Ab initio protein folding, 61
Ab initio quantum chemistry, 315
AB model, 184
Accessible surface area, 15
Activity coefficients, 240
Adjacent gaps, 98
Adjacent side chains, 118
Admissibility condition, 301
Algorithms for domain identification, 39
Aligned substructures, 29
Alignment, vii, 58, 90
Alignment order, 101
Alignment scores, 90
AlSCRIPT, 112
Alzheimer’s disease, 219
AMBER, 124, 133, 192, 200
Ambiguous electron density maps, 141
Amino acid sequences, 60, 116, 232
Amino acids, 5
Amphipathic molecules, 236
Amplitude information, 297
α-Amylase, 11
Analytical models, 181
Annotation-based searches, 61
Applications of wavelets in chemistry, 309
Aqueous solutions, 231, 239
Aristotle, 2
Artificial charge distribution, 247
Artificial neural networks (ANN), 70, 73, 313
ASTRAL, 13, 39
Atomic Non-Linear Environment Assessment (ANOLEA), 63
Atomic volumes, 144
Atomistic models, 241
Atomistic simulation, vii
Authors, 16
Autocorrelation function, 180
Automated alignment methods, 101
Automated classification, 40
Automatic identification of protein domains, 14
Average concentration, 281
Average crossing number, 34, 35
Average electric fields, 281
Average group clustering, 47
Average linkage clustering, 47
Average linkage hierarchical clustering, 43
Back-bone chain, 35
Backbone-dependent rotamer library, 126
Background signal, 309
Backtracking trees, 130
Bacteriorhodopsin, 8
Barrel structure, 10
β-Barrels, 10, 187, 235
Basis pdfs, 114, 115
Basis set expansions, 315
Basis set superposition error (BSSE), 315
Berendsen external heat-bath method, 134
Best basis, 307, 313
Best conformation, 129
Best model, vii, 60, 84, 124, 137
Bias, 116, 170
Biased sampling, 198
Biasing potential, 197, 216
Binding sites, 86, 89, 121, 174

Reviews in Computational Chemistry, Volume 22
edited by Kenny B. Lipkowitz, Thomas R. Cundari, and Valerie J. Gillet
Copyright © 2006 Wiley-VCH, John Wiley & Sons, Inc.
Conformational space, 170
Conformational states, ix
Conformations, 170, 179
Consensus fold, 44
Consensus model, vii, 121
Conserved domain, 66
Conserved Domain Architecture Retrieval Tool (CDART), 67
Conserved domain database (CDD), 67
Conserved regions, 121
Constructing protein models, 111
Contact maps, 29
Continuity equation, 274, 277
Continuous Fourier transform (CFT), 297
Continuous wavelet transform (CWT), 301
Continuum model, 274, 281, 283
Continuum of wavelet dilations, 303
Convection, 277
Cooperative folding process, 171, 190
Coordinate root mean square deviation (cRMS), 17, 27, 31
Core regions, 15
Core structures, 120, 146
Corey-Pauling-Koltun (CPK) models, 4
Correct protein structures, 141
Correctly folded protein, 138, 149
Correctly threaded matches, 82
Correlation matrix, 18, 19
Correspondence length, 24
Correspondence, 24
Coulomb force, 244, 258
Creutzfeld-Jacob disease, 219
Curated classification, 40
Current conservation, 278
Current density, x, 274, 276, 278
Current density vector, 274
Curse of dimensionality, 316
Cytochrome C, 195

DALI Domain dictionary (DDD), vi, 16, 43
DALI Fold Classification, 39
DALILIGHT, 25
Darwin, 2
Data alignment, 317
Data archiving, 313
Data mining, 14
Data variance, 316
Databases, 1, 61
Databases of protein structural domains, 16
Data-driven discovery, 3
Daubechies 6 wavelet, 300

DDBASE, 16
Dead-end elimination (DEE), 127
Debye length, 281
Decoy structures, 79
3Dee, 16
DeepView, 64
Defective protein, 145
Definition of Secondary Structure of Proteins (DSSP), 71
DEJAVU, 25
Denaturant, 178
Denatured protein, 170
Denatured state, 204
Denaturing conditions, 209
Denaturing simulations, 197
Denoising, xi
Denoising algorithm, 310
Density of states, 180, 182, 197
Descriptors, 33, 316
Descriptors of chemical data, 320
Detective, 16, 42
Deviations in atomic volumes, 145
DIAL, 16
Dielectric barrier, 243
Dielectric constant, 192, 259, 263, 268, 278
Dielectric discontinuities, 250
Dielectric medium, 239
Diffusion coefficient, 239, 263, 268, 274
Diffusion collision model, 171
Diffusivity, 234
Dilated wavelet, 301, 302
Dilation variable, 303
Dilations, 302
Dimension reduction, 317
Dirichlet boundary condition, 262
Discontinuous molecular dynamics, ix
Discrete Fourier transform (DFT), 298, 299
Discrete wavelet transformation (DWT), 303
Discretization errors, 280
Discretization grid, 249
Disjointed signal, 306
Dissimilarity, 47
Distance ALIgnment (DALI) algorithm, 4, 28
Distance geometry, 28
Distance map, 28
Distance matrices, 24
