INDEX

Absolute temperature scale, see Kelvin scale
Acid/alkaline denaturation
  calorimetry, 173, 174
  cooperativity, 174
  protonation, 173, 174
  titratable groups, 173
Acid–base equilibrium, 18–20
A-DNA, 92
Alpha-helix
  calorimetry, 95–105
  cooperativity, 97–101
  ellipticity, 97
  enthalpy, 102–104
  entropy, 103, 104
  Gibbs energy, 103–105
  heat capacity, 99–102
  hydration, 1–3, 105
  hydrogen bonding, 103–105
  stability, 103
  unfolding, 95–99
  van der Waals, 104, 105
  van’t Hoff enthalpy, 95, 96

Alpha-lactalbumin, 235
Amino acids
  d- and l-isomers, 76
  ionization, 74
  pK values, 74
  solubility, 88
  structure, 73–75
Anhydrous protein
  chymotrypsinogen, 203, 205
  heat capacity, 202–205
  hydrogen bonding, 208, 209
  packing density, 208
  polypeptide, 203
  rigidity, 210, 213
  thermal motion, 204
  unfolding enthalpy, 204–210
  unfolding entropy, 210–213
  van der Waals interactions, 208–209
  Antennanapedia homeodomain, see
  Homeodomains
  Apolar groups, see Nonpolar groups
Apomyoglobin
  cold denaturation, 170–171
  heat denaturation, 170–171
  molten globule, 234–240
Aqueous solutions, 16–18
Aromatic groups
  hydration enthalpy, 195–199
  hydration entropy, 195–199
  hydration heat capacity, 195–199
Association entropy
  cratic entropy, 273–275
  coiled-coil formation, 283–285
  experimental verification, 275–276
  Streptomyces subtilizin dimerization, 277–283
  translational entropy, 273–275
  vibrational entropy, 275
Association reaction
  association constant, 33
  binding isotherm, 34
  dissociation constant, 34
  enthalpy, 34
  ATF2/cJun bZIP, 313–317
  AT-hook/DNA, 322–326
Barnase
  heat capacity, 158, 159
  heat denaturation 158–160
  unfolding, 158, 159
B-DNA, 92–94
Bovine pancreatic trypsin inhibitor
  heat capacity, 203
  unfolding, 207
BPTI, see Bovine pancreatic trypsin inhibitor
bZIPS, see ATF2/cJun; GCN4
Calcium-binding proteins
  calmodulin, 258–262
  light chain of myosin, 258
  parvalbumin, 258–260
  troponin C, 258, 261
Calmodulin
  calorimetry, 261–263
  peptide recognition, 287–292
  structure, 258–262
Calorimetry, of polynucleotides 361–372
  DNA duplexes, 361–372
  DNA phage T2, 354–357
  Poly(a)Poly(U), 357–361
  tRNA 378–383
Calorimetry, of protein–DNA complexes
  ATF2/cJun bZIP, 313–316
  AT-hook, 322–326
  HMG boxes, 326–331
  homeodomains, 300–307
  NF-κB, 345, 346
  HMGAI, 345–346
Calorimetry, of proteins
  alpha-helix, 95–105
  calmodulin c, 259–263, 287–293
  coiled-coils, 106–110
  collagen, 135–141
  fibrinogen, 264–267
  fibronectin, 267–268
  leucine zipper, 118–123
  myosin light chain, 58
  myosin rod, 115, 116
  ovomucoid, 255–258
  papain, 250, 251
  paramyosin, 116, 117
  parvalbumin, 258–260
  pepsinogen, 251–255
  plasminogen, 263–264
  Streptomyces subtilisin, 277–283
  troponin, 117, 118
  troponin, 258, 261
Calorimetry experiment
  binding characteristics, 41–43
  complex heat capacity profiles, 60, 61
  correction on refolding, 61–63
  denaturation enthalpy, 56–58
  heat capacity, 53–54
  multicomponent transition, 59, 60
  van’t Hoff enthalpy, 58, 59
Calorimetry instruments
  batch calorimeter, 35
  flow-mix calorimeter, 35, 36
  heat capacity calorimeter (DSC), 43–53
  isothermal reaction calorimeter (ITC), 33–43
  pressure–perturbation calorimeter, 63–66
