suggests a host adaptation hotspot in RNA viruses. <b>2021</b> , 49, 1567-1580	2
563	Protein and Small Molecule Structure Determination by the Cryo-EM Method MicroED. <b>2021</b> , 2305, 323-342	2
562	3D Structural Determination of Macromolecules Using X-ray Crystallography Methods. <b>2021</b> , 119-140	
561	NMR and MD simulations reveal the impact of the V23D mutation on the function of yeast oligosaccharyltransferase subunit Ost4. <b>2021</b> , 31, 838-850	1
560	Posttranslational modifications of $\beta$ -conotoxins: sulfotyrosine and C-terminal amidation stabilise structures and increase acetylcholine receptor binding. <b>2021</b> , 12, 1574-1584	

559	Nonsteroidal ecdysone receptor agonists use a water channel for binding to the ecdysone receptor complex EcR/USP. <b>2021</b> , 46, 88-100	2
558	Integrating quantitative proteomics with accurate genome profiling of transcription factors by greenCUT&RUN. <b>2021</b> , 49, e49	2
557	A Simplified Amino Acidic Alphabet to Unveil the T-Cells Receptors Antigens: A Computational Perspective. <b>2021</b> , 9, 598802	
556	REDCRAFT: A computational platform using residual dipolar coupling NMR data for determining structures of perdeuterated proteins in solution. <b>2021</b> , 17, e1008060	2
555	Improving deep learning-based protein distance prediction in CASP14.	
554	Deciphering the structural attributes of protein-heparan sulfate interactions using chemo-enzymatic approaches and NMR spectroscopy. <b>2021</b> , 31, 851-858	0
553	Recognition of Histone H3 Methylation States by the PHD1 Domain of Histone Demethylase KDM5A. <b>2021</b> ,	5
552	pyconsFold: A fast and easy tool for modelling and docking using distance predictions.	1
551	Novel anti-repression mechanism of H-NS proteins by a phage $\Phi$ arly protein	
550	Patterns in Protein Flexibility: A Comparison of NMR "Ensembles", MD Trajectories, and Crystallographic B-Factors. <b>2021</b> , 26,	2
549	Determining the three-dimensional atomic structure of an amorphous solid. <b>2021</b> , 592, 60-64	57
548	Asterix/Gtsf1 links tRNAs and piRNA silencing of retrotransposons. <b>2021</b> , 34, 108914	5
547	Critical evaluation of a crystal structure of nitrogenase with bound N ligands. <b>2021</b> , 26, 341-353	6
546	Torpedo californica acetylcholinesterase is stabilized by binding of a divalent metal ion to a novel and versatile 4D motif. <b>2021</b> , 30, 966-981	3
545	Structure-based design of a Cortistatin analogue with immunomodulatory activity in models of inflammatory bowel disease. <b>2021</b> , 12, 1869	7
544	Mevo lectin specificity toward high-mannose structures with terminal $\text{Man}(1,2)\text{Man}$ residues and its implication to inhibition of the entry of Mycobacterium tuberculosis into macrophages. <b>2021</b> , 31, 1046-1059 <sup>0</sup>	
543	Crystal structure and functional implication of a bacterial cyclic AMP-AMP-GMP synthetase. <b>2021</b> , 49, 4725-4737	3
542	Synthesis of the Potent, Selective, and Efficacious $\beta$ secretase (BACE1) Inhibitor NB-360. <b>2021</b> , 64, 4677-4696	4

541	Molecular Interactions between Two LMP2A PY Motifs of EBV and WW Domains of E3 Ubiquitin Ligase AIP4. <b>2021</b> , 11,	0
540	Rational design of metal-binding sites in domain-swapped myoglobin dimers. <b>2021</b> , 217, 111374	1
539	Structural and functional characterization of a putative carbonic anhydrase from <i>Geobacillus kaustophilus</i> reveals its cambialistic function. <b>2021</b> , 547, 96-101	1
538	Xanthine-Guanine-Hypoxanthine Phosphoribosyltransferase-A Putative Target for Drug Discovery against Gastrointestinal Tract Infections. <b>2021</b> , 64, 5710-5729	1
537	Mechanism and dynamics of fatty acid photodecarboxylase. <b>2021</b> , 372,	28
536	Benzyl alcohol inhibits carbonic anhydrases by anchoring to the zinc coordinated water molecule. <b>2021</b> , 548, 217-221	4
535	NMR-Based Screening and Drug Discovery. 1-83	
534	Decoding microbiome and protein family linkage to improve protein structure prediction.	
533	Exploring the Conformational Landscape of the Neh4 and Neh5 Domains of Nrf2 Using Two Different Force Fields and Circular Dichroism. <b>2021</b> , 17, 3145-3156	6
532	Accurate prediction of protein torsion angles using evolutionary signatures and recurrent neural network.	
531	Advancements in macromolecular crystallography: from past to present. <b>2021</b> , 5, 127-149	3
530	Improving deep learning-based protein distance prediction in CASP14. <b>2021</b> ,	2
529	Current directions in combining simulation-based macromolecular modeling approaches with deep learning. <b>2021</b> , 16, 1025-1044	3
528	Influence of the 5'-terminal sequences on the 5'-UTR structure of HIV-1 genomic RNA. <b>2021</b> , 11, 10920	4
527	NMR solution structure and analysis of isolated S3b-S4a motif of repeat IV of the human cardiac sodium channel.	
526	NMR structural analysis of the yeast cytochrome c oxidase subunit Cox13 and its interaction with ATP. <b>2021</b> , 19, 98	1
525	OPUS-X: An Open-Source Toolkit for Protein Torsion Angles, Secondary Structure, Solvent Accessibility, Contact Map Predictions, and 3D Folding.	0
524	Crystal structure of enoyl-CoA hydratase from <i>Thermus thermophilus</i> HB8. <b>2021</b> , 77, 148-155	0

523	Rules for designing protein fold switches and their implications for the folding code.	0
522	Multiscale Quantum Refinement Approaches for Metalloproteins. <b>2021</b> , 17, 3783-3796	1
521	SAMF: a Self-adaptive Protein Modeling Framework. <b>2021</b> ,	1
520	Distance-based Reconstruction of Protein Quaternary Structures from Inter-Chain Contacts.	1
519	Discovery of Novel Chemical Series of OXA-48 $\beta$ -Lactamase Inhibitors by High-Throughput Screening. <b>2021</b> , 14,	0
518	Molecular Features of the Measles Virus Viral Fusion Complex That Favor Infection and Spread in the Brain. <b>2021</b> , 12, e0079921	4
517	Crystal structure of the ferredoxin reductase component of carbazole 1,9a-dioxygenase from <i>Janthinobacterium</i> sp. J3. <b>2021</b> , 77, 921-932	
516	Role of backbone strain in de novo design of complex $\beta$ -protein structures. <b>2021</b> , 12, 3921	9
515	DNCON2_Inter: predicting interchain contacts for homodimeric and homomultimeric protein complexes using multiple sequence alignments of monomers and deep learning. <b>2021</b> , 11, 12295	9
514	Quantum-refinement studies of the bidentate ligand of V-nitrogenase and the protonation state of CO-inhibited Mo-nitrogenase. <b>2021</b> , 219, 111426	3
513	Anthocyanin 5,3'-aromatic acyltransferase from <i>Gentiana triflora</i> , a structural insight into biosynthesis of a blue anthocyanin. <b>2021</b> , 186, 112727	0
512	Structural discrimination analysis for constraint selection in protein modeling. <b>2021</b> ,	
511	Introduction to a special issue of <i>Magnetic Resonance</i> in honour of Robert Kaptein at the occasion of his 80th birthday. <b>2021</b> , 2, 465-474	
510	Multiple regulatory intrinsically disordered motifs control FOXO4 transcription factor binding and function. <b>2021</b> , 36, 109446	4
509	The basicity of an active-site water molecule discriminates between tyrosinase and catechol oxidase activity. <b>2021</b> , 183, 1861-1870	3
508	Structures of the ApoL1 and ApoL2 N-terminal domains reveal a non-classical four-helix bundle motif. <b>2021</b> , 4, 916	1
507	Folding non-homologous proteins by coupling deep-learning contact maps with I-TASSER assembly simulations. <b>2021</b> , 1,	40
506	Structural Characterization of the PawL-Derived Peptide Family, an Ancient Subfamily of Orbitides.	

