

INDEX

- activated process, 54, 116, 131
 - reaction coordinate, 131, 172
 - simulation by activated molecular dynamics, 73–5
- activation volume, 135
- adiabatic mapping, 35–7, 46, 54–7, 117–18
- convergence, 55–7
 - DNA helix bending, 145–7
 - DNA helix twist, 125, 145–6
 - DNA melting, 125
 - global motions, 138
 - hinge bending: lysozyme, 140; tRNA, 147–9
 - large scale deformations, 54, 57, 139
 - myoglobin, 118
 - thermodynamic considerations, 47, 55
 - tyrosine ring flip, 54, 119–20
- adopted basis set Newton–Raphson method, 49
- allosteric transitions, 172
- alpha helix, 15
- AMBER, 181
- anharmonicity, 36, 59, 72, 82–4, 99, 107, 109–10, 116, 162
 - quasiharmonic approximation 67–8
- anisotropy, 81, 84, 107–9
- antibodies, 137
 - hinge bending, 149
- antibody–antigen interactions
 - flexibility, 169
- arabinose-binding protein
 - hinge bending, 141, 144, 169
 - ligand binding, 172
 - solvation, 150, 172
- argon, liquid, 62, 65
- array processors, 159
- atom type, 183, 185

- base pairing, 18–19
- base stacking, 19

- Beeman method, 174–5
- beta sheet, 15
- bond angle
 - potential function, 40
- Born–Oppenheimer treatment, 39, 42, 66
- Brownian dynamics, 37–8, 75–8, 161, 171
 - diffusional encounter, 152–4, 165, 170
 - DNA helix bending, 146
 - hydrodynamic interactions, 77
 - Langevin equation, relationship, 139
 - large scale motions, 139
 - local motions, 145
 - protein denaturation, 142
 - rate constant calculations, 77–8
- catabolite activator protein, 170
- CEDAR, 181
- CHARMM, 181
- collagen, 32
- collision frequency, 93–5, 190
- computer programs
 - description, 181–7
- computing methods
 - advances in hardware, 158–60
 - advances in methodology, 160–1
- conjugate gradient, 47–8, 51–3
 - convergence on quadratic surface, 51
 - efficiency, 52
- constraints
 - during molecular dynamics, 176–80
 - forces, 46
- coordinate file, 45, 183
- correlation function, time
 - definition, 84
 - Langevin oscillator, 95
 - range of validity, 94
- counterion condensation, 19
- covalent bond
 - potential function, 40
- crankshaft motions, 112

230 *Index*

- cutoff distance, 40, 184
 cytochrome c, 14, 80, 98
 collective motions, 82, 87–9, 91
- Debye–Hückel model, 153
 Debye–Waller factor, 97
 denaturation, 31, 33
 Brownian dynamics, 142
 local, 138, 142
 molecular dynamics, 97
 descent techniques, iterative, 50
 dielectric coefficient, 42
 distance-dependent, 42
 effective, 43–4
 scaling, 105
 dielectric constant, 153
 liquid hydrocarbons, 10
 water, 10
 dielectric screening, 40, 42–3, 97, 105, 150, 171
 diffusion, 26
 Brownian dynamics simulations, 37, 75–8, 152–4, 165, 170
 denaturation, 138, 142
 Einstein relationship, 26, 93
 flexible solutes, 27
 gated, 34, 155
 hydrodynamic interactions, effects of, 33, 76–7
 in solids, 132
 internal motions in macromolecules, 93
 intramolecular flexibility, 145: tRNA, 147
 ligand binding, 34, 154, 165
 molecular associations, 151–2, 170:
 superoxide dismutase, 152–4
 oxygen in protein, 104
 rotational, 93, 100
 diffusion coefficient, 26
 hydrodynamic models, 77
 relative, 33, 76
 water at protein surface, 86
 diffusional encounter, 33, 151–4
 dispersion forces, 16, 19
 distribution functions
 moments, 82, 107
- DNA
 A-DNA, 19
 atomic displacements, 107
 B-DNA, 19
 B–Z transition, 33, 130
 double helix, 19
 function, 1
 helix bending, 145–7
 helix twist, 125, 145–6
 hydration, 19
 left-handed, 3, 19
 molecular weight, 3
 secondary structure, 3, 18–19; melting, 125
 structure: reviews, 19;
 sequence-dependence, 3, 112–13
 sugar pucker, 125
 torsional stiffness, 114
 Z-DNA 19, 107, 111–14, 127; structure refinement, 162
- electron transfer, 39, 171
 electrostatic interactions
 diffusional encounter, 153–4
 polarization effects, 39, 42, 132–3, 135;
 modeling, 171
 potential function, 40
 solvent screening, 11, 19, 44, 153–4
 energy minimization, 36, 47–54
 Crystallographic refinement, 46
 molecular dynamics: relationship, 44–7
 thermodynamic considerations, 47
- enthalpy
 activation, 135
 entropy, 36, 47, 121
 activation, 135
 configurational, 66
 hydration, 9
 ligand binding, 118
 molecular association, 22–3, 169
 normal mode analysis, 67
 quasiharmonic approximation, 67
 thermodynamic cycle perturbation method, 166
 umbrella sampling, 69
 vibrational, 130
- enzyme activity, 167–8
 equations of motion, 46, 61–2
 numerical integration, 173–80
 experimental methods
 reviews, 5
 extended atoms, 58, 182
- flash photolysis, 123
 fluorescence depolarization, 104
 hinge bending motions, 144–5
 simulation, 146
 fluorescence quenching, 104
 free energy calculations, 66–73
 ligand binding, 166
 normal mode analysis, 67
 perturbation theory, 69–70
 potential of mean force, 69
 solvation, 70
 thermodynamic integration, 72
 umbrella sampling, 68, 120
 friction coefficient, 26, 77
 effect on reaction rate, 131
- gated process, 133–4, 170
 ligand binding, 123, 136, 155–6, 166, 169
 ring rotations, 133
 tyrosine ring flip, 121
 Gear method, 176