Calorie, see Energy units
CC concept, see Counterion condensation theory
Celsius scale, see Temperature scales
Chemical structure, of proteins
  amino acid residues, 71–76
  C-terminal, 72
  N-terminal, 72
  peptide bond, 72
Chymotrypsinogen anhydrous, 203, 205
Coiled-coils
  calorimetry, 106–110
  discreteness, 123
  entropy of formation, 283–285
  leucine-zipper GCN4, 118–123
  muscle proteins, 113–118
  three-stranded, 110, 113
  two-stranded, 105–110
  unfolding, 106–110
Cold denaturation
  apomyoglobin, 170, 171
  calorimetry, 169–171
  ellipticity, 169
  experimental observation, 168–173
  intrinsic viscosity, 169, 170
  lactoglobulin, 171
  myoglobin, 169, 170
  NMR, 169
  phosphoglycerate kinase, 169, 171
  protonation, 168
  staphylococcal nuclease, 171
Collagen
  calorimetry, 135–141
  chemical structure, 127, 128
  conformation, 127–127
  cooperativity, 132, 133
  melting enthalpy, 130, 135–140
  melting entropy, 133, 135–138
  flexibility, 129–131, 145–148
  hydration, 140–143
  hydrogen bonds, 129–131
  hydrogen exchange, 129, 130, 145–148
  Rich-Crick model, 129
  Ramachandran models, 129, 130, 131
  physical structure, 127–129
  role of pyrrolidines, 134, 135
  stability, 131–133, 148, 149
  thermodynamics, 133–135, 138–140
Completeness, of protein unfolding, 182–186
Conformation, of polypeptide chain
  alpha-helix, 83–85
  cis-trans isomers, 78
  conformational freedom, 79–81
  entropy, 79, 80
  local restrictions, 81–82
  long-range restrictions, 82, 83
  peptide unit, 77, 78
  polyproline helix, 85, 86
  random coiled, 81
  regular conformation, 82–86
Cooperativity, in protein unfolding, 225, 242, 243
Cratie entropy, 273–275
Denaturants
  calorimetry, 176–178
  denaturants, 154, 175–182
  enthalpy of binding, 180, 181
  Gibbs energy of binding, 180–181
  GuHCl–protein interaction, 175–182
  protein stability, 175, 176
  urea–protein interaction, 175–182
Denaturation of proteins, see Unfolding, of proteins
Discreteness, in proteins, 113–118, 268–271
Dissipative forces, 219–222
DNA
  A and B conformation, 92
  bending, 331–334, 375–376
  calorimetry, 354–357, 361–371
  chemical structure, 89, 90
  density, 372–375
  double helix, 92, 94
  grooves, 92
  hydration, 339–344, 372–375
  melting temperature, 356–357
  specificity of the AT sequences, 366–372
  thermodynamics, 366–367
DNA–binding proteins
  ATF2/Jun bZIP, 313–316
  AT-hook, 322–326, 346
  GCM4 bZIP, 307–313
  HMG boxes, 326–331
  HMGI/Y, 322
  homeodomains, 300–307
  IRF-3, 317–319
  NF-kB, 320–322, 346
DNA calorimetry
  correction on premelting, 364–366
  correction on residual structure, 363–366
  DSC, 354–357
  intrinsic melting enthalpy, 366–371
  intrinsic melting entropy, 371–372
  ITC, 362
DNA–protein interaction
  AT-hook, 322–326
  bZIPs, 307–316
  CC and PDB approach, 297–300, 346, 347
  GCN4, 307–313
  HMG boxes, 326–331
  homeodomains, 300–307
  hydration, 341–344
  IRF3, 317–322
  major groove binding, 300–322, 339–342
  minor groove binding, 322–331, 339–345
  multicomponent complexes, 345–346.
  non-sequence-specific binding, 331–336
  salt effect, 336–339
  sequence-specific binding, 331–336
Domains, in proteins, see Discreteness, in proteins
Dry protein, see Anhydrous protein
Dyn, see Force units
Energy units
  calorie, 7
  erg, 8
  joule, 8