505	OPUS-Rota4: A Gradient-Based Protein Side-Chain Modeling Framework Assisted by Deep Learning-Based Predictors.	
504	A SARS-CoV-2 neutralizing antibody selected from COVID-19 patients binds to the ACE2-RBD interface and is tolerant to most known RBD mutations. <b>2021</b> , 36, 109433	25
503	fHow ATP and dATP act as molecular switches to regulate enzymatic activity in the prototypic bacterial class Ia ribonucleotide reductase.	2
502	The X-ray structure of L-threonine dehydrogenase from the common hospital pathogen <i>Clostridium difficile</i> . <b>2021</b> , 77, 269-274	0
501	Structure of an open conformation of T7 DNA polymerase reveals novel structural features regulating primer-template stabilization at the polymerization active site. <b>2021</b> , 478, 2665-2679	3
500	Structure and dynamics of the quaternary hunchback mRNA translation repression complex. <b>2021</b> , 49, 8866-8885	0
499	Synthetic hookworm-derived peptides are potent modulators of primary human immune cell function that protect against experimental colitis in vivo. <b>2021</b> , 297, 100834	1
498	Design, synthesis and biochemical evaluation of novel carbonic anhydrase inhibitors triggered by structural knowledge on hCA VII. <b>2021</b> , 44, 116279	0
497	Macromolecular refinement of X-ray and cryoelectron microscopy structures with Phenix/OPLS3e for improved structure and ligand quality. <b>2021</b> , 29, 913-921.e4	12
496	Implications of critical nodes-dependent unidirectional cross-talk between Plasmodium and Human SUMO pathway proteins in Plasmodium infection.	
495	A common binding motif in the ET domain of BRD3 forms polymorphic structural interfaces with host and viral proteins. <b>2021</b> , 29, 886-898.e6	7
494	A Capped Tudor Domain within a Core Subunit of the Sin3L/Rpd3L Histone Deacetylase Complex Binds Nucleic Acids.	
493	Quaternary structure independent folding of voltage-gated ion channel pore domain subunits.	
492	Glycogen phosphorylase revisited: extending the resolution of the R- and T-state structures of the free enzyme and in complex with allosteric activators. <b>2021</b> , 77, 303-311	1
491	Anti-Fungal Hevein-like Peptides Biosynthesized from Quinoa Cleavable Hololectins. <b>2021</b> , 26,	2
490	A Step toward NRF2-DNA Interaction Inhibitors by Fragment-Based NMR Methods. <b>2021</b> , 16, 3576-3587	0
489	Novel anti-repression mechanism of H-NS proteins by a phage protein. <b>2021</b> , 49, 10770-10784	1
488	Current protein structure predictors do not produce meaningful folding pathways.	2

487	Substrate-induced product-release mechanism of lipocalin-type prostaglandin D synthase. <b>2021</b> , 569, 66-71	1
486	OPUS-X: An Open-Source Toolkit for Protein Torsion Angles, Secondary Structure, Solvent Accessibility, Contact Map Predictions, and 3D Folding. <b>2021</b> ,	1
485	Protonectin peptides target lipids, act at the interface and selectively kill metastatic breast cancer cells while preserving morphological integrity. <b>2021</b> , 601, 517-530	1
484	Schistocins: Novel antimicrobial peptides encrypted in the Schistosoma mansoni Kunitz Inhibitor SmKI-1. <b>2021</b> , 1865, 129989	2
483	Binding of vanadium ions and complexes to proteins and enzymes in aqueous solution. <b>2021</b> , 449, 214192	10
482	Multiobjective heuristic algorithm for protein design in a quantified continuous sequence space. <b>2021</b> , 19, 2575-2587	1
481	Guardians of the Cell: State-of-the-Art of Membrane Proteins from a Computational Point-of-View. <b>2021</b> , 2315, 3-28	
480	Structural and functional characterization of nylon hydrolases. <b>2021</b> , 648, 357-389	0
479	Small molecule targeting r(UGGAA) disrupts RNA foci and alleviates disease phenotype in Drosophila model. <b>2021</b> , 12, 236	8
478	Molecular basis for Ras suppressor-1 binding to PINCH-1 in focal adhesion assembly. <b>2021</b> , 296, 100685	1
477	Solution Structure and Conformational Dynamics of a Doublet Acyl Carrier Protein from Prodigiosin Biosynthesis. <b>2021</b> , 60, 219-230	3
476	Protein-Protein Modeling Using Cryo-EM Restraints. <b>2020</b> , 2112, 145-162	1
475	An Overview on Protein Structure Determination by NMR: Historical and Future Perspectives of the use of Distance Geometry Methods. <b>2013</b> , 377-412	5
474	Nuclear Magnetic Resonance Spectroscopy. <b>2013</b> , 113-173	2
473	NMR-based modeling and refinement of protein 3D structures. <b>2015</b> , 1215, 351-80	4
472	Automated structure determination from NMR spectra. <b>2015</b> , 1261, 303-29	9
471	Tools to assist determination and validation of carbohydrate 3D structure data. <b>2015</b> , 1273, 229-40	14
470	Using Molecular Replacement Phasing to Study the Structure and Function of RNA. <b>2016</b> , 1320, 233-57	5

469	Acknowledging Errors: Advanced Molecular Replacement with Phaser. <b>2017</b> , 1607, 421-453	30
468	A Practical Guide to the Simultaneous Determination of Protein Structure and Dynamics Using Metainference. <b>2019</b> , 2022, 313-340	3
467	Three-Dimensional Structure Determination of Peptides Using Solution Nuclear Magnetic Resonance Spectroscopy. <b>2020</b> , 2068, 129-162	11
466	Nuclear magnetic resonance-based modeling and refinement of protein three-dimensional structures and their complexes. <b>2008</b> , 443, 229-55	1
465	Cell-free protein synthesis for structure determination by X-ray crystallography. <b>2010</b> , 607, 149-60	19
464	Application of anomalous diffraction methods to the study of DNA and DNA-complexes. <b>2010</b> , 613, 133-52	2
463	Automated protein NMR structure determination in solution. <b>2010</b> , 673, 95-127	3
462	Strategies employed for the development of PARP inhibitors. <b>2011</b> , 780, 463-89	3
461	Comprehensive automation for NMR structure determination of proteins. <b>2012</b> , 831, 429-51	45
460	ARIA for solution and solid-state NMR. <b>2012</b> , 831, 453-83	38
459	Phasing electron diffraction data by molecular replacement: strategy for structure determination and refinement. <b>2013</b> , 955, 243-72	4
458	Structural Studies of a soluble monomeric Quinohemoprotein Alcohol Dehydrogenase from <i>Pseudomonas putida</i> HK5. <b>2000</b> , 213-218	1
457	Ribosomal Dynamics: Intrinsic Instability of a Molecular Machine. <b>2009</b> , 303-316	3
456	RNA Structure Determination by Structural Probing and Mass Spectrometry: MS3D. <b>2012</b> , 361-389	1
455	A Molecular Model of the Human Prothrombinase Complex. <b>2008</b> , 107-132	1
454	The Inverse Protein Folding Problem: Protein Design and Structure Prediction in the Genomic Era. <b>2012</b> , 121-140	1
453	Recent Advances in Low Resolution Refinement Tools in REFMAC5. <b>2013</b> , 231-258	5
452	Structural insights into the mechanism of c-di-GMPBound YcgR regulating flagellar motility in <i>Escherichia coli</i> . <b>2020</b> , 295, 808-821	3

451	Crystal Structure and Thermodynamic Analysis of Human Brain Fatty Acid-binding Protein. <b>2000</b> , 275, 27045-27054	124
450	A Novel Anti-tumor Cytokine Contains an RNA Binding Motif Present in Aminoacyl-tRNA Synthetases. <b>2000</b> , 275, 27062-27068	37
449	Sequestration of the Active Site by Interdomain Shifting. <b>2000</b> , 275, 27186-27196	47
448	Crystallographic Analysis of Calcium-dependent Heparin Binding to Annexin A2. <b>2006</b> , 281, 31689-31695	22
447	Crystal Structure of the RUN Domain of the RAP2-interacting Protein x. <b>2006</b> , 281, 31843-31853	6
446	Crystal Structures of Expressed Non-polymerizable Monomeric Actin in the ADP and ATP States. <b>2006</b> , 281, 31909-31919	44
445	Curcumin Allosterically Inhibits the Dengue NS2B-NS3 Protease by Disrupting Its Active Conformation. <b>2020</b> , 5, 25677-25686	12
444	Structure of the electron transfer complex between ferredoxin and ferredoxin-NADP+ reductase.	1
443	Structure of the Bcr-Abl oncoprotein oligomerization domain. <b>2002</b> , 9, 117-20	79
442	The SAM domain of polyhomeotic forms a helical polymer. <b>2002</b> , 9, 453-7	107
441	A method for validating the accuracy of NMR protein structures. <b>2020</b> , 11, 6321	12
440	A computationally designed chimeric antigen receptor provides a small-molecule safety switch for T-cell therapy. <b>2020</b> , 38, 426-432	42
439	Structural basis for autoinhibition and its relief of MOB1 in the Hippo pathway. <b>2016</b> , 6, 28488	23
438	Human ornithine transcarbamylase: crystallographic insights into substrate recognition and conformational changes. <b>2001</b> , 354, 501-9	32
437	Engineering of a glycosidase Family 7 cellobiohydrolase to more alkaline pH optimum: the pH behaviour of <i>Trichoderma reesei</i> Cel7A and its E223S/ A224H/L225V/T226A/D262G mutant. <b>2001</b> , 356, 19-30	22
436	The Crystal Structure of the Manganese Superoxide Dismutase from <i>Geobacillus stearothermophilus</i> : Parker and Blake (1988) Revisited. <b>2020</b> , 73, 145	1
435	Catalytic mechanism of quinoprotein methanol dehydrogenase: A theoretical and x-ray crystallographic investigation. <b>2001</b> , 98, 432-4	17
434	Crystal structure of the Holliday junction migration motor protein RuvB from <i>Thermus thermophilus</i> HB8. <b>2001</b> , 98, 1442-7	51