Distance root mean-squared deviation (dRMS), 27, 31
Distance-dependent dielectric, 192
Distance-geometry, viii, 113
Distantly similar sequences, 84
Distantly related proteins, 60
Distinguishable state, 182
Disulfide bonding, 89, 114, 127, 138
Disulfide bridges, 58, 126
Divide-and-Conquer, vii, 100
DNA, 35
Domain assignments, vi, 43
Domain classification, 68
Domain quality, 15
Domain sequence, 81
Domain-based pairwise alignment, 147
DomainParser, 16
Domains, 12, 38, 62, 146
DOMAK, 16, 42
Double-zeta basis sets, 314
DSSP, 13
Dynamic programming, 24, 95
eMOTIF, 39
Effective properties, 272
Electrical forces, 252
Electrodiffusion of ions, 274, 278
Electrodiffusive continuum, 270
Electron density gradients, 318
Electron density Laplacian, 318
Electron density maps, 116
Electron device simulation, 243
Electronegativity equalization scheme, 273
Electronic kinetic energy densities, 318
Electrophysiologic experiments, 231
Electrophysiology, 230
Electrostatic boundary conditions, 262, 271
Electrostatic moments, 272
Electrostatic potential, 250, 318
Electrostatic potential energy, 247
Electrostatics, 243
eMOTIF, 39
Empirical energy functions, 79
ENCAD, 195
Energy conservation, 278
Energy landscape theory, ix, 170, 172
Energy minimization, 132, 240
Engineering, x
Ensemble of single-chain conformations, 175
Ensemble of target proteins, 113
Ensembles of rotamers, 126
Entropy, 174
Entropy crisis, 174
ENZYME, vii, 62
Enzyme Committee (EC) number, 63
Equations of motion, 188, 273
Equilibrium molecular dynamics, 268
Equilibrium conditions, 195
Equilibrium distribution functions, 210
Equilibrium fluctuations, 209
Equilibrium sampling, 180
Ergodicity, 181
ERRAT, 138, 141, 147
Error, 280, 317
Error reduction, 254
Euclidian distances, 27
Euler integration, 265
Evaluating protein models, 138, 148
E-values, 66, 67
Evolutionary conserved residues, 90
Evolutionary distance, 80, 84, 90, 92
Evolutionary distant proteins, 70
Evolutionary history, 84
Evolutionary origin, 41
Evolutionary relatedness, 40
Evolutionary relationships between proteins, 35, 38, 57, 96
Evolutionary trends, 86
Ewald summation methods, x, 244, 247
Exact partition function, 181
Excess chemical potential, 262
Excluded volume, 182, 186
Expected value, 68
Expert Protein Analysis System (ExPASY), 62
Explicit solvation molecules, 137, 200, 267
Exposed regions, 108, 119
Extending gaps, 140
External boundary conditions, 263
External stimulus, 232
Factor analysis, 18
False positive, 65
False relationships, 317
Families of Structurally Similar Proteins (FSSP), 43
Family, vi, 38
Fast archiving, 313
Fast Fourier Transform (FFT), 249, 297
Fast multipole method (FMM), x, 244
Fasta, 99
FATCAT, 25
Feature isolation, 306
Feature pdf, 114, 115
Feature reduction, 317
Feature vectors, 35
Fibrous proteins, 7
Fick’s law, 274
<table>
<thead>
<tr>
<th>Subject Index</th>
<th>353</th>
</tr>
</thead>
<tbody>
<tr>
<td>Finite differences, 278</td>
<td></td>
</tr>
<tr>
<td>Finite difference grid, 250, 280</td>
<td></td>
</tr>
<tr>
<td>Finite difference iterative schemes, 252</td>
<td></td>
</tr>
<tr>
<td>Finite state machine, 73</td>
<td></td>
</tr>
<tr>
<td>Flawed models, 138</td>
<td></td>
</tr>
<tr>
<td>Flickers, 233</td>
<td></td>
</tr>
<tr>
<td>Fluctuating charge (FQ) model, 272</td>
<td></td>
</tr>
<tr>
<td>Fluctuation dissipation theorem, 188</td>
<td></td>
</tr>
<tr>
<td>Fluctuations, 277</td>
<td></td>
</tr>
<tr>
<td>Flux of charges, 274</td>
<td></td>
</tr>
<tr>
<td>Flux-based simulation, 239, 273</td>
<td></td>
</tr>
<tr>
<td>Fokker-Planck equation, 275</td>
<td></td>
</tr>
<tr>
<td>Fold, 38, 40, 41</td>
<td></td>
</tr>
<tr>
<td>Fold families, 35, 42</td>
<td></td>
</tr>
<tr>
<td>Fold overlap problem, 44</td>
<td></td>
</tr>
<tr>
<td>Fold recognition, 33</td>
<td></td>
</tr>
<tr>
<td>Folded protein, ix</td>
<td></td>
</tr>
<tr>
<td>Folded state, 175</td>
<td></td>
</tr>
<tr>
<td>Folding class, 10</td>
<td></td>
</tr>
<tr>
<td>Folding free energy barrier, 216</td>
<td></td>
</tr>
<tr>
<td>Folding kinetics, 12, 175, 183, 192</td>
<td></td>
</tr>
<tr>
<td>Folding nucleus, 207</td>
<td></td>
</tr>
<tr>
<td>Folding pathway, 197, 209</td>
<td></td>
</tr>
<tr>
<td>Folding process, ix</td>
<td></td>
</tr>
<tr>
<td>Folding progress, 179</td>
<td></td>
</tr>
<tr>
<td>Folding rate, ix, 170, 178</td>
<td></td>
</tr>
<tr>
<td>Folding routes, 175</td>
<td></td>
</tr>
<tr>
<td>Folding temperature, 175</td>
<td></td>
</tr>
<tr>
<td>Folding thermodynamics, 175, 183</td>
