

# Subject index

- A LA MODE*, 663  
A-DNA, 766  
A-tract bending, 783  
*Ab initio* phasing, 413  
  in molecular replacement, 360  
  low-resolution, 437  
  multisolution methods, 417  
Absolute configuration, 287, 372  
Absorption, 60  
Absorption coefficient  
  atomic, 373  
  atomic mass, 59  
  linear, 59  
Absorption corrections, 60  
  for lysozyme, 860  
Absorption edge, 54, 60  
Absorption factor, 59  
Accuracy, 499  
  of unit-cell parameters, 266, 653  
Acid–base equilibria, 733  
*ADIT*, 827  
*ADIT-NMR*, 827  
Affinity chromatography, 87  
Affinity tags, 92  
Alignment of phase sets, 440  
Alkylation of free cysteines, 96  
All-atom contact analysis, 688, 690–692, 694–695, 697, 699  
Alternative conformations, 492  
American method of crystal orientation, 263  
Amino acids  
  distribution of water molecules around, 802  
  hydrogen bonds in, 741  
  interactions with heavy-atom reagents, 320  
Amino-acid analogues as heavy-atom derivatives, 324  
Amino-aromatic hydrogen bonding, 728  
Ammonium sulfate, 86, 319  
Amplitude contrast, 595, 599  
Angular brightness of synchrotron radiation, 189  
Angular reconstitution, 627  
Angular refinement, 621  
Animation, 448, 456  
  of molecular-dynamics trajectories, 454  
Anion-exchange chromatography, 86  
Anisotropic atomic model, 486, 492  
Anisotropic mosaicity, 300  
Anisotropic scaling, 488  
Annealing, 243  
Annotation at the Protein Data Bank, 827  
*ANOLEA*, 664  
Anomalous correlation coefficient, 67  
Anomalous Cullis *R* factor, 69  
Anomalous difference Patterson map, 331  
Anomalous phasing power, 69  
Anomalous phasing with twinning, 548  
Anomalous *R* factor, 67  
Anomalous-scatterer labels for MAD, 377  
Anomalous scattering (dispersion), 55, 369, 373  
  data-collection strategies, 227  
  heavy-atom location, 367, 371  
  phase probability distribution, 370  
  phasing, 367  
  preparation of heavy-atom derivatives, 317  
  signal quality, 298, 300  
  sodium tartrate, 5  
  without isomorphous replacement, 371  
Anomalous scattering factors, 373  
  evaluation of, 373  
Anomalous substructure, 68  
Antibody Fv fragments in crystallization of  
  membrane proteins, 126  
Antifreezes, 241  
Antigen–antibody association, water molecules in,  
  815  
Archimedes' method, 154  
*ARCIMBOLDO*, 530  
Area detectors, 178–179, 183, 266  
  and cross fire, 163  
  and synchrotron radiation, 195, 198  
Argand diagram, 54  
Aromatic halogen bonds, 824–825  
*ARP/wARP*, 464, 525  
Asn/Gln/His flips, 695  
Astbury, W. T., 6  
Astigmatism, 625  
Asymmetric unit, 47  
  choice of, 217  
Atlas reports, 835  
Atomic absorption coefficient, 373  
Atomic charge distributions, 730  
Atomic displacement parameters (temperature  
  factors), 485  
  anisotropic, 56, 485  
  anisotropic, at atomic resolution, 492  
  anisotropic, refinement in *SHELXL*, 531  
  constraints, 490  
  effect of coordinate errors, 461  
  effect on coordinate uncertainty, 499  
  group *B* factors, 461  
  in structure validation, 656  
  isotropic, 56  
  refinement of, 461  
  restraints, 490, 522  
Atomic mass absorption coefficient, 59  
Atomic radii, 708  
  standard, 708  
  van der Waals, 708, 713  
Atomic resolution, 485  
  anisotropic atomic displacement parameters, 492  
  automatic location of water sites, 493  
  data collection, 228  
  data quality, 487  
  definition of, 487  
  deformation density, 494  
  hydrogen atoms, 491  
  ligands, 494  
  low-resolution data, 488  
  metal ions, 494  
  modelling alternative conformations, 492  
  ordered solvent, 493  
  structures for validation, 673, 684  
Atomic scattering factor, 54, 373  
  imaginary component, 373  
  real component, 373  
Atomic solvation parameters, 715  
Atomicity, 392, 486  
*AutoDep*, 827  
*Autographa californica* nuclear polyhedrosis virus  
  (AcNPV), 83  
Autoindexing, 263  
  basis vectors, 264  
  coordinate systems, 284  
  distribution of reciprocal-lattice vectors, 263  
  in *DENZO*, 283  
  misindexing, 284  
  twinning, 284  
Autoinduction, 142  
Automated convolution method for molecular-  
  boundary identification, 387  
Automated crystal mounting, 143  
Automated model building, 525  
Automated structure solution  