433	The crystal structure of the nitrogen regulation fragment of the yeast prion protein Ure2p. <b>2001</b> , 98, 1459-64	66
432	The structure of the ultraspiracle ligand-binding domain reveals a nuclear receptor locked in an inactive conformation. <b>2001</b> , 98, 1549-54	59
431	A method of incorporating rate constants as kinetic constraints in molecular dynamics simulations. <b>2021</b> , 118,	8
430	Structure of a soluble secreted chemokine inhibitor vCCI (p35) from cowpox virus. <b>1999</b> , 96, 12379-83	85
429	Crystal structure of PapA5, a phthiocerol dimycocerosyl transferase from Mycobacterium tuberculosis. <b>2004</b> , 279, 30634-42	58
428	Structural basis for interorganelle phospholipid transport mediated by VAT-1. <b>2020</b> , 295, 3257-3268	4
427	Insights into the binding mode of sulphamates and sulphamides to hCA II: crystallographic studies and binding free energy calculations. <b>2017</b> , 32, 1002-1011	25
426	Exploring benzoxaborole derivatives as carbonic anhydrase inhibitors: a structural and computational analysis reveals their conformational variability as a tool to increase enzyme selectivity. <b>2019</b> , 34, 1498-1505	5
425	Mutational analysis of the gephyrin-related molybdenum cofactor biosynthetic gene cnxE from the lower eukaryote <i>Aspergillus nidulans</i> . <b>2002</b> , 161, 623-32	13
424	Identification of amino acid residues required for ferric-anguibactin transport in the outer-membrane receptor FatA of <i>Vibrio anguillarum</i> . <b>2007</b> , 153, 570-584	15
423	The vaccinia virus A56 protein: a multifunctional transmembrane glycoprotein that anchors two secreted viral proteins. <b>2011</b> , 92, 1971-1980	12
422	Functional and structural studies of the vaccinia virus virulence factor N1 reveal a Bcl-2-like anti-apoptotic protein. <b>2007</b> , 88, 1656-1666	138
421	Accurate De Novo Prediction of Protein Contact Map by Ultra-Deep Learning Model.	6
420	Anti-diabetic drug binding site in KATP channels revealed by Cryo-EM.	1
419	Folding membrane proteins by deep transfer learning.	3
418	Amyloid fibril structure of islet amyloid polypeptide by cryo-electron microscopy reveals similarities with amyloid beta.	3
417	DeepDist: real-value inter-residue distance prediction with deep residual convolutional network.	8
416	A method for validating the accuracy of NMR protein structures.	1

415	Predicting interchain contacts for homodimeric and homomultimeric protein complexes using multiple sequence alignments of monomers and deep learning.	3
414	A SARS-CoV-2 neutralizing antibody selected from COVID-19 patients by phage display is binding to the ACE2-RBD interface and is tolerant to most known recently emerging RBD mutations.	8
413	Conformational dynamics of auto-inhibition in the ER calcium sensor STIM1.	1
412	Conformational control of translation termination on the 70S ribosome.	1
411	iScore: A novel graph kernel-based function for scoring protein-protein docking models.	1
410	CAIX forms a transport metabolon with monocarboxylate transporters in human breast cancer cells.	2
409	GSDB: a database of 3D chromosome and genome structures reconstructed from Hi-C data.	1
408	Less is more: Coarse-grained integrative modeling of large biomolecular assemblies with HADDOCK.	1
407	Pal stabilises the bacterial outer membrane during constriction by a mobilisation-and-capture mechanism.	1
406	Improved protein structure prediction using predicted inter-residue orientations.	17
405	Structure of the ribosome at 5.5 Å resolution and its interactions with functional ligands. <b>2001</b> , 66, 57-66	16
404	Structure of the full-length yeast Arp7-Arp9 heterodimer. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2014</b> , 70, 310-6	6
403	Structural analysis of Eglucosidase mutants derived from a hyperthermophilic tetrameric structure. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2014</b> , 70, 877-88	5
402	Exploiting large non-isomorphous differences for phase determination of a G-segment invertase-DNA complex. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2014</b> , 70, 685-93	4
401	Partial rotational lattice order-disorder in stefin B crystals. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2014</b> , 70, 1015-25	9
400	Anomalies in the refinement of isoleucine. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2014</b> , 70, 1037-49	3
399	Accurate macromolecular crystallographic refinement: incorporation of the linear scaling, semiempirical quantum-mechanics program DivCon into the PHENIX refinement package. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2014</b> , 70, 1233-47	40
398	Flexible torsion-angle noncrystallographic symmetry restraints for improved macromolecular structure refinement. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2014</b> , 70, 1346-56	13

397	Hierarchical () computation of small-angle scattering profiles and their associated derivatives. <b>2014</b> , 47, 755-761	3
396	py_convrot: rotation conventions, to understand and to apply. <b>2019</b> , 52, 869-881	2
395	Structural definition of polyspecific compensatory ligand recognition by P-glycoprotein. <b>2020</b> , 7, 663-672	12
394	Structure of the SPRY domain of the human RNA helicase DDX1, a putative interaction platform within a DEAD-box protein. <b>2015</b> , 71, 1176-88	6
393	Gyre and gimble: a maximum-likelihood replacement for Patterson correlation refinement. <b>2018</b> , 74, 279-289	13
392	Real-space refinement in PHENIX for cryo-EM and crystallography. <b>2018</b> , 74, 531-544	917
391	Refinement of protein structures using a combination of quantum-mechanical calculations with neutron and X-ray crystallographic data. <b>2019</b> , 75, 368-380	8
390	Combining random microseed matrix screening and the magic triangle for the efficient structure solution of a potential lysin from bacteriophage P68. <b>2019</b> , 75, 670-681	2
389	Macromolecular structure determination using X-rays, neutrons and electrons: recent developments in Phenix. <b>2019</b> , 75, 861-877	1527
388	Molecular replacement using structure predictions from databases. <b>2019</b> , 75, 1051-1062	10
387	Quantum refinement with multiple conformations: application to the P-cluster in nitrogenase. <b>2020</b> , 76, 1145-1156	4
386	Immunologic and structural analysis of eight novel domain-deletion beta3 integrin peptides designed for detection of HPA-1 antibodies. <b>2008</b> , 6, 366-75	10
385	Expression and Characterization of Stress Responsive Peptide-1; an Inducer of Antimicrobial Peptide Synthesis. <b>2019</b> , 4, 42-52	1
384	Crystal structure of the TRANCE/RANKL cytokine reveals determinants of receptor-ligand specificity. <b>2001</b> , 108, 971-9	139
383	The diabetogenic mouse MHC class II molecule I-Ag7 is endowed with a switch that modulates TCR affinity. <b>2010</b> , 120, 1578-90	31
382	Structure-guided engineering of a Thermobifida fusca cutinase for enhanced hydrolysis on natural polyester substrate. <b>2020</b> , 7,	4
381	Electron Cryomicroscopy and Image Reconstruction of Viral Nanoparticles. <b>2015</b> , 27-60	1
380	Resolving the paradox for protein aggregation diseases: a common mechanism for aggregated proteins to initially attack membranes without needing aggregates. 2, 221	7

379	Resolving the paradox for protein aggregation diseases: a common mechanism for aggregated proteins to initially attack membranes without needing aggregates. <b>2013</b> , 2, 221	6
378	Thiolation-enhanced substrate recognition by D-alanyl carrier protein ligase DltA from <i>Bacillus cereus</i> . <b>2014</b> , 3, 106	5
377	Mutant HIV-1 Protease Complexed with Tetrapeptide Inhibitor. Preliminary Report. <b>2002</b> , 101, 659-663	2
376	JAMM: a metalloprotease-like zinc site in the proteasome and signalosome. <b>2004</b> , 2, E2	170
375	Recognition and accommodation at the androgen receptor coactivator binding interface. <b>2004</b> , 2, E274	176
374	A <i>Drosophila</i> pattern recognition receptor contains a peptidoglycan docking groove and unusual L,D-carboxypeptidase activity. <b>2004</b> , 2, E277	77
373	Structural basis for a Munc13-1 homodimer to Munc13-1/RIM heterodimer switch. <b>2006</b> , 4, e192	84
372	Structural and functional analyses of PAS domain interactions of the clock proteins <i>Drosophila</i> PERIOD and mouse PERIOD2. <b>2009</b> , 7, e94	55
371	Elongation Factor Tu Prevents Misediting of Gly-tRNA(Gly) Caused by the Design Behind the Chiral Proofreading Site of D-Aminoacyl-tRNA Deacylase. <b>2016</b> , 14, e1002465	18
370	Structural Basis for Inhibitor-Induced Aggregation of HIV Integrase. <b>2016</b> , 14, e1002584	40
369	Markov State Models Reveal a Two-Step Mechanism of miRNA Loading into the Human Argonaute Protein: Selective Binding followed by Structural Re-arrangement. <b>2015</b> , 11, e1004404	39
368	Combining Evolutionary Information and an Iterative Sampling Strategy for Accurate Protein Structure Prediction. <b>2015</b> , 11, e1004661	15
367	Structure and evolutionary origin of Ca(2+)-dependent herring type II antifreeze protein. <b>2007</b> , 2, e548	55
366	X-ray structures of the signal recognition particle receptor reveal targeting cycle intermediates. <b>2007</b> , 2, e607	18
365	Structural and functional analyses of five conserved positively charged residues in the L1 and N-terminal DNA binding motifs of archaeal RADA protein. <b>2007</b> , 2, e858	18
364	Isolation, cloning and structural characterisation of boophilin, a multifunctional Kunitz-type proteinase inhibitor from the cattle tick. <b>2008</b> , 3, e1624	83
363	Odorranalectin is a small peptide lectin with potential for drug delivery and targeting. <b>2008</b> , 3, e2381	60
362	UPF201 archaeal specific family members reveal structural similarity to RNA-binding proteins but low likelihood for RNA-binding function. <b>2008</b> , 3, e3903	1