<td></td>
</tr>
<tr>
<td>Folding times, 174, 181, 186</td>
<td></td>
</tr>
<tr>
<td>Folding trajectories, 207, 208</td>
<td></td>
</tr>
<tr>
<td>FoldMiner, 25</td>
<td></td>
</tr>
<tr>
<td>Force, 250</td>
<td></td>
</tr>
<tr>
<td>Force fields, 125, 192, 268, 271</td>
<td></td>
</tr>
<tr>
<td>Force field parameterization, 192</td>
<td></td>
</tr>
<tr>
<td>Force field parameters, 271, 272</td>
<td></td>
</tr>
<tr>
<td>Four-helix bundles, 10</td>
<td></td>
</tr>
<tr>
<td>Fourier filtering, 309, 311</td>
<td></td>
</tr>
<tr>
<td>Fourier transform (FT), xi, 247, 296, 297</td>
<td></td>
</tr>
<tr>
<td>FRAGFINDER, 71</td>
<td></td>
</tr>
<tr>
<td>Fragment matching, 24</td>
<td></td>
</tr>
<tr>
<td>Fragment-base alignment, 87</td>
<td></td>
</tr>
<tr>
<td>Framework model, 171</td>
<td></td>
</tr>
<tr>
<td>Free energy, 176, 179, 270</td>
<td></td>
</tr>
<tr>
<td>Free energy calculation, 270</td>
<td></td>
</tr>
<tr>
<td>Free energy minimum, 216</td>
<td></td>
</tr>
<tr>
<td>Free energy surfaces, ix</td>
<td></td>
</tr>
<tr>
<td>Frequency domain, 297</td>
<td></td>
</tr>
<tr>
<td>Frequency information, 297</td>
<td></td>
</tr>
<tr>
<td>Friction coefficient, 264, 265, 281</td>
<td></td>
</tr>
<tr>
<td>Frustration, 173, 175, 214</td>
<td></td>
</tr>
<tr>
<td>Fukui function, 318</td>
<td></td>
</tr>
<tr>
<td>Full multigrid method, 257</td>
<td></td>
</tr>
<tr>
<td>Fully atomistic simulations, 190</td>
<td></td>
</tr>
<tr>
<td>Functional diversity, 11</td>
<td></td>
</tr>
<tr>
<td>Functional genomics projects, 3</td>
<td></td>
</tr>
<tr>
<td>Funnel-shaped free energy landscape, 170, 174</td>
<td></td>
</tr>
<tr>
<td>$\phi$-value analysis, ix, 201, 212</td>
<td></td>
</tr>
<tr>
<td>Gabor transform, 298</td>
<td></td>
</tr>
<tr>
<td>Gap, 23, 27, 68, 76, 87, 105, 110, 118</td>
<td></td>
</tr>
<tr>
<td>Gap penalty, 30, 90, 95</td>
<td></td>
</tr>
<tr>
<td>Gap residue parameters, 79</td>
<td></td>
</tr>
<tr>
<td>Gap-extending penalty (GEP), 98</td>
<td></td>
</tr>
<tr>
<td>Gapless fragments, 72</td>
<td></td>
</tr>
<tr>
<td>Gap-opening penalty (GOP), 98</td>
<td></td>
</tr>
<tr>
<td>Gapped alignment, 67</td>
<td></td>
</tr>
<tr>
<td>Gating, 242, 281</td>
<td></td>
</tr>
<tr>
<td>Gating ring, 235</td>
<td></td>
</tr>
<tr>
<td>Gauß-Seidel Method, 253</td>
<td></td>
</tr>
<tr>
<td>Gaussian multiwavelet basis, 315</td>
<td></td>
</tr>
<tr>
<td>GB/SASA, 192, 194</td>
<td></td>
</tr>
<tr>
<td>GenBank, 65</td>
<td></td>
</tr>
<tr>
<td>Gene sequence, 89</td>
<td></td>
</tr>
<tr>
<td>GeneDoc, 107, 122, 123</td>
<td></td>
</tr>
<tr>
<td>Generalized Born (GB) model, 192</td>
<td></td>
</tr>
<tr>
<td>Generalized ensemble methods, 180</td>
<td></td>
</tr>
<tr>
<td>Genetic algorithm, 24, 72, 319</td>
<td></td>
</tr>
<tr>
<td>Genetic algorithm/Partial least squares (GA/PLS), 319</td>
<td></td>
</tr>
<tr>
<td>Genetic code, 9</td>
<td></td>
</tr>
<tr>
<td>Genetic information, 3</td>
<td></td>
</tr>
<tr>
<td>Genome, v, 3, 61</td>
<td></td>
</tr>
<tr>
<td>GenTHREADER, 110</td>
<td></td>
</tr>
<tr>
<td>Geometric hashing, 24</td>
<td></td>
</tr>
<tr>
<td>Geometric properties, 33</td>
<td></td>
</tr>
<tr>
<td>Geometric similarity, 17</td>
<td></td>
</tr>
<tr>
<td>Glass transition temperature, 173, 175, 190</td>
<td></td>
</tr>
<tr>
<td>Global alignment, 66, 79, 86, 91, 99</td>
<td></td>
</tr>
<tr>
<td>Global energy minimum, 174</td>
<td></td>
</tr>
<tr>
<td>Global fluctuations, 209</td>
<td></td>
</tr>
<tr>
<td>Global minimum energy conformation, 125</td>
<td></td>
</tr>
<tr>
<td>Globin fold, 10</td>
<td></td>
</tr>
<tr>
<td>Globular proteins, 7, 9</td>
<td></td>
</tr>
<tr>
<td>Glycolipids, 237, 238</td>
<td></td>
</tr>
<tr>
<td>Gō-models, 190, 208</td>
<td></td>
</tr>
<tr>
<td>Gō-type potentials, 217</td>
<td></td>
</tr>
<tr>
<td>Gonnet matrices, 91, 95, 102, 140</td>
<td></td>
</tr>
<tr>
<td>Gramicidin A, x, 232</td>
<td></td>
</tr>
<tr>
<td>Grand canonical ensemble, 262</td>
<td></td>
</tr>
<tr>
<td>Graph theory, 132</td>
<td></td>
</tr>
<tr>
<td>Greediness, 88, 99</td>
<td></td>
</tr>
<tr>
<td>Greek key barrels, 10</td>
<td></td>
</tr>
</tbody>
</table>
Green's function, 245
Grid, 279
GROMOS, 124, 133, 192
GROMOS96, 63
Guide tree, 95
Haar wavelet, 305
Hartree-Fock equations, 315
Hartree-Fock exchange, 315
Helical proteins, 198
Heme group, 10
Hemerythrin, 10
Hemoglobin, 9, 35
Hen's egg-white lysozyme, 58, 85
Heteropolymer, 5
Heteroscedastic noise, 309
Heuristic approaches, 30