- Gibbs free energy, 67
 grid search, 48, 53
 GROMOS, 181
- Haemoglobin
 function, 1
 ligand binding, 154, 165
 protein exchange, 103
 harmonic oscillator, 59
 Langevin equation, 92–3, 110, 140
 multidimensional, 59
 Helmholtz free energy, 67, 70
 hexokinase
 hinge bending, 145
 hydration
 ionic, 10, 25–6
 ligand binding, 171
 nonpolar solutes, 8–9
 nucleic acids, 19
 potential functions, 42–3
 proteins, 14
 hydrodynamic models, 76–7
 hydrogen bond, 7, 182–4, 186
 geometry, 182
 in proteins, 15
 motions, 103–4, 110–11
 potential function, 41, 186
 hydrogen exchange
 DNA, 125–6
 models, 103
 nucleic acids, 33
 proteins, 102–4
 hydrophobic effect, 10–11, 13, 16, 19
- ice
 structure, 8
 immunoglobulins
 hinge bending, 145
 infrared absorption spectroscopy, 57
 intercalation, 34, 130
 internal coordinates, 45, 49, 182
 internal energy
 normal mode analysis, 67
 umbrella sampling, 69
 ions
 hydration, 10, 25–6
- lac repressor, 163
 hinge bending, 169–70
 Langevin equation, 27
 Brownian dynamics, relationship, 139
 effective friction constant, calculation, 94
 harmonic oscillator, 92–3, 110, 140
 internal motions, 35, 55, 92–4, 138, 140
 stochastic boundary conditions, 64
 leapfrog method, 174
 ligand binding, 67, 117, 165–6
 hydration effects, 171
 perturbation theory, 72
 proteins, 2–3
- liquid structure, 116
 lysozyme
 hinge bending, 90, 140–4
- mean square displacement matrix, 81
 minimum image convention, 63
 models, phenomenological, 27–8, 91–5, 165
 molecular association, 22–4, 33–4, 168–70
 dynamics, 151–6
 hydration changes, 34
 protein–DNA interactions, 23
 reviews, 24
 solvent effects, 43
 molecular dynamics, 6, 36–7, 60–6
 activated molecular dynamics, 73–5,
 117; oxygen in myoglobin, 165–6;
 tyrosine ring flip, 118–23
 activated processes, 37
 active site, 37, 64–5
 constant pressure, 64, 188–9, 191–3
 constant temperature, 64, 188–91
 constrained, 38, 176–80
 crystal environment, 84
 crystallographic refinement, 65, 162–3
 DNA, 146; instability, 105; table, 106
 energy conservation, 62
 energy minimization, 65; relationship,
 44–7
 equilibration, 187
 history, 62
 large scale deformations, 57, 139
 ligand binding, 165–6
 limitations, 65–6, 157
 low temperature, 65, 163
 Monte Carlo, comparison, 38, 66
 periodic boundary conditions, 45, 63, 160
 quantum corrections, 38–9
 rare events, 37
 solvent, 62, 159; effects, 84–5, 107;
 mobility, 85–6
 stochastic boundary conditions, 65, 160
 structure refinement, 65, 161–4
 thermodynamic considerations, 47
 thermodynamic ensembles, 64, 188–9
 warmup, 187
 molecular mechanics, 39, 44, 58
 Monte Carlo method, 6, 38
 efficiency, 38, 66
 molecular dynamics, comparison, 38, 66
 normal modes, 161
 Mossbauer spectroscopy, 102
 motions, intramolecular
 amplitude, 80–2, 87, 107, 115; solvent
 effects, 85–6; table, 29;
 time-dependence, 84, 87
 anharmonicity, 36, 59, 72, 82–4, 99, 107,
 109–10, 116, 162; quasiharmonic
 approximation, 67–8
 anisotropy, 81, 84, 107–9
 antigenicity, relationship, 169