361	N- and C-terminal domains of the calcium binding protein EhCaBP1 of the parasite <i>Entamoeba histolytica</i> display distinct functions. <b>2009</b> , 4, e5269	13
360	Structure of human DNA polymerase kappa inserting dATP opposite an 8-OxoG DNA lesion. <b>2009</b> , 4, e5766	46
359	Crystal structure of the C-terminal cytoplasmic domain of non-structural protein 4 from mouse hepatitis virus A59. <b>2009</b> , 4, e6217	12
358	HAAD: A quick algorithm for accurate prediction of hydrogen atoms in protein structures. <b>2009</b> , 4, e6701	20
357	Solution structure and phylogenetics of Prod1, a member of the three-finger protein superfamily implicated in salamander limb regeneration. <b>2009</b> , 4, e7123	57
356	Promoter recognition by a complex of Spx and the C-terminal domain of the RNA polymerase alpha subunit. <b>2010</b> , 5, e8664	42
355	Molecular modeling of mechanosensory ion channel structural and functional features. <b>2010</b> , 5, e12814	8
354	The "Phantom Effect" of the Rexinoid LG100754: structural and functional insights. <b>2010</b> , 5, e15119	55
353	Modifying the substrate specificity of <i>Carcinoscorpius rotundicauda</i> serine protease inhibitor domain 1 to target thrombin. <b>2010</b> , 5, e15258	3
352	Crystal structure of EHEC intimin: insights into the complementarity between EPEC and EHEC. <b>2010</b> , 5, e15285	17
351	Crystal structure of UBA2(ufd)-Ubc9: insights into E1-E2 interactions in Sumo pathways. <b>2010</b> , 5, e15805	38
350	Structure of HsdS subunit from <i>Thermoanaerobacter tengcongensis</i> sheds lights on mechanism of dynamic opening and closing of type I methyltransferase. <b>2011</b> , 6, e17346	17
349	X-ray structure of the human calreticulin globular domain reveals a peptide-binding area and suggests a multi-molecular mechanism. <b>2011</b> , 6, e17886	66
348	Structural asymmetry of phosphodiesterase-9, potential protonation of a glutamic acid, and role of the invariant glutamine. <b>2011</b> , 6, e18092	17
347	The structure of the NPC1L1 N-terminal domain in a closed conformation. <b>2011</b> , 6, e18722	36
346	Structural basis for dual-inhibition mechanism of a non-classical Kazal-type serine protease inhibitor from horseshoe crab in complex with subtilisin. <b>2011</b> , 6, e18838	10
345	The structure of <i>Helicobacter pylori</i> HP0310 reveals an atypical peptidoglycan deacetylase. <b>2011</b> , 6, e19207	13
344	Crystal structures of two aminoglycoside kinases bound with a eukaryotic protein kinase inhibitor. <b>2011</b> , 6, e19589	22

343	The crystal structure of the human co-chaperone P58(IPK). <b>2011</b> , 6, e22337	19
342	Structural differences between the <i>Streptococcus agalactiae</i> housekeeping and pilus-specific sortases: SrtA and SrtC1. <b>2011</b> , 6, e22995	29
341	Crystal structure of outer membrane protein NMB0315 from <i>Neisseria meningitidis</i> . <b>2011</b> , 6, e26845	13
340	A conformational switch in the active site of BT_2972, a methyltransferase from an antibiotic resistant pathogen <i>B. thetaiotaomicron</i> . <b>2011</b> , 6, e27543	1
339	Human anti-V3 HIV-1 monoclonal antibodies encoded by the VH5-51/VL lambda genes define a conserved antigenic structure. <b>2011</b> , 6, e27780	39
338	Protein 3D structure computed from evolutionary sequence variation. <b>2011</b> , 6, e28766	709
337	Crystal structure of a human single domain antibody dimer formed through V(H)-V(H) non-covalent interactions. <b>2012</b> , 7, e30149	12
336	Structural basis of Ets1 cooperative binding to widely separated sites on promoter DNA. <b>2012</b> , 7, e33698	17
335	Crystal structure of ChrR--a quinone reductase with the capacity to reduce chromate. <b>2012</b> , 7, e36017	48
334	NMR structure of lipoprotein YxeF from <i>Bacillus subtilis</i> reveals a calycin fold and distant homology with the lipocalin Blc from <i>Escherichia coli</i> . <b>2012</b> , 7, e37404	4
333	Intrinsically unstructured domain 3 of hepatitis C Virus NS5A forms a "fuzzy complex" with VAPB-MSP domain which carries ALS-causing mutations. <b>2012</b> , 7, e39261	34
332	Ipomoelin, a jacalin-related lectin with a compact tetrameric association and versatile carbohydrate binding properties regulated by its N terminus. <b>2012</b> , 7, e40618	10
331	Crystal structure of TNF- $\beta$ -inducing protein from <i>Helicobacter pylori</i> in active form reveals the intrinsic molecular flexibility for unique DNA-binding. <b>2012</b> , 7, e41871	5
330	Crystal structures of the network-forming short-arm tips of the laminin $\alpha$ and $\beta$ chains. <b>2012</b> , 7, e42473	42
329	Solution structural analysis of the single-domain parvulin TbPin1. <b>2012</b> , 7, e43017	6
328	Site specific cleavage mediated by MMPs regulates function of agrin. <b>2012</b> , 7, e43669	17
327	Crystal structure of <i>Cryptosporidium parvum</i> pyruvate kinase. <b>2012</b> , 7, e46875	10
326	Solution structure of a phytocystatin from <i>Ananas comosus</i> and its molecular interaction with papain. <b>2012</b> , 7, e47865	17

325	The pentameric channel of COMPcc in complex with different fatty acids. <b>2012</b> , 7, e48130	11
324	A divalent ion is crucial in the structure and dominant-negative function of ID proteins, a class of helix-loop-helix transcription regulators. <b>2012</b> , 7, e48591	14
323	Exploring ORFan domains in giant viruses: structure of mimivirus sulfhydryl oxidase R596. <b>2012</b> , 7, e50649	13
322	Structural and functional insights into (S)-ureidoglycolate dehydrogenase, a metabolic branch point enzyme in nitrogen utilization. <b>2012</b> , 7, e52066	3
321	Structural insights into cellulolytic and chitinolytic enzymes revealing crucial residues of insect $\beta$ N-acetyl-D-hexosaminidase. <b>2012</b> , 7, e52225	12
320	Crystal structure and computational modeling of the fab fragment from a protective anti-ricin monoclonal antibody. <b>2012</b> , 7, e52613	11
319	Solution structure of an archaeal DNA binding protein with an eukaryotic zinc finger fold. <b>2013</b> , 8, e52908	10
318	Structural and functional analysis of the DEAF-1 and BS69 MYND domains. <b>2013</b> , 8, e54715	18
317	Use of a molecular decoy to segregate transport from antigenicity in the FrpB iron transporter from <i>Neisseria meningitidis</i> . <b>2013</b> , 8, e56746	19
316	Structures of coxsackievirus, rhinovirus, and poliovirus polymerase elongation complexes solved by engineering RNA mediated crystal contacts. <b>2013</b> , 8, e60272	54
315	Structural and phylogenetic studies with MjTX-I reveal a multi-oligomeric toxin--a novel feature in Lys49-PLA2s protein class. <b>2013</b> , 8, e60610	14
314	Structural insights into a wildtype domain of the oncoprotein E6 and its interaction with a PDZ domain. <b>2013</b> , 8, e62584	15
313	Plant Kinesin-Like Calmodulin Binding Protein Employs Its Regulatory Domain for Dimerization. <b>2013</b> , 8, e66669	4
312	The serine protease domain of MASP-3: enzymatic properties and crystal structure in complex with ecotin. <b>2013</b> , 8, e67962	18
311	Crystal structure and substrate specificity of D-galactose-6-phosphate isomerase complexed with substrates. <b>2013</b> , 8, e72902	3
310	Structural analysis of peptide-analogues of human Zona Pellucida ZP1 protein with amyloidogenic properties: insights into mammalian Zona Pellucida formation. <b>2013</b> , 8, e73258	29
309	Transmembrane and Juxtamembrane Structure of $\beta$ Integrin in Bicelles. <b>2013</b> , 8, e74281	14
308	The crystal structure of the orphan nuclear receptor NR2E3/PNR ligand binding domain reveals a dimeric auto-repressed conformation. <b>2013</b> , 8, e74359	26

307	Structural, biochemical and genetic characterization of dissimilatory ATP sulfurylase from <i>Allochromatium vinosum</i> . <b>2013</b> , 8, e74707	23
306	Reaction trajectory revealed by a joint analysis of protein data bank. <b>2013</b> , 8, e77141	10
305	Single, double and quadruple alanine substitutions at oligomeric interfaces identify hydrophobicity as the key determinant of human neutrophil alpha defensin HNP1 function. <b>2013</b> , 8, e78937	20
304	High resolution crystal structure of human $\beta$ -glucuronidase reveals structural basis of lysosome targeting. <b>2013</b> , 8, e79687	41
303	Identification of a new epitope in uPAR as a target for the cancer therapeutic monoclonal antibody ATN-658, a structural homolog of the uPAR binding integrin CD11b (M). <b>2014</b> , 9, e85349	24
302	Solution structure of CXCL5--a novel chemokine and adipokine implicated in inflammation and obesity. <b>2014</b> , 9, e93228	24
301	Cyanuric acid hydrolase from <i>Azorhizobium caulinodans</i> ORS 571: crystal structure and insights into a new class of Ser-Lys dyad proteins. <b>2014</b> , 9, e99349	8
300	Structural insights of the ssDNA binding site in the multifunctional endonuclease AtBFN2 from <i>Arabidopsis thaliana</i> . <b>2014</b> , 9, e105821	5
299	Crystal structure of Cruxrhodopsin-3 from <i>Haloarcula vallismortis</i> . <b>2014</b> , 9, e108362	11
298	Crystal structure of human importin- $\beta$ (Rch1), revealing a potential autoinhibition mode involving homodimerization. <b>2015</b> , 10, e0115995	14
297	Lpg0393 of <i>Legionella pneumophila</i> is a guanine-nucleotide exchange factor for Rab5, Rab21 and Rab22. <b>2015</b> , 10, e0118683	9
296	Structure determination of feline calicivirus virus-like particles in the context of a pseudo-octahedral arrangement. <b>2015</b> , 10, e0119289	4
295	Rheostat re-wired: alternative hypotheses for the control of thioredoxin reduction potentials. <b>2015</b> , 10, e0122466	13
294	A Kazal-Type Serine Protease Inhibitor from the Defense Gland Secretion of the Subterranean Termite <i>Coptotermes formosanus</i> Shiraki. <b>2015</b> , 10, e0125376	7
293	Crystallographic Study of the LUMI Intermediate of Squid Rhodopsin. <b>2015</b> , 10, e0126970	8
292	Structure of Staphylococcal Enterotoxin E in Complex with TCR Defines the Role of TCR Loop Positioning in Superantigen Recognition. <b>2015</b> , 10, e0131988	11
291	Structural Basis for the Inhibition of a Phospholipase A2-Like Toxin by Caffeic and Aristolochic Acids. <b>2015</b> , 10, e0133370	24
290	Probing the ATP Site of GRP78 with Nucleotide Triphosphate Analogs. <b>2016</b> , 11, e0154862	13