Heuristic search, 65
Hidden Markov models (HMMs), vii, 70, 73
Hierarchic classification, 40
Hierarchical clustering, 47, 197
Hierarchical simulation strategy, 283
High performance computing, 230
High-frequency noise, 309
Hinged proteins, 125
HIV reverse-transcriptase, 319
Homologous protein structures, 118
Homologous proteins, 113
Homologous sequences, 71
Homology modeling, vii, 57
Homoscedastic noise, 309
HOMSTRAD, 39, 62
Horse hemoglobin α, 58
Horse hemoglobin β, 58, 151
HP models, 182
HT model, 189
Human α-lactalbumin, 151
Human genome project, v
Human proteome, v
Hydrated ion, 235
Hydrated membrane/channel system, 242
Hydration shell, 239
Hydrogen bonds, 8, 28, 71, 138, 199, 233
Hydropathy index, 105
Hydropathy plots, vii, 108
Hydropathy profile, 108
Hydropathy score, 108
Hydrophilic amino acid residues, 98
Hydrophilic region, 98, 108
Hydrophobic collapse model, 171
Hydrophobic core, 7, 8, 10, 183, 198, 200
Hydrophobic effects, 174
Hydrophobic interactions, 190
Hydrophobic regions, 108
Hydrophobic residues, 108, 171, 183, 188
Hydrophobic sheets, 198
Hydrophobic sidechains, 232
Hydrophobic thickness, 238
Hypothesis-driven research, 3
Image charges, 282
Immunoglobins, 11
Implicit membrane models, 240
Implicit solvent treatment, 133, 192, 264
Implicit water models, 240
Importance sampling, ix, 197
Improving alignments, 104
In vivo folding, 219
Incorrect stereochemistry, 143
Incorrectly folded proteins, 138, 149, 219
Incorrectly threaded matches, 82
Informatics, x
Information, 301
Information compression, 295
Information cost, 308
Information entropy, 313
Information-rich descriptors, 317
Infrared spectral analysis, 320
Infrared spectral libraries, 313
Infrared spectroscopy, 311, 313
Inhomogeneous charge distributions, 262
Integration time step, 265
Internal distances matrix, 28
Internal electrostatic interactions, 263
International Union of Biochemistry and Molecular Biology (IUBMB), 63
InterPro, 39
Inverse wavelet transform, 302
Ion channel simulation, 230
Ion channels, ix, 229, 231
Ion permeation, 268
Ion pump, 9
Ion transport, ix, 8
Ionic charge transport, 229
Ionic concentration, 274
Ionic drift, 274
 Ionic flux, 231, 276
Ionic permeation, 281
 Ionic velocity, 277
Irregular property distributions, xi, 295
Ising model, 15
Isoelectric point, 108
Iterative methods, 254
Iterative Search, 69
JalView, 107, 112
3D-JIGSAW, 113, 119
Jelly roll barrels, 10
J-walking, 180

K2, 25
K2SA, 25
K-channel, 242
KcsA channel, 234
Kendrew models, 4
Keratin, 7
Kinetic $\phi$-values, 213
Kinetic traps, 183
K-means clustering, 47
Knot theory, 33, 35
Knowledge base, 113
Knowledge discovery, 14
Knowledge-based evaluation, 150
Knowledge-based potentials, 78
Knowledge-based rules, 121
Kohlrausch’s law, 274
KvAP channel, 234

Lactose intolerance, 85
Lagrange multipliers, 18
Langevan dynamics, ix, 211
Langevin equation, 188, 264, 265, 275
Langevin temperature equilibration, 134
Large proteins, 12
Large-scale fluctuations, 189
Latent frustration, 175
Lattice models, ix, 171, 179, 182
Lattice Monte Carlo simulations, 181
Lattice move sets, 185
Lattice site, 182
Learning, Observing and Outputting Protein Patterns (LOOPP), 78
Lennard-Jones potential, 188, 190, 192, 259
Levinthal paradox, ix, 170, 174
Like contacts, 184
Linnaeus, 2
Lipid bilayer, 231, 234, 236, 238
Lipid membrane, 229
Lipid mobility, 237
Lipid molecules, x
Lipid/protein interface, 241
LOAD (Library of Ancient Domains), 67
Local alignment, 79, 86, 99
Local average ionization potential, 318
Local energy minima, 180
Local fluctuations, 209
Local free energy minimum, 175

Local geometry matching, 24
Local interactions, 172
Local polarization fields, 283
Local resolution, 314
Local secondary structure, 28, 78
Local similarity, 24, 67, 84
Localized electric fields, 244
LOCK2, 25
Long-range electrostatics, 231
Long-range force, 244
Long-range interactions, x, 247
Long-time process, 194
Loops, 90, 105, 235
Loop regions, 11, 58, 78, 111, 120
Loop segments, 119
Low energy sequence, 183
Low-energy collapsed state, 186
Low-energy conformations, 135
LSQRMS, 25

Machine learning, 313, 316
Macromolecular Crystallographic Information File (mmCIF), 69
Macroscopic polarization behavior, 268
Main-chain conformation, 117
Mainly $\beta$ proteins, 9, 40
Many-body effects, 272
Markov models, 70, 71
Markov transition model, 28
Markovian random forces, 264
Mass spectrometry, 311, 313
Matching segments, 117
MATRAS, 25