  for MAD and MIR, 379  
  in *PHENIX*, 544  
Automatic location of water sites, 493  
Automatic particle picking, 625  
Automation in crystallography, 140  
Automation of crystallization, 107  
Automounters, 231  
Averaging of reflection intensities, 298  
  *R* factors, 298  
*AVGSYS*, 361  
B-DNA, 766  
  A-tract bending, 783  
  minor-groove width, 780  
  sequence-dependent bendability, 781  
  sequence-dependent deformability, 780, 783, 785  
*BABCOCK*, 770  
Babinet inverted structure, 360  
Babinet's principle of complementarity, 499  
Back-projection reconstruction, 621  
Backbone geometry, 697  
Backbone tracing, in *SHELXE*, 530  
Background, determination of, 267  
Background corrections, 60  
Backrub, 691–692  
Bacterial diseases, 16, 19  
Bacteriophages, filamentous, 589  
Bacteriorhodopsin, 123  
  electron diffraction studies, 559–560  
Baculovirus expression systems, 83  
  AcNPV, 83  
  BmNPV, 83  
‘Baking’, 418  
Balasubramanian plot, 655  
Base pairing, 767  
  Hoogsteen, 769  
  Watson–Crick, 769  
Basis vectors, 45  
  in autoindexing, 264  
  standard, 46  
Batch methods of crystallization, 105  
Baton building, 443  
Beam divergence, 214  
Beer's law, 59  
Beever, C. A., 6  
Beever–Lipson strips, 6  
Bending magnets, 161  
Bernal, J. D., 5–6  
Bessel functions, 584  
  spherical, 345  
Best Fourier, 330, 369  
Best phase, 330  
Bias  
  and restraints, 474  
  avoidance, in *PHENIX*, 542  
  in refinement, 405, 459  
  model, 401, 404, 466, 472, 651  
Biaxial crystals, 147  
Bidentate hydrogen bonding, 756  
Bifurcated hydrogen bonding, 721  
Bijvoet, J. M., 5  
Bijvoet differences, 375  
Bijvoet pairs, 60, 374, 380  
Bijvoet Patterson map, 9  
*BILDER*, 449  
Binary integer programming, 439  
Binding energies, 715–716  
  electrostatic contributions to, 734  
Biological halogen bonds, 822  
Biological Macromolecule Crystallization Database  
  (BMCD), 838  
BioMagResBank (BMRB), 831  
Birefringence, 147  
Blind region, 220, 273  
Blindness, 23  
Block-matrix approximation, 488, 505  
Blow, D. M., 7, 9  
Blow & Crick method, 368  
Boltzmann model, 731  
*Bombyx mori* nuclear polyhedrosis virus (BmNPV),  
  83  
Bond-angle restraints, 474, 477, 479  
Bond-length restraints, 474, 476–477  
Bond lengths from the CSD, 738  
Bovine  $\alpha$ -lactalbumin, molecular-dynamics  
  simulation, 645  
Bovine pancreas ribonuclease A, molecular-dynamics  
  simulation, 645  
Bovine pancreatic trypsin inhibitor (BPTI)  
  molecular-dynamics simulation, 633, 645  
  solvent structure, 815  
Bragg, W. H., 5  
Bragg, W. L., 5–7, 845  
Bragg's law, 5, 56, 65, 213  
Bravais lattice, 52, 279  
*Bremsstrahlung*, 159, 162  
Britton plot, 314  
5-Bromouracil, 822

## SUBJECT INDEX

- 5-Bromouridine, 378  
 Buckingham energy function, 587  
 Buffers, 319  
   acetate, 319  
   citrate, 319  
   Tris buffer, 319  
 Bulk solvent, modelling of, 493  
 Bunn, C. W., 5  
 Buried water molecules, 726, 810
- $C^\alpha$ -only model, 655  
 $C^\beta$  deviation, 697  
 C41 strain, 93  
 C43 strain, 93  
 C—H...O hydrogen bonds, 727, 742  
 C—H...X hydrogen bonds, 741  
 Calcium-binding proteins, 757  
   calmodulin, 757  
   staphylococcal nuclease, 757  
 Calibration of CCD detectors, 184  
 Calmodulin, 757  
 Cambridge Structural Database (CSD), 736  
   bond lengths, 738  
   composite crystal-field environments, 742  
   conformational libraries, 740  
   conformations, 739  
   data acquisition, 737  
   data completeness, 737  
   energies, 739  
   hydrogen-bonding motifs, 743  
   in structure validation, 662  
   IsoStar, 743–744  
   knowledge-based structural libraries, 738, 740  
   metal coordination, 740  
   relevance to protein crystallography, 736–737  
   restraints from, 474  
   software, 737  
   *SuperStar*, 745  
   van der Waals radii, 709
- Cancers, 22  
 Carbohydrate-binding proteins, 755  
 Carbonyl–carbonyl interactions, 742  
 Carboxypeptidase, 9  
 Cardiovascular disorders, 23  
 Cartesian molecular dynamics, 469  
 CATH, 749–751  
 CCD detectors. *See* Charge-coupled device detectors  
 CCP4 (Collaborative Computational Project, Number 4), restraints, 662  
 Cell-free expression systems, 93  
 Cell lysis, 94  