289	A Model for Dimerization of the SOX Group E Transcription Factor Family. <b>2016</b> , 11, e0161432	3
288	Sarkosyl-Induced Helical Structure of an Antimicrobial Peptide GW-Q6 Plays an Essential Role in the Binding of Surface Receptor OprI in <i>Pseudomonas aeruginosa</i> . <b>2016</b> , 11, e0164597	7
287	<i>Staphylococcus aureus</i> single-stranded DNA-binding protein SsbA can bind but cannot stimulate PriA helicase. <b>2017</b> , 12, e0182060	10
286	Compatible topologies and parameters for NMR structure determination of carbohydrates by simulated annealing. <b>2017</b> , 12, e0189700	3
285	<i>Neisseria meningitidis</i> Type IV Pili Composed of Sequence Invariable Pilins Are Masked by Multisite Glycosylation. <b>2015</b> , 11, e1005162	42
284	Structure Elucidation of Coxsackievirus A16 in Complex with GPP3 Informs a Systematic Review of Highly Potent Capsid Binders to Enteroviruses. <b>2015</b> , 11, e1005165	13
283	Crystal Structure of the Pre-fusion Nipah Virus Fusion Glycoprotein Reveals a Novel Hexamer-of-Trimers Assembly. <b>2015</b> , 11, e1005322	41
282	A Bat-Derived Putative Cross-Family Recombinant Coronavirus with a Reovirus Gene. <b>2016</b> , 12, e1005883	70
281	Timeless couples G-quadruplex detection with processing by DDX11 helicase during DNA replication. <b>2020</b> , 39, e104185	27
280	Structures of ISCth4 transpososomes reveal the role of asymmetry in copy-out/paste-in DNA transposition. <b>2021</b> , 40, e105666	2
279	Spectroscopic characterization of bacteriorhodopsin's L-intermediate in 3D crystals cooled to 170 K. <b>2001</b> , 74, 794-804	24
278	Ibrutinib targets mutant-EGFR kinase with a distinct binding conformation. <b>2016</b> , 7, 69760-69769	33
277	Roles of charged residues in pH-dependent redox properties of cytochrome from Miyazaki F. <b>2006</b> , 2, 45-56	1
276	An Improved Integration of Template-Based and Template-Free Protein Structure Modeling Methods and its Assessment in CASP11. <b>2015</b> , 22, 586-93	9
275	Progress in protein crystallography. <b>2016</b> , 23, 201-10	18
274	Solution Structure and Expression Profile of an Insect Cytokine: <i>Manduca sexta</i> Stress Response Peptide-2. <b>2017</b> , 24, 3-11	3
273	From Recognition to Reaction Mechanism: An Overview on the Interactions between HIV-1 Protease and its Natural Targets. <b>2020</b> , 27, 2514-2549	7
272	The role of herpes simplex virus-1 thymidine kinase alanine 168 in substrate specificity. <b>2008</b> , 2, 60-6	9

271	Novel avian influenza H7N3 strain outbreak, British Columbia. <b>2004</b> , 10, 2192-5	154
270	In vitro and in vivo effect of parathyroid hormone analogue (1-14) containing -amino-iso-butyric acid residue (Aib) <sub>1,3</sub> . <b>2006</b> , 47, 214-22	3
269	Three Dimensional Structure of Pseudomonas aeruginosa Tsi2: a Novel Species-specific Antitoxin-like Protein With Coiled Coil Conformation*. <b>2012</b> , 39, 640-646	1
268	Macromolecular crystallographic structure refinement. <b>2015</b> , 191, a219	3
267	Crystal Structure of MJ0684 from Methanococcus jannaschii, a Novel Archaeal Homolog of Kynurenine Aminotransferase. <b>2008</b> , 29, 173-176	1
266	Biochemical and Structural Analysis of Hormone-sensitive Lipase Homolog EstE7: Insight into the Stabilized Dimerization of HSL-Homolog Proteins. <b>2010</b> , 31, 2627-2632	3
265	Unambiguous Determination of Intermolecular Hydrogen Bond of NMR Structure by Molecular Dynamics Refinement Using All-Atom Force Field and Implicit Solvent Model. <b>2010</b> , 31, 2717-2720	6
264	X-ray Crystallographic Structure of TIR-Domain from the Human TIR-Domain Containing Adaptor Protein/MyD88-Adaptor-Like Protein (TIRAP/MAL). <b>2012</b> , 33, 3091-3094	8
263	Characterization of peptide deformylase2 from B. cereus. <b>2007</b> , 40, 1050-7	4
262	Structural analysis of sialyltransferase PM0188 from Pasteurella multocida complexed with donor analogue and acceptor sugar. <b>2008</b> , 41, 48-54	21
261	Analysis of the solution structure of the human antibiotic peptide dermcidin and its interaction with phospholipid vesicles. <b>2010</b> , 43, 362-8	16
260	Structure of a pore-blocking toxin in complex with a eukaryotic voltage-dependent K(+) channel. <b>2013</b> , 2, e00594	139
259	Three-dimensional electron crystallography of protein microcrystals. <b>2013</b> , 2, e01345	234
258	Mechanism of chiral proofreading during translation of the genetic code. <b>2013</b> , 2, e01519	29
257	A conserved MCM single-stranded DNA binding element is essential for replication initiation. <b>2014</b> , 3, e01993	65
256	Analysis of the crystal structure of an active MCM hexamer. <b>2014</b> , 3, e03433	47
255	Autoinhibition of Bruton's tyrosine kinase (Btk) and activation by soluble inositol hexakisphosphate. <b>2015</b> , 4,	53
254	Coordination of peptidoglycan synthesis and outer membrane constriction during Escherichia coli cell division. <b>2015</b> , 4,	127

253	STIL binding to Polo-box 3 of PLK4 regulates centriole duplication. <b>2015</b> , 4,	81
252	CarD uses a minor groove wedge mechanism to stabilize the RNA polymerase open promoter complex. <b>2015</b> , 4,	43
251	Binary architecture of the Nav1.2- $\beta$ signaling complex. <b>2016</b> , 5,	31
250	Motility and microtubule depolymerization mechanisms of the Kinesin-8 motor, KIF19A. <b>2016</b> , 5,	36
249	Advances in X-ray free electron laser (XFEL) diffraction data processing applied to the crystal structure of the synaptotagmin-1 / SNARE complex. <b>2016</b> , 5,	18
248	Structure of protein O-mannose kinase reveals a unique active site architecture. <b>2016</b> , 5,	23
247	Tandem hnRNP A1 RNA recognition motifs act in concert to repress the splicing of survival motor neuron exon 7. <b>2017</b> , 6,	34
246	Model-based local density sharpening of cryo-EM maps. <b>2017</b> , 6,	113
245	Structures reveal opening of the store-operated calcium channel Orai. <b>2018</b> , 7,	56
244	Structure of the gene therapy vector, adeno-associated virus with its cell receptor, AAVR. <b>2019</b> , 8,	30
243	Crystal structure of the 3C protease from Southern African Territories type 2 foot-and-mouth disease virus. <b>2016</b> , 4, e1964	6
242	Solution and crystal structures of a C-terminal fragment of the neuronal isoform of the polypyrimidine tract binding protein (nPTB). <b>2014</b> , 2, e305	8
241	Multi contact-based folding method for de novo protein structure prediction. <b>2021</b> ,	
240	Biophysical Methods to Investigate Hydration Structures of Proteins. <b>2021</b> , 25-59	
239	Structural Characterization of the PawL-Derived Peptide Family, an Ancient Subfamily of Orbitides. <b>2021</b> , 84, 2914-2922	
238	Three-dimensional atomic packing in amorphous solids with liquid-like structure. <b>2021</b> ,	3
237	Discovery of Umibecestat (CNP520): A Potent, Selective, and Efficacious $\beta$ -Secretase (BACE1) Inhibitor for the Prevention of Alzheimer's Disease. <b>2021</b> , 64, 15262-15279	2
236	Structural evidence for visual arrestin priming via complexation of phosphoinositols. <b>2021</b> ,	1