Energy
  definition, 5
  conservation law, 5
  Gibbs free energy, 13

Engrailed homeodomain, 300–306, 332
Enhanceosome, 345–347
Enhancer DNA, 345

Enthalpy
  alpha helix, 103, 104
  base-pairing, 383
  collagen, 135–138
  definition, 6
  DNA, 354–357, 369–372
  hydration, 24, 194–199, 207
  polynucleotides, 357–361
  protein–DNA interactions, 303–341
  protein unfolding, 155–181, 214, 215
  tRNA, 378–383
  van’t Hoff, 15

Entropy
  conformational, 210–213
  definition 11–13
  hydration, 24, 211–213
  rotation, 273–275
  translation, 273–275
  vibration, 275

Equine lysozyme, 236, 237

Erg, see Energy units

Evolution, of proteins, 254–256, 260, 267, 271

Fahrenheit scale, see Temperature scales

Fibrinogen, 264–267
Fibronectin, 267–268

Flexibility, of protein structure
  collagen, 129–131, 148, 149
  globular proteins, 228, 229
  hydrogen exchange, 226–228
  microunfoldings in protein, 225–228
  protein–DNA interaction, 298–341
  hydration, 24–32, 197, 198

Globular proteins, see also Proteins
  cold denaturation, 167–173
  compactness, 153
  denaturation, 153–181
  disulfide crosslinks, 159, 183
  ellipticity, 169, 175, 184, 185
  flexibility, 169
  heat capacity, 155, 158–161
  heat denaturation, 155–167
  pH titration, 174
  protonation/deprotonation, 168
  stability, 161–167, 175, 176, 186–190
  standard entropy, 187, 189
  thermodynamic characteristics, 186–189
  unfolded state, 154, 159, 182–186
  unfolding, 155–182
  viscosity, 170, 183, 184

GuHCl–protein interaction, 175–182

Heat capacity
  definition, 8
  hydration, 24, 25
  molar, 9
  partial, 20–23
  specific, 8, 9
  water, 18

Heat capacity, of proteins
  alpha helix, 99, 102
  anhydrous, 202–204
  BPTI, 202
  chymotrypsinogen, 203, 205
  collagens, 136
  cytochrome c, 203
  globular proteins, 155–162
  hydration effect, 24, 25, 194–196
  molar, 9
  myosin rod, 115, 116
  paramyosin 116
  partial, 20–23
  specific, 8, 9
  tropomyosin, 117
  unfolding increment, 205
  water, 18
Heat capacity, of polynucleotides and their complexes
DNA phage T4, 354
DNA duplex, 361–364
polynucleotides, 357–361
protein–DNA complexes, 302, 305, 328

Heat denaturation, of proteins
apo-cytochrome, 157, 181
apomyoglobin, 170, 171
barnase, 158, 160
cooperativity, 156–158
heat capacity increment, 158–160
lactoglobulin, 171
lysozyme, 157, 164, 174, 176–178, 184, 186, 189
myoglobin, 161–166, 168–171, 184, 189
phosphoglycerate kinase, 171, 172
reversibility, 155
stability, 161–167
staphylococcal nuclease, 171
thermodynamic specification, 186–189
ubiquitin, 160

Hierarchy, in proteins
primary structure, 71–76
quaternary structure, 88, 89
secondary structure, 82–86
tertiary structure, 88–88

Hydration
collagen, 140–143
folded protein, 199, 200
Gibbs energy, 24, 32
heat capacity effect, 21, 22
protein groups, 193–199
unfolded proteins, 200–201
water accessible area, 201

Hydrogen bonds
alpha-helix, 103–105, 216–218
enthalpy, 216, 217
Gibbs energy, 217
network hydrogen bonds, 216
reduced hydrogen bonds, 216
van der Waals contribution, 215
water, 16–18

Hydrogen exchange
collagens, 129, 130, 145–148
globular proteins, 226–228
Hydrophobic effect, 25–28, 218, 219, 242

Interactions, in proteins
electrostatic, 208, 209
hydrogen bonding, 216, 217, 219, 220
hydrophobic, 25–28, 218–223
van der Waals, 204–210, 219–220

IRF3 transcription factor
C-terminal domain, 317, 318
DNA bending, 319
DNA binding sites, 317
linker, 318
N-terminal domain, 317, 318
isothermal titration calorimeter (ITC)
data analysis, 41–43
experiment, 38–41
instruments, 36–38

Joule, see Energy units

Kinetics, of protein folding, 233
Kirchhoff’s relation, 9

Leucine-zipper, see GCN4 bZIP
Leventhal paradox, 233

Light chain, of myosin, 258

Lysozyme
acid denaturation, 173, 174
calorimetry, 158, 164, 174, 176–178, 184, 186, 189
GuHCl denaturation, 176–178
heat capacity, 203, 205
heat denaturation, 158
hydration, 207, 211
intrinsic viscosity, 183–184
isothermal titration, 173–175
unfolding enthalpy, 10–11, 186, 214
unfolding Gibbs energy, 186–189

Matt2 homeodomain, 300–306, 332

Microunfoldings, in proteins, see Hydrogen exchange

Molten globule
alpha-lactalbumin, 235
apomyoglobin, 239, 240
concept, 234–240
equine lysozyme, 236, 237
staphylococcal nuclease, 236, 238

Multidomain proteins
discreteness in proteins, 268–271
fibrinogen, 264–267
fibronectin, 267–268
light chain, of myosin, 258
ovomucoid, 255–258
papain, 250, 251
parvalbumin, 258–260
Multidomain proteins (cont’d)
plasminogen, 263–264
troponin, 258, 261

Muscle proteins, 113–118
discreteness, 113–115
myosin rod, 115, 116
paramyosin, 116, 117
troponyosin, 117, 118