Maximal common subgraph detection, 24, 65
Maximal segment pair (MSP), 67
Mean field approximation, x, 24, 274, 281
Mean structural properties, 274
Measures of similarity, 26, 27
Mechanical wire model, 58
Mechanical work, 235
Mechano-sensitive channels, 232
Melting curves, 176
Membrane, 231, 236
Membrane potential, 234
Membrane proteins, 7
Membrane-spanning pore, 235
MEMSAT, 110
Metafolds, 44
Metrics, 17
Metropolis Monte Carlo method, 171, 186
Meyer wavelet, 305
Mirror transformation, 29
Misalignment, 99, 101
Misaligned regions, 63
Misfolded compact states, 183
Misfolded proteins, 78
Misfolded regions, 63
Misplacement of side chains, 141
Mixed α-β proteins, 9, 40
Mobile ions, 243
MODELLER, 113, 119, 121, 122, 123, 187
MOE, 113, 119, 121, 122
Molecular dynamics, ix, 125, 133, 135, 147, 181, 199, 235, 236, 247, 267
Molecular mechanics, 115, 125, 132
Molecular pdf, 114, 115
Molecular superposition methods, 311
Molecules to Go, 13
MOLSCRIPT, 4
MONSTER, 79
Monte Carlo, ix, 24, 181, 186, 268
Monte Carlo step, 186
Most homologous template, 110
Mother wavelet, 301, 311
Motif-based secondary structure prediction, 110
Move set, 183, 185
MSD, 13
MthK channel, 234
Multicanonical sample, 180, 212
Multidomain protein structures, 14, 42
Multigrid iteration, 257
Multigrid methods, x, 254, 256, 280
Multiple folding nuclei, 209
Multiple folding pathways, 172
Multiple sequence alignment, 90, 100, 110
Multiple sequences, 84
Multiple template methods, vii, 65, 70, 72, 113, 118
Multipole expansion, 245
Multiresolution analysis (MRA), 304, 309, 312
Multistate folders, 177
Multistate models, 176
Mutants, 230, 236
Mutant channels, 243
Mutated residues, 89
Mutation, 90, 91, 212
Mutation probability scores, 91
Myoglobin, 4, 9, 35, 86

NAMD, 124, 133
Narrow channels, 282
National Center for Biotechnology Information (NCBI), 65
Native conformation, 143
Native contacts, 190, 207, 214
Native state, vii, viii, 182, 189, 204
Native structure, 7
NCBI-BLAST, 65
Nearest-grid-point (NGP) charge, 251
Neighbor-joining (NJ) tree, 87
Nernst-Planck equation, x, 274, 278
Nest iteration method, 257
Neumann method, 262
Newtonian dynamics, x
Newtonian mechanics, 265
Newton’s equations of motion, 172, 191
NMR-based protein structures, 69
NMRC LUST, 138, 146, 147
NMRCORE, 146, 147
Noise, 23, 296, 309
Noise of changing variance, 309
Noise types, 310
Noise wavelets, 309
Noncooperative folding mechanism, 189
Nonlinear wave functions, 314
Non-native conformations, 183
Non-native state minima, 180
Nonoptimal stereochemistry, 138
Nonperiodic boundary conditions, 262
Nonperiodic functions, 298
Nonpolar amino acid side chains, 8
Non-Redundant (NR) database, 65
Nonstationary signals, 298
NRL_3D, 13
Nuclear magnetic resonance (NMR) spectroscopy, 9, 23, 68, 232, 313
Nucleation, 207
Nucleation condensation model, 171, 194
Nucleic acids, 1, 68
Nucleic Acid Research, 61
Number of native contacts, 205

Off-lattice models, ix, 171, 172, 179, 187
OLDERADO, vii, 138, 146, 147, 148
Opening gaps, 140
OPLS, 192
Optimal alignment, 14, 23, 101
Optimal correspondence, 24
Optimal fit bias, 31
Optimal fitting, 301
Optimal signal representation, 308
Optimal wavelet, 306, 311
Optimally aligned residues, 86
Optimization method, 135
Order parameters, 203, 214
Organelles, 2
Ornstein-Zernike equation, 262
Orthogonal wavelet, 305
Outliers, 27, 31

Pairwise alignment, 90
Pairwise residue matches, 99
Pairwise superposition, 146
PAM1, 92
PAM250, 92
Parallel tempering, 180
Parsimonious models, 317
Partial least squares (PLS), 319
Particle-based simulations, 263
Particle-mesh Ewald (PME) method, 249
Particle-Particle-Particle-Mesh (P3M) method, 244
Partition function, 182
Patch-clamp fluorescence microscopy, 233
Pattern recognition, 316, 320

**Pattern-Hit Initiated BLAST (PHI-BLAST), 66**

PDB at a Glance, 13
PDB ID, 69
PDB90, 43
PDBSum, 13
PDP, 16
Penalty functions, 147
Peptide bond, 5
Peptides, 68
Periodic boundary conditions, 243, 246, 261
Periodic systems, 249
Pfam, 39, 62
Phase space, 263
Phase transition, 173, 174
PHD, 110
pH-gated channels, 236
Phosphatidylcholine, 237
Phosphoglycerides, 237
Phospholipids, 237
Phospholipid bilayer, 7
Photoacoustic spectroscopy, 311
PHYLIP, 96, 97
Phylogenetic trees, 96, 99
phylogeny, 2
Physicochemically similar proteins, 84
PISCES, 13
Pittsburgh Supercomputer Center, 122
Plasma simulations, 263
Point dipole (PD) model, 272
Point mutation, 212
Point-Accepted Mutation (PAM) matrices, 91, 92, 140