- 235 From Angstroms to Nanometers: Measuring Interatomic Distances by Solid-State NMR. **2021**, 6
- 234 Mechanistic insights into an atypical interaction between ATG8 and SH3P2 in. **2021**, 1-17 1
- 233 Applications of Molecular Modeling in NMR Structure Determination. **2001**,
- 232 Analyzing Three-Dimensional Structures of Variant Enzymes. **2003**,
- 231 Structure of the  $\alpha$ -Carbanion/Enamine Reaction Intermediate. **2003**,
- 230 The mechanism for acetylcholine receptor inhibition by  $\alpha$ -neurotoxins and species-specific resistance to  $\alpha$ -bungarotoxin revealed. **2004**, 45-54
- 229 CNS.
- 228 CNS. **2004**,
- 227 Structures of R- and T-state Escherichia coli Aspartokinase III. **2006**, 281, 31544-31552 6
- 226 Structure and Function of Two Prostaglandin (PG) Synthases for Drug Design. **2007**, 47, 036-043
- 225 Targeting the PDZ Domains of Molecular Scaffolds of Transmembrane Ion Channels. **2008**, 139-148
- 224 Crystal Structures of the NblA Protein. **2008**, 237-241
- 223 Transmembrane protein models based on high-throughput molecular dynamics simulations with experimental constraints. **2008**, 443, 213-27 1
- 222 NMR: Applications in Chemical Biology.
- 221 Coarse-Grained Elastic Normal Mode Analysis and Its Applications in X-Ray at Moderate Resolutions Crystallographic Refinement. **2008**, 255-266
- 220 Interpreting The Observed Substrate Selectivity And The Product Regioselectivity In Orf2-Catalyzed Prenylation From X-Ray Structures. **2009**, 351-375
- 219 Structural Basis for Novel Interactions between Human TLS Polymerases and PCNA. **2009**, 51, 286-291
- 218 Neutron Diffraction Experiments for Protein. **2010**, 59, 263-277 1

- 217 Chapter 7:Protein Crystallography for Metalloproteins. **2010**, 212-238
- 216 Macromolecular Crystallographic Computing. **2010**, 1-36
- 215 Chapter 7:Structural Studies of Viral Proteins [X-ray Crystallography]. **2010**, 121-134
- 214 Chapter 6:X-ray Crystallography of Virus Capsids. **2010**, 100-120
- 213 Methods. **2011**, 19-30
- 212 Solution Structure of Water-soluble Mutant of Crambin and Implication for Protein Solubility. **2011**, 32, 1640-1644 1
- 211 References. 575-608
- 210 Combining Biochemical and Structural Information to Model RNA-Protein Complex Assembly. **2013**, 169-186
- 209 BetaMDGP: Protein Structure Determination Algorithm Based on the Beta-complex. **2014**, 130-155
- 208 Materials and Methods. **2014**, 25-40
- 207 Bibliography. **2015**, 243-260
- 206 Protocols for Studies of Bypass of DNA Damage by DNA Polymerase. **2015**, 35-43
- 205 Deformable complex network for refining low-resolution X-ray structures. *Acta Crystallographica Section D: Biological Crystallography*, **2015**, 71, 2150-7 2
- 204 High-Resolution 3D Structure Determination of Kaliotoxin by Solid-State NMR Spectroscopy. **2016**, 125-139
- 203 COMPARS: a stand-alone program for map comparison using quantile rank scaling. **2016**, 49, 2270-2275
- 202 Identification of a Highly Conserved Hypothetical Protein TON\_0340 as a Probable Manganese-Dependent Phosphatase. **2016**, 11, e0167549
- 201 Cryo-EM structure of the ATP-sensitive potassium channel illuminates mechanisms of assembly and gating. 1
- 200 Computational and Experimental Studies of ADP-Ribosylation. **2017**, 1608, 475-513

199 Iterative model-based density improvement yields better atomic structures from cryo-EM maps.

198 Introduction. **2018**, 1-27

197 Application of the immunoregulatory receptor LILRB1 as a novel crystallisation chaperone for class I peptide-MHC complexes.

196 Identification of residue pairing in interacting  $\beta$ strands from a predicted residue contact map.

195 Simultaneous Determination of Protein Structure and Dynamics Using Cryo-Electron Microscopy. 1

194 Patterns in protein flexibility: a comparison of NMR  $\beta$ ensembles, MD trajectories and crystallographic B-factors.

193 Chapter 3:Structural and Dynamic Characterization of Protein Domains using Paramagnetic Data. **2018**, 85-106

192 3D protein structure from genetic epistasis experiments. 4

191 Dynamic interactions of type I cohesin modules fine-tune the structure of the cellulosome of *Clostridium thermocellum*. 0

190  $^{13}\text{C}$  Chemical Shifts in Proteins: A Rich Source of Encoded Structural Information. **2019**, 659-698

189 Structure and ligand binding of As-p18, an extracellular fatty acid binding protein from the eggs of a parasitic nematode. **2019**, 39, 3

188 Recognition of histone H3 methylation states by the PHD1 domain of histone demethylase KDM5A.

187 Flagella methylation promotes bacterial adhesion and host cell invasion.

186 Structural basis for the binding selectivity of human CDY chromodomains.

185 Structure-based design of a Cortistatin analog with improved immunoregulatory activity against inflammatory bowel disease (IBD).

184 Defining the familial fold of the vicilin-buried peptide family.

183 The genetic origin of evolidine, the first cyclopeptide discovered in plants, and related orbitides.

182 pH dependent inhibition from ammonium ions in the *Pseudomonas mevalonii* HMG-CoA Reductase crystallization environment. 1

- 181 REDCRAFT: A Computational Platform Using Residual Dipolar Coupling NMR Data for Determining Structures of Perdeuterated Proteins Without NOEs.
- 180 Structural determinants within the adenovirus early region 1A protein spacer region necessary for tumorigenesis.
- 179 Structural insight into hormone recognition and transmembrane signaling by the atrial natriuretic peptide receptor. 0
- 178 Asterix/Gtsf1 links tRNAs and piRNA silencing of retrotransposons.
- 177 Experimental and computational studies on molecular mechanism by which Curcumin allosterically inhibits Dengue protease.
- 176 A common binding motif in the ET domain of BRD3 forms polymorphic structural interfaces with host and viral proteins.
- 175 Accurate prediction of protein torsion angles using evolutionary signatures and recurrent neural network. **2021**, 11, 21033 0
- 174 Improved Protein Structure Prediction Using a New Multi-Scale Network and Homologous Templates. **2021**, e2102592 11
- 173 Distance-based reconstruction of protein quaternary structures from inter-chain contacts. **2021**, 1
- 172 Workflow for Protein N-terminal Acetylation and C-terminal Amidation Application using CcpNmr Analysis v2.4 Platform and Aria2.3 Structure Calculation Software.
- 171 Timeless couples G quadruplex detection with processing by DDX11 during DNA replication.
- 170 Evidence for binary Smc complexes lacking kite subunits in archaea. **2020**, 7, 193-206 0
- 169 Fe-S protein assembly involves bipartite client binding and conformational flexibility in the CIA targeting complex.
- 168 A global Ramachandran score identifies protein structures with unlikely stereochemistry. 1
- 167 Conformational dynamics of auto-inhibition in the ER calcium sensor STIM1. **2021**, 10, 4
- 166 CTD of SARS-CoV-2 N protein is a cryptic domain for binding ATP and nucleic acid that interplay in modulating phase separation. **2021**, 1
- 165 Crystal structure and site-directed mutagenesis of circular bacteriocin plantacyclin B21AG reveals cationic and aromatic residues important for antimicrobial activity. 0
- 164 Deep Homology-Based Protein Contact-Map Prediction.

163	Plasticity, ligand conformation and enzyme action of <i>Mycobacterium smegmatis</i> MutT1. <b>2020</b> , 76, 982-992	
162	Structure and dynamics of the quaternary hunchback mRNA translation repression complex.	
161	Molecular basis for gating of cardiac ryanodine receptor: underlying mechanisms for gain- and loss-of function mutations.	
160	Unraveling the mechanism of recognition of the 3' splice site of the adenovirus major late promoter intron by the alternative splicing factor PUF60. <b>2020</b> , 15, e0242725	0
159	Peptide-in-groove interactions link target proteins to the beta-propeller of clathrin. <b>2000</b> , 97, 1096-100	128
158	Molecular basis for CD40 signaling mediated by TRAF3. <b>2000</b> , 97, 10395-9	50
157	Insights into the functional architecture of the catalytic center of a maize beta-glucosidase Zm-p60.1. <b>2001</b> , 127, 973-85	10
156	Crystal structures of two forms of a 14-mer RNA/DNA chimer duplex with double UU bulges: a novel intramolecular U*(A x U) base triple. <b>2001</b> , 7, 1425-31	4
155	Structural basis of pyrimidine specificity in the MS2 RNA hairpin-coat-protein complex. <b>2001</b> , 7, 1616-27	33
154	Detailed analysis of RNA-protein interactions within the bacterial ribosomal protein L5/5S rRNA complex. <b>2002</b> , 8, 1548-57	22
153	Structural basis of Ets1 cooperative binding to palindromic sequences on stromelysin-1 promoter DNA. <b>2010</b> , 9, 3054-62	21
152	A new crystal form of mouse thiamin pyrophosphokinase. <b>2011</b> , 2, 111-8	2
151	Structural analysis of NADPH depleted bovine liver catalase and its inhibitor complexes. <b>2011</b> , 2, 67-77	1
150	Structural evidence for the order of preference of inorganic substrates in mammalian heme peroxidases: crystal structure of the complex of lactoperoxidase with four inorganic substrates, SCN, I, Br and Cl. <b>2011</b> , 2, 328-39	11
149	Crystal structure of peptidyl-tRNA hydrolase from <i>mycobacterium smegmatis</i> reveals novel features related to enzyme dynamics. <b>2012</b> , 3, 58-69	9
148	Structural basis of heparin binding to camel peptidoglycan recognition protein-S. <b>2012</b> , 3, 86-94	4
147	Advances in protein NMR provided by the NIGMS Protein Structure Initiative: impact on drug discovery. <b>2010</b> , 13, 335-49	7
146	A conserved Ebulge glycine residue facilitates folding and increases stability of the mouse Edefensin cryptdin-4. <b>2022</b> , 114, e24250	