Myoglobin

- cold denaturation, 169, 170
effect, 169
- enthalpy of unfolding, 214
- heat capacity, 161, 171, 203, 205
- heat denaturation 161–166, 168–171, 184, 189
- hydration enthalpy, 207
- hydration entropy, 211
- intrinsic viscosity, 184
- stability, 166, 189
- unfolding, 162

Myosin rod

- calorimetry, 115, 116
discreteness, 113–118

Newton, see Force units

NF-κB transcription factor, 320–322

NK-2 homeodomain, 300–306, 332

Nonpolar groups

- hydration enthalpy, 195
- hydration entropy 195
- van der Waals interaction, 208

Nucleic acids

- chemical structure, 70, 89, 90
- nucleotides, 90
- physical structure, 91–94
- thermodynamics, 353–383

Ovomucoid, 255–258

Packing density, 229–231

Papain, 250, 251

Paramyosin, 116, 117

Partial heat capacity, see Heat capacity

Parvalbumin, 258–260

Peptide bond, see Proteins

Peptide unit, 77, 78

Phase transitions in proteins, 243, 244

Phosphoglycerate kinase, 171, 172

Plasminogen, 263–264

Poisson-Boltzman (PB) equation, 298, 346, 347

Polar groups

- hydration enthalpy, 196
- hydration entropy, 197
- hydration heat capacity, 196

Polynucleotides

- DSC, 358, 359
- ITC, 360
- unfolding, 357–361

Polypeptide chain

- amino acid residues, 71–76
- conformation, 76–81
- C-terminal, 72
- N-terminal, 72,
- peptide bonds, 72
- peptide unit, 72

Polyproline coiled-coils, see Collagen

Pressure perturbation calorimetry (PPC)

- background, 63–65
- experiment, 65–67
- thermal expansion coefficient, 63–65

Primary structure, of proteins, see Chemical structure, of proteins

Protein folding

- cooperativity, 225, 226
- forces, 220–223
- intermediate states, 233
- kinetics, 233
- mechanisms of cooperation, 242, 243

Protein interior

- packing density, 229–232
- flexibility, 226–228

Proteins

- anhydrous, 202–213
- chemical structure, 71–76
- conformations, 76–85
- domain organization, 113–118, 268–271
- entropy, 79–80
- evolution, 69–71
- flexibility, 226–228
- globular, 153–189
- hierarchy, 86–88
- hydration, 88, 193–202
- physical structure, 76–81
- primary structure, 71–76
- quaternary structure, 88, 89
- random coil, 81
- regular conformations, 82–86
- stability, 225, 226
- tertiary structure, 86–88

Purines, 90

Pyrimidins, 90

Quaternary structure, of proteins, see Hierarchy, in proteins

Ramachandran plot, 81–83

Ribonuclease A

- GuHCl effect, 180
- heat capacity, 161, 179, 203, 205
hydration enthalpy, 207
hydration entropy, 211
intrinsic viscosity, 184
stability, 189
unfolding, 162
RNA
chemical structure, 89, 90
physical structure, 91–94
poly(A)poly(U), 357–361
tRNA, 376–383
Sacker-Tetrod equation, 274
Stability, of protein
coooperativity, 242, 243
macro stability, 225, 226
micro-stability, 226–228
thermodynamic states, 243, 244
Staphylococcal nuclease, 236, 238
Streptomyces subtilisin
calorimetry, 277–283
entropy of dimerization, 277–283
structure, 277
Temperature
definition, 6
absolute scale, 7
Celsius scale, 7
Fahrenheit scale, 7
Kelvin scale, 7
Thermodynamic states, of protein, 186–189, 243, 244
Three-stranded-coiled-coil, 110–113
Transcription factors
bZIP, 307–313
HMG boxes, 325–331
homeodomains, 300–307
IRF3, 317–319
NF-κB, 320–322
Translational entropy, see Association entropy
tRNA
base-pairing, 383
calorimetry, 378–380
melting profiles, 380, 381
structures, 377
thermodynamic analysis, 381–385
Tropomyosin, 113–118
Troponin, 258, 261
Two-stranded coiled-coils
calorimetry, 106–110
structure, 105, 106
Unfolding, of proteins
cold denaturation, 167–173
completeness, 182–186
cooperaativity, 156–158
denaturant effect, 175–182
e ellipticity, 184, 185
heat capacity increment, 158–161
heat denaturation, 155–167
pH denaturation, 173–175
reversibility, 155–156
stability, 161–167, 167–173
unfolded state, 182–186
viscosity, 170, 183, 184
Urea–protein interaction, 179–182
enthalpy of binding, 180, 181
Gibbs energy of binding, 180–181
Van’t Hoff equation, 15
Voronoi polyhedron, 229, 230
Water
heat capacity, 18
hydrogen bonds, 18
structure, 16–18