Poisson-Boltzmann equations, 192
Poisson-Nernst-Planck (PNP) method, x, 278
Poisson’s equations, x, 231, 245, 248, 252, 275
Polarizable-SPC (PSPC) model, 272
Polarization, 272, 281
Polarization field, 272
Polypeptide approximate conformation, 117
Polypeptide loops, 122
Polysaccharides, 85
Pores, 232
Porin channels, 239
Porins, x, 8, 235
Position-specific scoring matrix (PSSM), 66
Postsmoothing, 256
Potassium channels, 234
Potential energy function, 191
Potential energy surface (PES), 191
Potential gradient, 274
Potential of mean force (PMF), 142, 147, 197, 270
Power series expansion, 266
PREDATOR, 110
Predicting protein structure, 9
Prepeptide, 89
Preprotein, 89
Presmoothing, 256
PRIDE, 25
Primary structure, 7, 90
Primitive Cartesian Gaussian basis functions, 314
Principle of microscopic reversibility, ix, 195
Principle of minimum frustration, 175
PRINTS, 39
PRISM, 25
Probability density functions (PDFs), 113, 275
Probability fluxes, 276
Probability tables, 140
Probable sequences, 67
Probable templates, 71, 82
PROCHECK, vii, 133, 138, 147
PRODOM, 39
PROF, 110
Profiles, 28, 66, 73, 91
Progressive alignment, 87, 95, 98
Prolongation, 256
ProSa, vii, 124, 142, 147, 153
PROSITE, vii, 39, 62
PROSUP, 25
Protein building blocks, 5
Protein channel, 231
Protein conformation space, 32
Protein conformations, 179
Protein crystallization, vi
Protein Data Bank (PDB), vii, 8, 13, 38, 63, 65, 68, 88, 120
Protein domain assignment, 16
Protein domain class, 40
Protein domains, vi, 12
Protein engineering, 216, 243
Protein fold space, viii
Protein folding, 61, 194
Protein folding class, 10
Protein folding mechanism, 171
Protein folding process, 170
Protein folding thermodynamics, 189
Protein function, 60
Protein gates, 229
Protein $\alpha$-helix, 7, 58, 105, 187, 232
Protein Information Resource (PIR), 39, 65
Protein models, 179
Protein packing, 78
Protein relaxation times, 179
Protein Research Foundation (PRF), 65
Protein $\alpha$-sandwich, 187
Protein secondary structure, 73
Protein shape descriptors, 33, 35
Protein $\beta$-sheets, 7, 105, 187, 198, 232
Protein $\beta$-strands, 7, 90, 235
Protein structural domains, 15
Protein structure, 1, 4, 61, 170
Protein structure alignment programs, 25
Protein structure classifications, vi, 1, 35, 62
Protein structure comparisons, vi, 14, 35
Protein structure hierarchy, 5
Protein Structure Initiative (PSI), v
Protein structure resources, 13
Protein structure similarity, 14
Protein structure space, 44
Protein structure superposition, 23, 26
Protein transition states, 201
Protein unfolding, 195
Protein-nucleic acid complexes, 68
Proteins, v, 1, 231
$\alpha$ Proteins, 9, 40
ProtoMap, 39, 144
PROVE, vii, 138, 147
Pseudo-metric, 35
Pseudo-protein models, 74
PSI-PRED, 81, 110
3D-PSSM, 113, 119
PUU, 16, 42, 43
Pyramid algorithm, 304
Quantitative Structure Activity Relationship (QSAR), xi, 73, 296, 316
Quantitative Structure Property Relationship (QSPR), xi, 296, 316
Quantum chemistry, xi, 296, 314
Quaternions, 18
QuickSearch, 69
Radial distribution function (RDF), 268
Radius of curvature, 33, 217
Radius of gyration, 90, 105
Random coil, 90, 105
Random energy model (REM), 174
Random heteropolymers, 173
Random noise, 188
Random search through conformational space, 183
Rate-limiting step in protein folding, 189, 202
RCSB consortium, 13
Reaction coordinate, 176, 197, 202
Reaction models, 176
Real space, 245
Reciprocal space, 245
Reduced amino acid representations, 181
Reduced protein models, 187
Reduced redundant transformations, 302
Reference force, 259
Refinement, 119, 124
Refolding process, 178
Regression, xi, 316, 320
Relational database, 14
Relaxation time, 180, 238
Replica methods, 174
Replica-exchange (REX), ix, 199, 200
Replica-exchange molecular dynamics (REMD), 200
Residue burial, 76
Residue pattern, 66
Residues, 5, 58
Resources for classification of protein sequences, 39
Restraining potential, 216
Restriction, 256
Retinal binding proteins, 116
Reverse position-specific BLAST (RPS-BLAST), 66
Reverse transform, 301
Ribosome, 89
Ridges, 302
Rigid-body transformation, 16
RMS/coverage plot, 33
Rotamer library, 121, 126
Rotamer searches, 125
Rough energy landscape, 173
Rugged energy landscape, 187
Salt bridges, 5
Sampling methods, 199
SAM-T02, 119
Sandwich topologies, 11
SARF2, 25
Satisfaction of Spatial Restraints, 113
Savitzky-Golay smoothing, 309, 311
Scaffold, 74, 76, 78, 119, 197
Scaled Gauss metric (SGM), 35
Scaling, 230