145	Structure of HIV-1 Vpr in complex with the human nucleotide excision repair protein hHR23A. <b>2021</b> , 12, 6864	
144	Interaction between a fluoroquinolone derivative and RNAs with a single bulge. <b>2021</b> ,	0
143	Towards the automatic crystal structure solution of nucleic acids: automated model building using the new CAB program. <b>2021</b> , 77, 1602-1613	1
142	Atomic structure of the regulatory TGS domain of Rel protein from Mycobacterium tuberculosis and its interaction with deacylated tRNA. <b>2021</b> , 595, 3006	0
141	Simultaneous Assignment and Structure Determination of Proteins From Sparsely Labeled NMR Datasets.. <b>2021</b> , 8, 774394	1
140	Structural Determination of Uridine Diphosphate Glycosyltransferases Using X-Ray Crystallography. <b>2022</b> , 2396, 227-241	0
139	Ten things I 'hate' about refinement. <b>2021</b> , 77, 1497-1515	0
138	Structural basis of anti-SARS-CoV-2 activity of HCQ: specific binding to N protein to disrupt its interaction with nucleic acids and LLPS. 1-37	0
137	Structures of additional crystal forms of Satellite tobacco mosaic virus grown from a variety of salts. <b>2021</b> , 77, 473-483	0
136	Novel disintegrin-like peptides derived from an amphibian skin cDNA sequence of <i>Hypsiboas punctatus</i> . <b>2021</b> , e3382	
135	De novo protein design by deep network hallucination. <b>2021</b> ,	33
134	A Benzenesulfonamide GW8510 Rejuvenates Mice and Yeast Through Interaction with P21-Activated Kinases.	
133	Experimental and theoretical study on converting myoglobin into a stable domain-swapped dimer by utilizing a tight hydrogen bond network at the hinge region.. <b>2021</b> , 11, 37604-37611	0
132	Structural basis for effector recognition by an antibacterial type IV secretion system.. <b>2022</b> , 119,	0
131	Incorporating NOE-Derived Distances in Conformer Generation of Cyclic Peptides with Distance Geometry.. <b>2022</b> ,	
130	Advances in liquid-state NMR spectroscopy to study the structure, function, and dynamics of biomacromolecules. <b>2022</b> , 237-266	1
129	Complete Model of Vinculin Suggests the Mechanism of Activation by Helical Super-Bundle Unfurling.. <b>2022</b> , 41, 55	0
128	Insights into two-metal-ion catalytic mechanism of cap-snatching endonuclease of Ebinur Lake virus in .. <b>2022</b> , jvi0208521	1

127	T-hairpin structure found in the RNA element involved in piRNA biogenesis.. <b>2022</b> ,	0
126	Myricetin Allosterically Inhibits the Dengue NS2B-NS3 Protease by Disrupting the Active and Locking the Inactive Conformations.. <b>2022</b> , 7, 2798-2808	0
125	Xtrapol8: automatic elucidation of low-occupancy intermediate-states in crystallographic studies.	0
124	Structural Analysis of Hen Egg Lysozyme Refolded after Denaturation at Acidic pH.. <b>2022</b> , 41, 71	
123	Ecdysis triggering hormone peptide in the African malaria mosquito Anopheles gambiae: The peptide structure for receptor activation.. <b>2022</b> ,	0
122	Structures and function of a tailoring oxidase in complex with a nonribosomal peptide synthetase module.. <b>2022</b> , 13, 548	0
121	Energetics and -coupling constants for Ala, Gly, and Val peptides demonstrated using ABEEM polarizable force field and an aqueous solution.. <b>2022</b> ,	
120	Current structure predictors are not learning the physics of protein folding.. <b>2022</b> ,	3
119	A Capped Tudor Domain within a Core Subunit of the Sin3L/Rpd3L Histone Deacetylase Complex Binds to Nucleic Acid G-Quadruplexes.. <b>2021</b> , 101558	
118	Concurrent Identification and Characterization of Protein Structure and Continuous Internal Dynamics with REDCRAFT.. <b>2022</b> , 9, 806584	
117	Structural and functional insights into inhibition of human voltage-gated sodium channels by Econotoxin KIIIA disulfide isomers.. <b>2022</b> , 101728	2
116	Decoding the link of microbiome niches with homologous sequences enables accurately targeted protein structure prediction. <b>2021</b> , 118,	2
115	Single-atom catalysts supported on ordered porous materials: Synthetic strategies and applications.	3
114	Exploring cryo-electron microscopy with molecular dynamics.. <b>2022</b> ,	0
113	A Novel Family of Winged-Helix Single-Stranded DNA-Binding Proteins from Archaea.. <b>2022</b> , 23,	0
112	Predicting the structure of large protein complexes using AlphaFold and sequential assembly.	1
111	Structural and Biochemical Basis for Development of Diketo Acid Inhibitors Targeting the Cap-Snatching Endonuclease of the Ebinur Lake Virus (Order: ).. <b>2022</b> , e0217321	1
110	Membrane contact probability: An essential and predictive character for the structural and functional studies of membrane proteins.. <b>2022</b> , 18, e1009972	1

- 109 PD-1 N58-Glycosylation-Dependent Binding of Monoclonal Antibody Cemiplimab for Immune Checkpoint Therapy.. **2022**, 13, 826045 2
- 108 Halogen Bonds Exist between Noncovalent Ligands and Natural Nucleic Acids.. **2022**, 1 1
- 107 Minor differences in peptide presentation between chicken MHC class I molecules can explain differences in disease susceptibility.
- 106 Re-evaluation of protein neutron crystallography with and without X-ray/neutron joint refinement.. **2022**, 9, 342-348 0
- 105 Phosphosite-dependent presentation of dual phosphorylated peptides by MHC class I molecules.. **2022**, 25, 104013
- 104 Dissecting the stability determinants of a challenging de novo protein fold using massively parallel design and experimentation. 0
- 103 A mosaic bulk-solvent model improves density maps and the fit between model and data.
- 102 Cryo-EM Analyses Permit Visualization of Structural Polymorphism of Biological Macromolecules. **2021**, 1, 0
- 101 Aray Mutasyonların Protein Etkileşimlerine Tesirini Tahmin Eden Algoritmalarla HADDOCK'ın Performanslarının Karşılaştırılması. 0
- 100 Myricetin allosterically inhibits Dengue NS2B-NS3 protease as studied by NMR and MD simulations.
- 99 OPUS-Rota4: a gradient-based protein side-chain modeling framework assisted by deep learning-based predictors.. **2021**, 2
- 98 Solution Structure of the BPSL1445 Protein of Reveals the SYLF Domain Three-Dimensional Fold.. **2021**, 0
- 97 The aphid BCR4 structure and activity uncover a new defensin peptide superfamily.
- 96 The flexible N-terminal motif of uL11 unique to eukaryotic ribosomes interacts with P-complex and facilitates protein translation.. **2022**, 0
- 95 Conservation of the unusual dimeric JmjC fold of JMJD7 from *Drosophila melanogaster* to humans.. **2022**, 12, 6065 0
- 94 A deep reinforcement learning approach to reconstructing quaternary structures of protein dimers through self-learning.
- 93 Table1.PDF. **2018**,
- 92 Presentation1.PDF. **2018**,

- 91 Data\_Sheet\_1.pdf. **2019**,
- 90 Data\_Sheet\_1.PDF. **2019**,
- 89 Data\_Sheet\_1.ZIP. **2019**,
- 88 Image\_1.JPEG. **2019**,
- 87 Image\_2.JPEG. **2019**,
- 86 Image\_3.JPEG. **2019**,
- 85 Image\_4.png. **2019**,
- 84 DataSheet\_1.pdf. **2019**,
- 83 Data\_Sheet\_1.PDF. **2017**,
- 82 Structural and functional insight into mismatch extension by human DNA polymerase  $\beta$  **2022**, 119, e2111744119
- 81 Conformational ensemble of the TNF-derived peptide solnatide in solution. **2022**, 20, 2082-2090 ○
- 80 Design, Synthesis, and Antisickling Investigation of a Nitric Oxide-Releasing Prodrug of 5HMF for the Treatment of Sickle Cell Disease. **2022**, 12, 696 ○
- 79 True-atomic-resolution insights into the structure and functional role of linear chains and low-barrier hydrogen bonds in proteins.. **2022**, 2
- 78 Different Mutations in the HHV-6 DNA Polymerase Gene Accounting for Resistance to Foscarnet. **2007**, 12, 877-888 29
- 77 An electrostatically-steered conformational selection mechanism promotes SARS-CoV-2 Spike protein variation. **2022**, 167637 ○
- 76 Solid-state Nanopore Analysis on Conformation Change of DNA Polymerase I induced by DNA Substrate. ○
- 75 Minimal Increments of Hydrophobic Collapse within the N-Terminus of the Neuropeptide Galanin. ○
- 74 Molecular basis for gating of cardiac ryanodine receptor explains the mechanisms for gain- and loss-of function mutations. **2022**, 13, ○