 Cellular imaging, 234  
 Central limit theorem, 402–403  
 Centred (non-primitive) unit cell, 46  
 Centrosymmetric heavy-atom distributions, 371  
 Centrosymmetric point groups, 50  
 Channelling radiation, 159  
 Chaperones  
   use in crystallization, 110  
   use in protein folding, 81  
 Charge-coupled device (CCD) detectors, 183  
   calibration, 184  
   dark-current subtraction, 185  
   flat-field corrections, 185  
   for cryoTEM, 594, 599, 606  
   geometric distortion, 185  
   obliquity correction, 186  
 Charge distributions, atomic, 730  
 Charge-transfer bonds, 823  
 Charge-transfer equilibria, 733  
 Cheshire group, 349  
 Chiral volume, 654  
 Chirality, 145, 654  
 Chromatography, 86  
   affinity, 87  
   anion-exchange, 86  
   dye-ligand, 86  
   hydrophobic interaction, 86  
   hydroxyapatite, 86  
   immuno-affinity, 87  
   size-exclusion, 86  
 Chymotrypsin, 9  
 CIF (crystallographic information file), 737  
 Circular variance plots, 656
- Clashscore, 695  
 Class A metals, 318  
 Class B metals, 318, 321  
 Clotting factor Xa, 825  
 Cluster analysis, 739  
   of phase sets, 441  
 CMC (critical micelle concentration), 94, 122, 125  
 Codon usage, effect on expression levels, 79  
 Coherent neutron scattering, 575  
 Coherent X-ray diffraction microscopy (CXDM), 234  
 Collaborative Computational Project, Number 4 (CCP4), restraints, 662  
 Combined molecular replacement, 349  
 Comparison of phase sets, 439  
 Complete rolling algorithm, 714  
 Complex formation, water molecules in, 815  
 Composite crystal-field environments, 742  
 Compton effect, 52  
 Compton scattering, 59  
 Concanavalin A, 502  
 Concentration of membrane proteins, 95  
 Conceptual clustering, 739  
 Conformational equilibria, NMR studies of, 618  
 Conformational heterogeneity, 131  
 Conjugate-gradient method, 397, 463, 488  
   algorithms, 621  
   comparison with simulated annealing, 471  
   preconditioned, 463, 522–523  
 Connected rolling algorithm, 714  
 Connolly surface, 451, 714  
 Constraints, 461  
   atomic displacement parameter, 490  
   coordinate, 490  
   for phase improvement, 396  
   geometrical, 461  
   in density modification, 386  
   in *SHELXL*, 531  
   nonlinear, 396  
   real-space, 418  
 Contact surface, 707, 713  
 Contrast, 70  
 Contrast matching, 577, 580  
 Contrast-transfer function, 559, 596, 599, 606, 620  
   correction, 621, 625  
   in *EMAN*, 631  
 Contrast variation, 577, 580  
 Convex hull, 706  
 Cooperative hydrogen bonding, 721, 755, 758  
 Coordinate errors, 507  
   effect on atomic displacement parameters, 461  
   estimation of, 404, 657, 667  
   estimation of, using *SFCHECK*, 667  
   from cross validation, 466  
   variable, probability distributions, 402  
 Coordinate systems, 284  
 Coordinate systems in *DENZO*  
   beam-gravity, 284  
   beam-spindle, 284  
   beam- $2\theta$ , 285  
   data, 284  
 Coordinate uncertainty, 499  
   approximate methods, 505  
   block-matrix calculations, 505  
   low-resolution structures, 506  
   modified Fourier method, 505
- Coot*, 443  
 CorA, 95  
 Corey–Pauling–Koltun (CPK) models, 450  
 $\gamma$  correction, 395  
   perturbation- $\gamma$  approach, 395, 409  
 Correlation-coefficient translation function, 347  
 Correlation coefficients  
   anomalous, 67  
   CC(all), 68  
   CC( $F_{\text{obs}}$ ,  $F_{\text{calc}}$ ), 71  
   CC( $I_{\text{obs}}$ ,  $I_{\text{calc}}$ ), 71  
   CC(weak), 68  
   chain trace, 70  
 Coulombic potential, 731  
 Covariances, 499  
 Crambin  
   deformation density, 494  
   solvent structure, 814  
 Crick, F. H. C., 6–7
- Critical angle for total external reflection, 165  
 Critical micelle concentration (CMC), 94, 122, 125  
 Critical wavelength, 161, 190  
 Cross-correlation function, 625  
 Cross fire, 162–163  
 Cross linking, 320  
 Cross-rotation function, 341  
   and noncrystallographic symmetry, 335  
 Cross-translation function and noncrystallographic symmetry, 335  
 Cross validation, 464, 466, 491, 657  
   in estimation of  $\sigma_A$  values, 405  
   in maximum-likelihood refinement, 468  
   restraints, 474  
 Cross vectors, 328–329  
 Crossed polarizers, 147  
 Crowther, R. A., 9  