Scaling function, 303
Schrödinger equation, 314
Scientific classification, 2
Score, 95
Scoring functions, 26, 27
SearchStatus, 69
SearchFields, 69
SearchLite, 69
Secondary structure, 7, 41, 76, 79, 86, 89, 126, 132, 176, 200
Secondary structure elements (SSE), 8, 24, 40, 90, 118
Secondary structure prediction, 78, 110
Segment match modeling, 115, 116
Selecting templates, 104
Selectivity, 232
Selectivity filter, 234, 271
Self-consistency, 263, 279
Self-consistent simulation programs, 252
Self-force, 251
Sequence, 7, 10
Sequence alignment, 65, 70, 84
Sequence Alignment and Modeling (SAM), 70, 119
Sequence alignment methodologies, 86
Sequence identity, 81
Sequence similarity, 13, 57, 61, 73
Sequence to Coordinates (S2C) website, 88
Sequence-dependent thermodynamics, 183
Sequential folding, 172
SHAKE, 192
Shape descriptors, 33, 35
SHEBA, 26
Short time scales, 172
Short-range forces, x, 244, 258
Short-range interaction, 238, 271
Short-time Fourier transform (STFT), 298, 299
Side chains, 5, 105, 117, 119, 121
Side-chain conformational libraries, 126
Side-chain conformers, 137
Side-chain geometries, 125
Side-chain packing, 28
Side-Chains with Rotamer Library (SCWRL), vii, 125
Signal basis, 307
Signal characterization, 312
Signal cleaning, 296, 309
Signal components, 296
Signal compression, xi, 306, 313
Signal critical points, 312
Signal feature isolation, xi, 312
Signal information, 313
Signal noise, 309
Signal processing methods, xi, 295
Signal representation, 307
Signaling segment, 89
Silk, 7
Similarity, 14, 24, 29, 47, 66
Similarity matrix, 67, 86, 90, 91
Similarity measures, 43
Similarity score, 27, 32
Simple exact models, 181
Simple Modular Architecture Research Tool (SMART), 39, 67
Simple point charge (SPC) model, 269
Simulated annealing, 24, 125, 135
Simulated tempering, 180
Simulation box, 261
Simulation of protein folding, 169
Simulation techniques, 179
Single linkage clustering, 42, 47
Single template structure, 118
Single-domain proteins, 176
Singular value decomposition (SVD), 17, 18
Site-directed mutagenesis, 212
Size-dependent decomposition (SVD), 17, 18
Size-dependent artifacts, 262
Skeletal models, 4
Skeleton wavelets, 302
Smoluchowski equation, 276
Smoothing, xi
Smoothing algorithm, 310
Solvation effects, 242
Solvation state, 271
Solvent, 267
Solvent accessibility, 28
Solvent exposure, 76
Solvent viscosity, 188
Solvent-accessible surface area (SASA), 78, 140, 192
Space scales, x, 241
Space-filling models, 4
Spatial inhomogeneities, 263
Spatial restraints, 113
SPC/E, 133, 269
Specialized proteomic databases, 80
Spectral compression, 313
Spectroscopy, xi
Sperm whale myoglobin, 58, 83, 85, 122, 151
Spherical harmonics, 246
Sphingolipids, 237
Spin glass systems, ix, 172, 174, 199
Spline wavelet, 305
Spurious relationships, 319
SRS, 13
SSAP, 26, 28, 42
SSM, 26
Statistically sound model, 60
Stereochemical assignments, 138
Stochastic difference equation (SDE), ix, 194
Stochastic separatrix, 204
Stopped-flow kinetics, 177
STRIDE notation, 71, 89
STRUCTAL, 29, 30
Structural biology, vi, 2
Structural classification methods, 38
Structural Classification of Proteins (SCOP), vi, 3, 32, 39, 40, 44
Structural domains, 14
Structural family, 120
Structural features, 86
Structural genomics projects, 3, 35
Structural molecular biology, 1
Structural relatedness, 40
Structural similarities, 16
Structural variance, 146
Structurally conserved regions (SCRs), 90, 118
Structurally variable regions (SVRs), 90, 118
Structure alignment, vi, vii
Structure databases, 1, 35
Structure of water, 239
Structure-based alignment, 90
Substructure, 23, 24
Successive overrelaxation (SOR) method, 254
Supercoiled DNA, 35
Superfamily, vi, 38, 40
Super-secondary structures, 7
Surface property distributions, 318
Surface Volume (SurVol), 144
Swiss Institute for Bioinformatics, 62
SWISS-MODEL, vii, 62, 119
SWISS-PROT, vii, 62, 65
Symmlet wavelet, 305
Systematic classifications, 2
SYSTERS, 39
Target, 58, 59, 67, 84, 116
Target protein, 68
Target sequence, 90
Target-template alignments, 80, 122
Taylor expansion, 246, 275
T-Coffee, vii, 99, 102, 112
Temperature, 200
Template, 57, 58, 59, 84, 90, 116
Template protein, 88
Template selection, 122
Template structure, 104
Temporal information, 297
Tertiary structure, 7, 90, 101, 115, 140, 176
Theoretical protein models, 68
Thermodynamic equilibrium, 179
Thermodynamic φ-values, 213
THREADER, 78, 81
Threading, vii, 71, 73
Threading algorithm, 79