232 *Index*

- motions, intramolecular – *cont.*
 base pair melting, 33
 charge effects, 32
 collective, 87–91, 115–16
 comparison of proteins and nucleic acids, 32
 correlations, 84, 88–9, 98, 110–12, 116
 damping, 30–1, 75, 80, 93, 115–17, 137, 149–50; DNA bending, 146; lysozyme hinge bending, 141; tRNA, 149
 elastic, 30–2, 137–8, 140, 144, 146, 149
 experimental comparisons, 96–105, 115, 142, 144–5, 147
 global, 30–2, 137–50; biological significance, 137; nucleic acids, 145–9; proteins, 139–45
 helix-coil transition, 31, 142–4
 hinge bending, 29–32, 139–45;
 arabinose-binding protein, 141, 144, 169; lac repressor, 169–70; ligand binding, 155; lysozyme, 90, 140–4; ribonuclease, 90; tRNA, 147–9
 hydrogen bonds, 103–4, 110–11
 ligand binding, 154–5, 165–6
 local unfolding, 31, 142–5
 methyl groups, 100–2
 nucleic acids, 31–3
 packing rearrangements, 30
 proteins, 28–31
 rapid, 28, 31, 79–116; nucleic acids, 105–15; proteins, 80–105
 secondary structure, effects, 32
 sugar repuckering, 32, 126–9
 table, 29
 time scale, 115; table, 29
 torsions, 111–12, 117
 tyrosine rotation, 28, 31, 54, 118–23, 172; experiments, 124
 moving pictures, 108, 113
 multiple minima
 effects on dynamics, 83
 multiple minimum problem, 164
 muscle contraction, 137
 myoglobin
 collective motions, 89
 ligand binding, 57, 68, 118, 123, 135, 154, 165–6
 local motion, 98–9
 methyl group motions, 101
 Mossbauer spectroscopy, 102
 structure refinement, 162
 myosin
 hinge bending, 145

 neutron scattering, 104
 Newton–Raphson method, 48–9
 nonbonded exclusions, 184
 nonbonded interactions
 cutoff distance, 40, 184
 hydration effects, 42–3
 potential function, 40
 nonbonded pair list, 184
 normal mode analysis, 36, 57–60, 99, 138
 anharmonic effects, 36, 59, 67, 83–4, 91, 105
 damping effects, 105
 DNA, 107, 113–15, 146
 hinge bending, 140
 low frequency motions, 89–90
 Monte Carlo methods, 161
 moving pictures, 60
 solvent effects, 37
 torsion space, 89–90
 thermodynamic parameters, 67
 nuclear magnetic resonance
 dynamic information, 100–5, 123–4
 structure refinement, 163–4
 nuclear Overhauser effect, 100, 163–4
 nucleic acids
 dynamics, 4, 31–3
 function, 1–2
 structure, 3, 16–22; primary, 16–17; reviews, 22; secondary, 18–21; tertiary, 19–21
 nucleosome, 137, 146

 order parameter, 100–2

 parameter file, 45, 184
 partial charges, 185
 scaling, 42, 105
 path integrals, 39, 43
 penicillopepsin, 155
 periodic boundary conditions, 45, 63
 fluctuating, 160, 191–3
 longitudinal, 105
 perturbation theory, 69–72
 hydration, 71
 polar hydrogen, 182
 polyelectrolyte, 34, 105
 potential energy, 187
 potential energy function, 39–45, 58
 approximations, 170–1
 hydration effects, 42
 polarization effects, 170
 potential of mean force, 39–40, 42, 55, 59, 67, 83, 92–3, 120, 131, 138–9, 142, 150, 160, 165, 171
 umbrella sampling, 69
 potential of mean torque, 92
 proteins
 dynamics, 4, 28–31
 function, 1–2
 structure, 3, 11–16; prediction, 164; primary, 11–12; reviews, 16; secondary, 15; tertiary, 16
 pseudodihedral, 53
 pseudorotation pathway, 126, 129