 Crowther resolution, 237  
 Cryocrystallography, 241, 249, 256  
   and MAD, 376  
   antifreezes, 241  
   apparatus, 244, 249  
   cooling rates, 242  
   cryogens, 242, 252  
   cryoprotectants, 241, 249  
   crystal mounting, 250, 252  
   crystal storage, 253  
   crystal transfer, 247, 253  
   dual-stream apparatus, 245  
   effect of crystal cooling on resolution, 243  
   flash cooling, 252  
   ice formation, 241–242, 249  
   ice nucleation, 241  
   preparation of crystals for, 249  
   solvent modification, 241  
   techniques, 249  
   temperature calibration, 246  
 Cryo-electron microscopy, 620, 624  
 Cryo-electron tomography, 42–43  
 Cryogenic data collection, 231  
 Cryogens, 252  
 Cryoprotectants, 241, 249  
   ethylene glycols, 241, 249  
   glycerol, 249  
   2-methylpentane-2,4-diol (MPD), 241, 249  
   polyethylene glycol (PEG), 249  
 Cryotongs, 247  
 CRY SOL, 567  
 Crystal-density measurement, 152  
   Archimedes' method, 154  
   by flotation, 154  
   by pycnometry, 154  
   by tomographic crystal-volume measurement, 155  
   by volumetry, 154  
 Ficoll density gradients, 155–156  
 gradient-tube method, 155  
 immersion microbalance, 154  
 Crystal engineering, 742  
 Crystal faces, 145  
   indexing, 146  
   properties of, 146  
 Crystal growth  
   atomic force microscopy, 112  
   conditions, 838  
   diffusion, 102, 104–107  
   electron microscopy, 112  
   growth regime, 112  
   habits, 145  
   in convection-free media, 107  
   interferometry, 112  
   kinetics, 106, 110–112  
   nucleation, 99, 103, 111, 115  
   optical microscopy, 111–112  
   phase diagrams, 99  
   prediction of crystallizability, 107, 111, 114–115  
   prenucleation, 111  
   screw dislocation, 112  
   two-dimensional islands, 112  
 Crystal habit, 145  
   measurement of, 146  
 Crystal monochromators  
   for neutrons, 170  
   for X-rays, 166  
   highly ordered pyrolytic graphite (HOPG), 166

## SUBJECT INDEX

- Crystal morphology, 145  
 Crystal mounting, 145, 148  
   for cryocrystallography, 250, 252  
   loop mounting, 251  
   mechanical stability of, 243  
 Crystal orientation  
   accuracy of, for data integration, 266  
   American method, 263  
   determination of, 263  
 Crystal orientation matrix, 263  
 Crystal quality, 135, 145  
   evaluation of, 108, 111, 113  
   mosaicity, 103, 113  
   perfection, 112, 115  
 Crystal rotation, uneven, 290  
 Crystal seeding, 110  
 Crystal systems, 47, 52  
   hexagonal, 52  
   monoclinic, 47  
   orthorhombic, 47  
   tetragonal, 52  
   triclinic, 47  
   trigonal, 52  
 Crystal-to-detector distance, choice of, 221  
 Crystallants, 100  
 Crystallization, 838  
   automation of, 107  
   batch methods, 105  
   by water evaporation, 106  
   counter-diffusion method, 107  
   dialysis methods, 105  
   dynamic light scattering, 104, 111  
   effect of electric field, 102, 107, 110  
   effect of magnetic field, 107, 110  
   effect of pH, 101, 106  
   effect of pressure, 105, 107, 110  
   effect of temperature, 101, 105–106, 110  
   fluorescence spectroscopy, 111  
   hanging-drop method, 106  
   high-throughput method, 105, 109–110  
   in gels, 108  
   in microfluidic devices, 109  
   interface diffusion method, 104, 107  
   ionic liquids, 101, 103  
   of lysozyme, 101, 103, 108, 110–111, 113, 846  
   of membrane proteins, 122–123  
   phase diagrams, 99, 114  
   precipitants, 123  
   promotion of, 140  
   screening, 113  
   sitting-drop method, 106  
   solubilities, 99, 101, 114–115  
   supersaturation, 99  
 Crystallization additives, 102, 123  
 Crystallization database, 114  
 Crystallization chaperones, 110  
   noncovalent, 132  
 Crystallization robots, 142  
 Crystallization screens, 840  
 Crystallization strategies, 838  
 Crystallizing agents, 100  
 Crystallographic competition assay, 824  
 Crystallographic information file (CIF), 737  
 Crystallographic *R* factor, 71  
*Crystallography & NMR System (CNS)*, 463, 472  
 CSD. *See* Cambridge Structural Database  
 Cubic bicontinuous lipidic phases, 126  
 Cullis *R* factor, 69  
 Curved single-crystal monochromators, 196  
*CURVES*, 770  
 Cyclooxygenase 1, 124  
 Cyclooxygenase 2, 124  