Threading Expert, 81
Threading Onion Model (THOM), 79
Three-state model, 176, 189
TIGRFAMS, 39
TIM (triose phosphate isomerase), 12
TIM barrel, 12
Time domain, 297
Time scale, x, 172, 189, 192, 232, 240, 241
Time step, 192, 265
Time-dependent wave function, 315
Tinker, 124, 133
TIP3P, 133, 198
TIP4P, 133
TIP4P-Ew, 133
TIP4P-FQ, 273
TOPS, 10, 13, 26
TOPSCAN, 26
Training sets, 72
Transferable atom equivalent (TAE) descriptors, 317
<table>
<thead>
<tr>
<th>Subject Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>Transferable intermolecular potential functions (TIPS), 269</td>
</tr>
<tr>
<td>Transformed wavelet, 301, 302</td>
</tr>
<tr>
<td>Transition path sampling, 210, 212</td>
</tr>
<tr>
<td>Transition state, ix, 199, 201, 202, 206, 211, 216</td>
</tr>
<tr>
<td>Transition state ensemble (TSE), ix, 201</td>
</tr>
<tr>
<td>Transition state theory (TST), 202</td>
</tr>
<tr>
<td>Translation variable, 303</td>
</tr>
<tr>
<td>Transmembrane helices, 234</td>
</tr>
<tr>
<td>Transport equations, 276</td>
</tr>
<tr>
<td>Tree of protein fragments, 14</td>
</tr>
<tr>
<td>TrEMBL, 62</td>
</tr>
<tr>
<td>Triangular inequality, 32</td>
</tr>
<tr>
<td>Triangular-shaped-cloud (TSC) charge, 251</td>
</tr>
<tr>
<td>TRIBES, 39</td>
</tr>
<tr>
<td>Triple-zeta basis sets, 314</td>
</tr>
<tr>
<td>Tsallis ensemble, 180</td>
</tr>
<tr>
<td>Turn regions, 41</td>
</tr>
<tr>
<td>Two-dimensional models, 182</td>
</tr>
<tr>
<td>Two-grid iteration, 256</td>
</tr>
<tr>
<td>Two-hit search method, 67</td>
</tr>
<tr>
<td>Two-state folders, 177, 201, 212</td>
</tr>
<tr>
<td>Two-state folding, 183</td>
</tr>
<tr>
<td>Two-state kinetics, ix</td>
</tr>
<tr>
<td>Two-state models, 176</td>
</tr>
<tr>
<td>Type II diabetes, 219</td>
</tr>
<tr>
<td>UCSF Chimera, 85, 112, 138</td>
</tr>
<tr>
<td>Ultra violet circular dichroism (UVCD), 176</td>
</tr>
<tr>
<td>Ultraviolet-visible spectroscopy, 311, 313</td>
</tr>
<tr>
<td>Umbrella sampling, 212, 271</td>
</tr>
<tr>
<td>UNDERTAKER, 70</td>
</tr>
<tr>
<td>Unfolded state, 174, 175, 176, 200</td>
</tr>
<tr>
<td>Unfolding rate, 178, 206</td>
</tr>
<tr>
<td>Unfolding trajectories, ix, 195</td>
</tr>
<tr>
<td>Unfolding transition states, 206</td>
</tr>
<tr>
<td>UniProt, 39, 62</td>
</tr>
<tr>
<td>Unlike contacts, 184</td>
</tr>
<tr>
<td>Unsuitable geometries, 142</td>
</tr>
<tr>
<td>Valence regions, 314</td>
</tr>
<tr>
<td>van der Waals forces, 258</td>
</tr>
<tr>
<td>van der Waals surface, 241</td>
</tr>
<tr>
<td>van’t Hoff derived enthalpies, 176</td>
</tr>
<tr>
<td>Variable regions, 116, 121, 137</td>
</tr>
<tr>
<td>Variable target function method (VTFM), 115</td>
</tr>
<tr>
<td>Vassiliev knot invariants, 35</td>
</tr>
<tr>
<td>VAST, 26</td>
</tr>
<tr>
<td>Verify3D, vii, 124, 138, 140, 147, 151</td>
</tr>
<tr>
<td>Verlet algorithm, 188, 267</td>
</tr>
<tr>
<td>Verlet integration, 266, 269</td>
</tr>
<tr>
<td>Viruses, 68</td>
</tr>
<tr>
<td>Visualization, 4</td>
</tr>
<tr>
<td>VMD, 4, 138, 233, 236</td>
</tr>
<tr>
<td>Voltage-activated gate, 235</td>
</tr>
<tr>
<td>Voltage-sensor paddle, 235</td>
</tr>
<tr>
<td>Voltammetry, 311</td>
</tr>
<tr>
<td>Voronoi method, 144</td>
</tr>
<tr>
<td>Wang Landau method, 180</td>
</tr>
<tr>
<td>Washington University-BLAST (WU-BLAST), 68, 71</td>
</tr>
<tr>
<td>Water, 192, 263, 267</td>
</tr>
<tr>
<td>Water models, 268, 273</td>
</tr>
<tr>
<td>Water transport, 233</td>
</tr>
<tr>
<td>Wave function, 314</td>
</tr>
<tr>
<td>Wavelets, 295</td>
</tr>
<tr>
<td>Wavelet analysis, 305</td>
</tr>
<tr>
<td>Wavelet coefficient descriptors (WCDs), 317</td>
</tr>
<tr>
<td>Wavelet coefficients, 305, 310</td>
</tr>
<tr>
<td>Wavelet compression, 313</td>
</tr>
<tr>
<td>Wavelet families, 305</td>
</tr>
<tr>
<td>Wavelet function, 300, 303</td>
</tr>
<tr>
<td>Wavelet neural network (WNN), 313</td>
</tr>
<tr>
<td>Wavelet packet transform (WPT), 307</td>
</tr>
<tr>
<td>Wavelet selection, 306</td>
</tr>
<tr>
<td>Wavelet space, 296, 302, 303, 318</td>
</tr>
<tr>
<td>Wavelet thresholding, 310</td>
</tr>
<tr>
<td>Wavelet transform (WT), x, 295, 300</td>
</tr>
<tr>
<td>Weighted histogram analysis method (WHAM), 180, 181, 187, 190</td>
</tr>
<tr>
<td>Weighted superpositions, 21</td>
</tr>
<tr>
<td>Writhe, 33</td>
</tr>
<tr>
<td>X-ray absorption, 313</td>
</tr>
<tr>
<td>X-ray crystallography, 9, 23, 68, 144, 146</td>
</tr>
<tr>
<td>X-ray spectroscopy, 234</td>
</tr>
<tr>
<td>Z-scores, 43, 76, 81, 143</td>
</tr>
</tbody>
</table>