73	Quaternary structure independent folding of voltage-gated ion channel pore domain subunits.	1
72	Atomic solution structure of Mycobacterium abscessus F-ATP synthase subunit F <sub>1</sub> and identification of Ep1 Mab F1 as a targeted inhibitor.	0
71	A Powassan virus domain III nanoparticle immunogen elicits neutralizing and protective antibodies in mice. <b>2022</b> , 18, e1010573	2
70	The complex of Fas-associated factor 1 with Hsp70 stabilizes the adherens junction integrity by suppressing RhoA activation.	1
69	Williams-Beuren Syndrome Related Methyltransferase WBSCR27: From Structure to Possible Function. 9,	
68	Neurotoxic and cytotoxic peptides underlie the painful stings of the tree nettle <i>Urtica ferox</i> . <b>2022</b> , 102218	1
67	CARD8 negatively regulates NLRP1 inflammasome activation level by interaction with NLRP1.	
66	Crystal Structures of Flavivirus NS5 Guanylyltransferase Reveal a GMP-Arginine Adduct.	0
65	Xtrapol8 enables automatic elucidation of low-occupancy intermediate-states in crystallographic studies. <b>2022</b> , 5,	1
64	Structure and dynamic association of an assembly platform subcomplex of the bacterial type II secretion system.	0
63	Zinc finger structure determination by NMR: why zinc fingers can be a handful. <b>2022</b> ,	0
62	Multifaceted Computational Modeling in Glycoscience.	7
61	Dynamics of lipid displacement inside the hydrophobic cavity of a nonspecific lipid transfer protein from <i>Solanum melongena</i> . 1-11	0
60	Complete structure elucidation of a functional form of the <i>Bacillus thuringiensis</i> Cry4Ba Endotoxin: Insights into toxin-induced transmembrane pore architecture. <b>2022</b> , 620, 158-164	0
59	Crystallography of polysaccharides: Current state and challenges. <b>2022</b> , 70, 102183	1
58	Exploring the use of cobalt(II) dipolar shifts in refining the structure of a zinc finger peptide. <b>2022</b> , 235, 111912	
57	Molecular and Biochemical Differences of the Tandem and Cold-Adapted PET Hydrolases Ple628 and Ple629, Isolated From a Marine Microbial Consortium. 10,	1
56	An N <sup>+</sup> H <sup>-</sup> N low-barrier hydrogen bond preorganizes the catalytic site of aspartate aminotransferase to facilitate the second half-reaction.	

55	Structural insight into ASH1L PHD finger recognizing methylated histone H3K4 and promoting cell growth in prostate cancer. 12,	1
54	UNC-45 assisted myosin folding depends on a conserved FX3HY motif implicated in Freeman Sheldon Syndrome.	
53	The neuropeptide galanin adopts an irregular secondary structure. <b>2022</b> , 626, 121-128	
52	An N-capping asparagine-lysine-proline (NKP) motif contributes to a hybrid flexible/stable multifunctional peptide scaffold. <b>2022</b> , 13, 9410-9424	0
51	Solid-State NMR Spectroscopy on Microbial Rhodopsins. <b>2022</b> , 181-206	0
50	Biochemical, structural, and computational studies of a $\beta$ -carbonic anhydrase from the pathogenic bacterium <i>Burkholderia pseudomallei</i> . <b>2022</b> , 20, 4185-4194	2
49	Improved methodology for protein NMR structure calculation using hydrogen bond restraints and ANSURR validation: the SH2 domain of SH2B1.	0
48	OPUS-Fold3: a gradient-based protein all-atom folding and docking framework on TensorFlow.	0
47	Unusual Cytochrome c552 from <i>Thioalkalivibrio paradoxus</i> : Solution NMR Structure and Interaction with Thiocyanate Dehydrogenase. <b>2022</b> , 23, 9969	0
46	NMR determination of the 2:1 binding complex of naphthyridine carbamate dimer (NCD) and CGG/CGG triad in double-stranded DNA. <b>2022</b> , 50, 9621-9631	0
45	Reweighting methods for elucidation of conformation ensembles of proteins. <b>2022</b> , 77, 102470	0
44	Design and characterization of a protein fold switching network.	0
43	Discovery of a cysteine-rich peptide with glycation modification from <i>Achyranthes bidentata</i> Blume. <b>2022</b> , 105338	0
42	Aphid BCR4 Structure and Activity Uncover a New Defensin Peptide Superfamily. <b>2022</b> , 23, 12480	1
41	Antiviral drug design based on structural insights into the N-terminal domain and C-terminal domain of the SARS-CoV-2 nucleocapsid protein. <b>2022</b> ,	0
40	AI-guided cryo-EM probes a thermophilic cell-free system with succinyl-coA manufacturing capability.	0
39	Design, Synthesis, and Investigation of Novel Nitric Oxide (NO)-Releasing Aromatic Aldehydes as Drug Candidates for the Treatment of Sickle Cell Disease. <b>2022</b> , 27, 6835	0
38	Predicting the structure of large protein complexes using AlphaFold and Monte Carlo tree search. <b>2022</b> , 13,	3

37	Phosphorylation of the DNA repair scaffold SLX4 drives folding of the SAP domain and activation of the MUS81-EME1 endonuclease. <b>2022</b> , 41, 111537	0
36	HIF1 $\beta$ AS1 is a DNA:DNA:RNA triplex-forming lncRNA interacting with the HUSH complex. <b>2022</b> , 13,	2
35	Conformationally Defined Rexinoids for the Prevention of Inflammation and Nonmelanoma Skin Cancers.	0
34	A NR2E1-interacting peptide of LSD1 inhibits the proliferation of brain tumour initiating cells.	0
33	The CARD8 T60 variant associates with NLRP1 and negatively regulates its activation. 13,	0
32	The protein conformational basis of isoflavone biosynthesis. <b>2022</b> , 5,	0
31	Venomics survey of six myrmicine ants provides insights into the molecular and structural diversity of their peptide toxins. <b>2022</b> , 103876	1
30	Sampling of structure and sequence space of small protein folds. <b>2022</b> , 13,	0
29	Upstream of N-Ras C-terminal cold shock domains mediate poly(A) specificity in a novel RNA recognition mode and bind poly(A) binding protein during translation regulation.	0
28	Structural basis of transcription regulation by CNC family transcription factor, Nrf2. <b>2022</b> , 50, 12543-12557	3
27	Artificial intelligence for template-free protein structure prediction: a comprehensive review.	0
26	Structural and functional insights into CST tethering in <i>Tetrahymena thermophila</i> telomerase. <b>2022</b> , 30, 1565-1572.e4	0
25	Protein Engineering of Glucosylglycerol Phosphorylase Facilitating Efficient and Highly Regio- and Stereoselective Glycosylation of Polyols in a Synthetic System. <b>2022</b> , 12, 15715-15727	0
24	Insights into pyrrolysine function from structures of a trimethylamine methyltransferase and its corrinoid protein complex. <b>2023</b> , 6,	0
23	Structure and dynamic association of an assembly platform subcomplex of the bacterial type II secretion system. <b>2022</b> ,	0
22	Cryo-EM structure of adeno-associated virus 4 at 2.2 Å resolution. <b>2023</b> , 79, 140-153	1
21	Structural mechanism of BRD4-NUT and p300 bipartite interaction in propagating aberrant gene transcription in chromatin in NUT carcinoma. <b>2023</b> , 14,	0
20	Design and characterization of a protein fold switching network. <b>2023</b> , 14,	0

- 19 Discovery, Characterization, and Engineering of Lv1C, an  $\alpha$ /4-Conotoxin That Selectively Blocks Rat  $\alpha$ 3/ $\beta$ 4 Nicotinic Acetylcholine Receptors. **2023**, 66, 2020-2031 ○
- 18 The Molecular Basis of Heat-Stable Enterotoxin for Vaccine Development and Cancer Cell Detection. **2023**, 28, 1128 1
- 17 Upstream of N-Ras C-terminal cold shock domains mediate poly(A) specificity in a novel RNA recognition mode and bind poly(A) binding protein. ○
- 16 A Wider and Deeper Peptide-Binding Groove for the Class I Molecules from B15 Compared with B19 Chickens Correlates with Relative Resistance to Marek's Disease. ○
- 15 Targeting Enterococcus faecalis HMG-CoA reductase with a non-statin inhibitor. **2023**, 6, ○
- 14 The RRM-mediated RNA binding activity in T. brucei RAP1 is essential for VSG monoallelic expression. **2023**, 14, ○
- 13 The mechanism underlying toxicity of a venom peptide against insects reveals how ants are master at disrupting membranes. **2023**, 26, 106157 ○
- 12 A Combined in Silico and Structural Study Opens New Perspectives on Aliphatic Sulfonamides, a Still Poorly Investigated Class of CA Inhibitors. **2023**, 12, 281 ○
- 11 Detailed analysis of distorted retinal and its interaction with surrounding residues in the K intermediate of bacteriorhodopsin. **2023**, 6, ○
- 10 Facilitating the structural characterisation of non-canonical amino acids in biomolecular NMR. **2023**, 4, 57-72 ○
- 9 Residues of Legume AG41 Peptide Crucial to Its Bio-Insecticidal Activity. **2023**, 13, 446 ○
- 8 A cataract-causing Y204X mutation of CRYB1 promotes C-terminal degradation and higher-order oligomerization. ○
- 7 A potential long-range RNA-RNA interaction in the HIV-1 RNA. 1-9 ○
- 6 The TINCR ubiquitin-like microprotein is a tumor suppressor in squamous cell carcinoma. **2023**, 14, ○
- 5 The Automatic Solution of Macromolecular Crystal Structures via Molecular Replacement Techniques: REMO22 and Its Pipeline. **2023**, 24, 6070 ○
- 4 Taipan Natriuretic Peptides Are Potent and Selective Agonists for the Natriuretic Peptide Receptor A. **2023**, 28, 3063 ○
- 3 Biological Screening and Crystallographic Studies of Hydroxy  $\beta$ -Lactone Derivatives to Investigate PPAR $\alpha$  Phosphorylation Inhibition. **2023**, 13, 694 ○
- 2 Pyrrolysine-Inspired in Cellulo Synthesis of an Unnatural Amino Acid for Facile Macrocyclization of Proteins. **2023**, 145, 10249-10258 ○



- 1 Unusual substructure conformations observed in crystal structures of a dicistrovirus RNA-dependent RNA polymerase suggest contribution of the N-terminal extension in proper folding. **2023**,

o