 Cylindrical averaging in fibre diffraction, 583  
 Cylindrical coordinates, 584  
 Cylindrically averaged Patterson function, 586  
 Cytochrome *bc*<sub>1</sub> complex, 123  
 Cytochrome *c*, 9  
 Cytochrome *c* oxidase, 123  
   crystallization of, 126  
  
 $D_{m,m'}$  matrices, 345  
 D<sub>2</sub>O – H<sub>2</sub>O difference maps, 554–555, 801  
 DALI, 749–751  
 DALI domain dictionary, 751, 753  
  
*Daresbury Laue Software Suite*, 207  
 Dark-current subtraction for CCD detectors, 185  
 DARPIn chaperones, 133  
 Data collection, 65  
   exposure time, 224  
   fine slicing, 215  
   geometries, 212  
   in electron diffraction, 557  
   in fibre diffraction, 585  
   in SAXS, 570  
   low-temperature, 241, 249  
   monochromatic, 211  
   rotation method, 213  
   rotation range, 215–217, 219  
   still exposure, 213  
   strategies, 226  
   wide slicing, 215  
 Data completeness, 66, 211  
   and direct methods, 414  
   and refinement, 460  
   and structure validation, 653  
   in the rotation method, 217  
 Data integration, 266  
   accuracy, 266  
   background determination, 267  
   by profile fitting, 266, 268  
   by summation, 266–267  
   for fibre diffraction, 586  
   standard profiles, 268  
 Data processing  
   autoindexing, 263  
   for lysozyme, 850, 859  
   in electron diffraction, 558  
   in fibre diffraction, 585  
   in SAXS, 571  
   integration, 266  
   partially recorded reflections, 296  
   *DENZO* and *SCALEPACK*, 282  
 Data quality, 65  
 Data redundancy, 206–207, 217, 227, 376, 653  
 Data resolution  
   and direct methods, 413  
   and refinement, 460  
   and structure validation, 653  
   effective, 653  
   nominal, 653  
 Data-to-parameter ratio in fibre diffraction, 587  
 Databases  
   Cambridge Structural Database, 736  
   for crystallization, 114  
   heavy-atom data bank, 317, 325  
   Nucleic Acid Database, 833  
   Protein Data Bank, 827  
 Debye equation, 567, 575  
 Debye function, 565  
 Debye–Scherrer arcs, 584  
 Decay *R* factor, 68  
 3Dee, 749–750  
 Defocus series, 620  
 Deformation density, 494  
   in crambin, 494  
 Delaunay triangulation, 705  
*DEMON/ANGEL*, 361  
 Density modification, 385  
   constraints, 386  
   in *DM/DMMULTI*, 407  
   in *PHENIX*, 544  
   quality indicators for, 69  
   *R* factors, 70  
   reciprocal-space interpretation of, 393  
   scaling of observed structure factors, 390  
 Density-modification free *R* factor, 70  
 Density-modification real-space free residuals, 70  
*DENZO*, 263, 269, 282  
 De-orthogonalization matrix, 355  
 Deposition sites for the Protein Data Bank, 827  
 Detectable quantum efficiency (DQE), 177, 183  
 Detector calibration, 184, 266  
 Detector distortions, 289  
 Detector overloads, 224, 271  
 Detectors  
   accuracy, 177  
   area, 178–179, 183, 266  
   CCD, 183  
   dynamic range, 178  
   film, 180  
   flat-field corrections, 178  
   gas discharge (wire) counters, 180  
   geometric distortion, 178  
   image plates, 172, 180  
   line spread function, 177  
   multiwire proportional counters, 171, 180  
   neutron, 171  
   photon counters, 179  
   photon integrators, 179–180  
   pixel array, 181  
   point, 179  
   point spread function, 177  
   reverse-biased semiconductor, 180  
   scintillator/photomultiplier, 179  
   signal-to-noise ratio, 177  
   spatial resolution, 177  
   stopping power, 178  
   storage phosphors, 180  
   synchrotron-radiation, 195  
   television, 181  
   two-dimensional, 212  
   X-ray, 177, 183  
 Detergents, 122, 125  
   as solubilization agents, 103  
   for membrane-protein solubilization, 94  
   in membrane-protein crystallization, 123  
 Detwinning, 548  
   model-based, 550  
 Diabetes, 23  
 Diagonal-approximation method, 397, 488  
 Dialysis methods of crystallization, 105  
 Dickerson, R. E., 7  
 Dielectric constant, 730  
   effective, 732  
 Difference density quality, 658  
 Difference distance matrix plot, 454  
 Difference Fourier maps, 329  
   in fibre diffraction, 588  
 Difference Fourier syntheses for heavy-atom location, 371  
 Differential phase residual, 601  
 Diffraction-component precision index (DPI), 73, 506–507, 658, 667  