Index

233

- quantum effects, 38–9, 60, 66, 96
 simulation, 167
- quasiharmonic approximation, 36, 67–8,
 138, 160
 effects of multiple minima, 36
- Raman spectroscopy, 57
- rate constant, 135
- reaction coordinate, 46, 54–5, 66–7, 73
 choice of, 74, 172
 transition state, 131
 tyrosine ring flip, 119
- ribonuclease
 hinge bending, 90
 hydrogen exchange, 103
- SHAKE, 174–80
- site-directed mutagenesis, 167
- Smoluchowski theory, 151–2
- solutions, aqueous
 nonpolar solutes, 8–9
 polar solutes, 10
- steepest descent, 47–53
 efficiency, 51
 step size, 50
- Stokes law, 26
- internal molecular motion, 141
- structure
 dependence on time scale, 6
 refinement by computer simulation, 65,
 161–4
- sugar pucker, 21, 129
 DNA helix twist, 125
 fluctuations, 111, 127–30
 purines vs pyrimidines, 125–7
 repuckering, 126–30
- supercomputers, 158–60
- superoxide dismutase, 152–4, 165
- surface area, solvent-accessible, 43
 correlated to motions, 108
- temperature factor, 91, 97, 162
 antigenicity, relationship, 169
 contributions to, 97
 correlations, 162
 hydrogen exchange, relationship, 104
 simulation, 162
 tRNA, 107
- theoretical methods, 35–78
 reviews, 4
- thermodynamic cycle perturbation method,
 71–3
 enzyme activity, 167–8
 ligand binding, 72, 166
 umbrella sampling, comparison, 71
- topology file, 45, 183, 186
- torsions
 backbone: nucleic acids, 17; proteins, 11
 improper, 183
 potential function, 40
 sugar, 129
- trajectory, 46
- transition state theory, 131–6
 nonequilibrium effects, 135
- transitions, local, 117–36
 biological relevance, 134
 damping, 133
 nucleic acids, 124–31
 proteins, 118–24
 time scale, 117
- transmission coefficient, 73, 131–2
 calculation, 75
 tyrosine ring flip, 121
- triosephosphate isomerase, 155
- tRNA
 anticodon–codon interaction, 2
 crystal structures, 20
 hinge bending, 147–9
 hydrogen bond motions, 110–11
 local motions, 106–11
 molecular dynamics, 106, 185–7
 molecular weight, 3
 structure, 19–21
- tropomyosin, 32
- trypsin, 85, 145, 155
 enzyme activity, 167
 ligand binding, 166
 molecular dynamics, 159
- trypsin inhibitor, 80
 collective motions, 89, 91
 global motions, 139
 hydration, 84–5, 94, 100
 local motions, 80–1, 83
 methyl group motions, 100–2
 neutron scattering, 104
 normal mode analysis, 60, 83, 89–90,
 104
 structure refinement, 162, 164
 tyrosine librations, 31, 91–5, 104
 tyrosine ring flip, 54, 118–24
- trypsinogen, 145
- umbrella sampling, 68–9, 74
 large scale deformations, 139
 thermodynamic cycle perturbation
 method, comparison, 71
 tyrosine ring flip, 120
- variable metric method, 53–4, 163
- Verlet method, 173–4
 constrained, 176–80
- vibrational motions
 normal mode analysis, 58
- virtual bonds, 53
- virus coat proteins, 137
- viscosity, 26
 and ligand binding, 123, 136

234 *Index*

Water

dielectric constant, 10
diffusion, 86
dynamics, 25–8
hydrogen bonding, 7
molecular dynamics, 62
molecule, 7
structure, 7–8; reviews, 11; solute effects,
8–11, 25–6

X-ray crystallography

dynamic information, 96–100
structure refinement by computer
simulation, 65, 161–3

Young's modulus

DNA helix twisting, 114
protein hinge bending, 140