   examples, 507  
 Diffraction-pattern prediction, in *DENZO*, 288  
 Diffraction-pattern symmetry, 60  
 Diffraction physics, 52, 282  
 Diffraction ripples in Patterson maps, 62  
 Diphtheria toxin, structure validation, 681  
 Direct methods, 68, 413  
   and maximum entropy, 433  
   false minima, 422  
   limitations, 435  
   minimal function, 417  
   multisolution methods, 417  
   parameter-shift method, 418  
   peak picking, 418  
   peaklist optimization, 418  
   tangent formula, 417  
 Directed evolution, 130  
 Directional atomic contact analysis, 655  
 Disorder, 462  
   dynamic, 462, 485  
   modelling in *SHELXL*, 532  
   rotational, 584  
   screw, 584  
   static, 462, 485  
   translational, 584  
 Displaying information, 454  
 Displaying structures, 448–449  
   animation, 456  
   CPK models, 450  
   direct volume rendering, 453  
   geometric representation, 450  
   illustration, 455  
   isosurfaces, 452  
   physical models, 456  
   ray tracing, 451  
   stereolithography, 456  
   three-dimensional printing, 456  
   volumetric representation, 452

## SUBJECT INDEX

- Distance matrix plot, 454  
Distance measurements, 579–580  
*DM/DMMULTI*, 361, 407  
DNA, 6, 766, 778  
  A, B and Z helices, 777  
  A-DNA, 766  
  B-DNA, 766  
  B-to-Z interconversion, 778  
  handedness of helices, 774  
  hydrogen bonding in, 726  
  interactions with proteins, 757, 759  
  major groove, depth of, 774  
  minor groove, depth of, 774  
  Nucleic Acid Database, 833  
  torsion angles, 771  
  treatment in *PHENIX*, 541  
  Watson–Crick Z-DNA, 778  
  Z-DNA, 766  
DNA/RNA hybrids, 766  
*DOCK*, 745  
Dodecylphosphatidylcholine, 96  
Double-crystal monochromators, 196  
DPI. *See* Diffraction-component precision index  
*DPS*, 265  
DQE (detective quantum efficiency), 177, 183  
*DREAR*, 415  
Drug delivery, 41  
Drug design, 15, 135  
  use of the CSD, 745  
Drug metabolism, 25  
Drug resistance, 18  
Dual-axis tomography, 43  
Dual-space methods, 68  
Duplex RNA, 766  
Dye–ligand chromatography, 86  
Dynamic disorder, 462, 485  
Dynamic processes  
  NMR studies of, 615, 618  
  SAXS studies of, 563  
*E. coli* expression systems, 77, 79  
Early structure determinations, 6, 8  
  carboxypeptidase, 9  
  chymotrypsin, 9  
  cytochrome *c*, 9  
  globular proteins, 6–7  
  glyceraldehyde-3-phosphate dehydrogenase, 10  
  haemoglobin, 6–8  
  insulin, 6, 9  
  lactate dehydrogenase, 9  
  lysozyme, 9, 845  
  membrane proteins, 9  
  myoglobin, 6, 8  
  papain, 9  
  penicillin, 5  
  pepsin, 6  
  ribonuclease, 9  
  sodium tartrate, 5  
  tobacco mosaic virus, 6  
  viruses, 9  
  vitamin B<sub>12</sub>, 5  
EDSAC1 and 2, 8  
Effective dielectric constant, 732  
Effective resolution, 66  
Elastase, solvent structure, 809  
Elastic scattering, 52  
Electron cryomicroscopy (cryoTEM), 593  
  Protein Data Bank, 827  
  specimen preparation, 597  
  types of specimens, 597  
  vitrification of specimens, 597  
Electron crystallography, 557  
  of membrane proteins, 561  
Electron density  
  calculation of, 60  
  skewness of, 70  
Electron-density averaging, 352, 390–391  
  computer programs, 361  
  convergence, 359  
  in *DM/DMMULTI*, 409, 411  
  multidomain, 360  
  multiple-crystal-form, 358, 360  
Electron diffraction, 557  
  bacteriorhodopsin, 559–560  
  data collection, 557  
  data processing, 558  
  data sampling, 558  
  radiation damage, 558  
  refinement, 560  
  specimen preparation, 557  
  structure factors, 559  
  tubulin, 560–561  
Electron microscopy, 557, 593  
  amplitude contrast, 599  
  contrast-transfer function, 559, 599  
  electron sources, 557  
  field emission gun, 595  
  impact on structural biology, 42  
  minimal (low-dose) procedure, 558  
  phase contrast, 599  
  recording media, 557  
  signal-to-noise ratio, 596  
  spatial coherence of electron beam, 595  
  spherical aberration, 599  
Electron pair distribution function, 565–566  
Electron scattering, 557, 593  
  elastic, 593–594  
  inelastic, 593–594  
Electron tomography, 620  
Electron-transfer equilibria, 733–734  
Electrostatic energy, 732  
Electrostatic fields, response of proteins to, 730  
Electrostatic force, 732  
Electrostatic free energy, 732  
Electrostatic interactions in proteins, 730  
Electrostatic polarization, 730  
Electrostatic potential  
  calculation of, 732  
  distributions, 730, 732  
Electrostatics, 535, 730  
  acid–base equilibria, 733  
  Boltzmann model, 731  
  Coulombic potential, 731  
  dielectric constant, 730  
  effective dielectric constant, 732  
  electron-transfer equilibria, 733–734  
  electrostatic polarization, 730  
  ion binding, 733–734  
  Langevin model, 730–731  
  linear solvent dielectric models, 731  
  point inducible dipole, 730  
  Poisson–Boltzmann equation, 731  
  polarity, 731  
  polarizability, 730–731  
  reaction potential, 731  
  screening potential, 731  
  self-potential, 731  
  solvation potential, 731  
*EMAN*, 629  
Enantiomorph, 360  
  discrimination with *SHELXE*, 530  
  selection of correct, 377  
Enantiomorphic point groups, 47–48  
Enantiomorphism, 46  
Ensemble, 433  
ENTREZ, 749, 751  
Entropy, 433  
  Shannon's theorems, 433  
*ENVELOPE*, 361  
Environment profiles, 663  
Enzyme catalysis, role of metal ions, 756  
Epitaxial twinning, 311  
*ERRAT*, 678  
Error model, 67  
Error-reduction algorithm, 234  
Errors  
  coordinate, 507  
  coordinate, estimation of, 404, 657, 667  
  coordinate, from cross validation, 466  
  coordinate, probability distributions for, 402  
  detector, 268  
  effect on MAD phasing, 376  
  in protein-structure models, 520, 649, 651–652, 677  
  instrument, 268  
  position, 507  
  systematic, in profile-fitted intensities, 271  
Estimated standard deviation (e.s.d.), 499, 501  
Ethylene glycols, 241, 249  
Euler parameterization, 345  
Ewald, P. P., 5  
Ewald sphere, 57–58, 205, 213, 272  
  partial reflections, 296, 301–302  
Expected intensity factor, 402  
Exposure, uneven, 290  
Exposure time, 224  
Expression systems, 76–77  
  baculoviruses, 83  
  constitutive, 78  
  constructs, 76  
  *E. coli*, 77, 79  
  fermentation, 80  
  growth media, 80  
  inducible, 78  
  insect cell–virus, 83  
  mammalian cells, 84  
  misfolded proteins, 80  
  plasmids, 78  
  post-translational modifications, 75–76, 82, 89  
  preparation of cDNA clones, 76  
  T7 polymerase, 78  
  yeasts, 82  
Extended-atom parameters, 642  
Extended atoms, 715  
Extinction, 59  
<sup>19</sup>F NMR, 821  
F<sub>1</sub> ATPase, synchrotron-radiation studies of, 198  
Fab antibody fragments, 95  
False minima, 422  
Fankuchen, I., 6  
Fast Fourier transform (FFT), 489  
  in *TNT*, 522  
Fast rotation function, 342  
  angular resolution, 343  
Fast screen, 838  
FepA, 124  
Few-atoms model, 439  
FhuA, 124  
Fibre diffraction, 583–584  
  background subtraction, 586  
  cylindrical averaging, 583  
  data collection, 585  
  data integration, 586  
  data processing, 585  
  Debye–Scherrer arcs, 584  
  difference Fourier maps, 588  
  early studies, 6  
  large assemblies, 590  
  layer lines, 584  
  polynucleotides, 589  
  polypeptides, 588  
  polysaccharides, 589  
  profile fitting, 586  
  refinement, 587  
  rotational disorder, 584  
  screw disorder, 584  
  selection rule, 584  
  simulated annealing, 588  
  structure determination, 586  
  structure factors, 584  
  time-resolved studies, 585  
  tobacco mosaic virus, 587  
  translational disorder, 584  
Fibre-optic tapers, 183  
Fibres, 583  
  noncrystalline, 583  
  polycrystalline, 583  
  preparation of, 585  
Ficoll density gradients, 155–156  
Figure-of-merit weighting for model phases, 404  
Figures of merit, 69–70  
Filamentous bacteriophages, 589  
Fine slicing, 215  
Flash cooling, 252  
Flat-field corrections for CCD detectors, 185  
*FLEX*, 745  
*FLEX*, 745  
Flood-field detector calibration, 287  
Flotation method, 154  
Flux of synchrotron radiation, 189

## SUBJECT INDEX

- Focusing collimators  
 capillary optics, 165  
 for microfocus sources, 165
- Force constants, 475
- Force-feedback devices, 457
- Force fields, 644  
*CHARMM*, 662  
*CHARMM22*, 644  
*GROMOS96*, 633–634, 640  
 modifications for structure determination, 644  
 parameterization of, 644
- Fourier maps, difference, 329
- Fourier methods, 5
- Fourier refinement, 419
- Fourier shell correlation, 43, 601–602, 621
- Fourier summation, 62
- Fourier syntheses, histogram of, 438
- Fourier transformation, 60  
 in *DM/DMMULTI*, 411  
 inverse, 60
- Fourier–Bessel structure factor, 584
- Fourier–Bessel syntheses, 584
- Fractional atomic coordinates, 60
- Frame shift, 649
- Franklin, R., 7
- Free-atom model, 525
- Free-electron model, 373
- Free lunch algorithm, in *SHELXE*, 530
- Free phase residual, 561
- Free *R* factor, 71, 466, 506, 651, 657, 665  
 for density modification, 70  
 precision of, 665
- FREEHELIX*, 770
- Fresnel zone, 54
- Friedel pairs, 60, 375
- FRODO*, 449
- Frost prevention, 245
- Full-matrix inversion  
 restrained, 502  
 unrestrained, 502, 504
- Fully recorded reflections, 214
- Fungi, 17, 21
- Fusion chaperone, 132
- Fusion proteins, 77, 131, 140
- Future of crystallography, 39
- Future of science, 39
- G* factors, 656
- GAP*, 361
- Gauss–Bonnet theorem, 715
- Geis, I., 766, 871
- Gelder's law, 449
- Gels, crystallization in, 108
- General purpose graphics processing unit, in *EMAN*, 630
- Generation of phase sets, 438
- Genetic algorithms, 330, 567
- Genetic diseases, 14
- Geometric distortion in CCD detectors, 185
- Glide*, 534, 537
- Global minimum, 466
- Glutaraldehyde, 320
- Glyceraldehyde-3-phosphate dehydrogenase, 10
- Glycerol, 249
- Glycosyl bond geometry, 773–774  
*anti*, 774
- Glycosylation, 75, 82–83, 133
- GOLD*, 745
- Goodness of fit, 501
- Gouraud shading, 451
- Gradient-tube method, 155
- GRAMPS/GRANNY*, 449
- GRASP*, 450, 714, 718
- GRID*, 745
- GRIP*, 449
- Gripper, 232
- GROMOS96*, 633–634, 640
- GST tag, 92
- Guinier plot, 565, 577
- h*-cell, 354
- HAD (heavy-atom data bank), 317, 325
- Haemoglobin, 6–8  
 dimeric, water molecules in, 816
- $\alpha$ -Haemolysin, 124
- Halogen-bond acceptors, 823–824
- Halogen-bond geometry, 823
- Halogen bonds *versus* hydrogen bonds, 824
- Halogen interactions, 821  
 in the Protein Data Bank, 822
- Halogens, *in vivo* incorporation of, 821
- Hamilton, Rollett and Sparks method, 296
- for partial reflections, 296  
 singular-value decomposition of the normal-equations matrix, 296
- Hamilton's significance test, 588
- Hammett  $\sigma$  constants, 821–822
- Handedness, 145, 329, 360, 371, 382
- Hanging-drop method, 106
- Hard cations, 321
- Hard ligands, 318
- Hard metals, 756
- Harker, D., 7
- Harker lines, 63
- Harker phase diagram, 368
- Harker planes, 63
- Harker sections, 328
- Hassel, O., 822
- HBPLUS*, 722
- HEAVY*, 330
- Heavy-atom data bank (HAD), 317, 325
- Heavy-atom derivatives  
 amino-acid analogues, 324  
 of lysozyme, 846, 855  
 preparation of, 317
- Heavy-atom distributions, centrosymmetric, 371
- Heavy-atom location, 327, 367, 371  
 and direct methods, 425
- Heavy-atom reagents, 318  
 class B metals, 321  
 effect of concentration, 320  
 effect of pH, 318–319  
 effect of precipitants and buffers, 319  
 effect of temperature, 320  
 effect of time of soak, 320  
 electrostatic binding of, 323  
 hard cations, 321  
 hydrophobic, 323  
 interactions with amino acids, 320  
 lability, 318  
 oxidation states, 318  
 polynuclear, 324  
 solubility, 319  
 stability, 318
- Helical particles, 603
- Helical symmetry, 333, 584
- Helical viruses, 589
- $\alpha$ -Helices, 6
- Helices, hydrogen bonding in, 723
- Helix capping, 725
- Helix parameters  
*BABCOCK*, 770  
*CURVES*, 770  
*FREEHELIX*, 770  
 horizontal displacement, 770  
 in nucleic acids, 766, 770  
 inclination, 770  
*NEWHELIX*, 770  
 propeller, 770, 775  
 rise, 775  
 rise per base pair, 770  
 roll, 770  
 twist, 770, 775  
*x* displacement, 770
- Helix-termination motifs, 724
- Helminths, 18, 21
- Hemihedral twinning, 146, 312
- Hendrickson–Lattman coefficients, 394, 407
- Hetero groups, structure validation, 663
- Hexagonal crystal system, 52
- High-throughput cloning, 140–141
- High-throughput crystallization, 142
- High-throughput crystallography, 140
- High-throughput screening methods, 134
- Highly ordered pyrolytic graphite (HOPG), 166
- Histogram of a Fourier synthesis, 438
- Histogram matching, 388  
 in *DM/DMMULTI*, 407–408, 411
- HKL*, 282
- Hodgkin, D. C., 5
- Holliday junction, 822
- Holmes, K. C., 7
- HOMSTRAD, 749–750
- Hoogsteen base pairing, 588, 769
- Hoppe, W., 10
- Huber, R., 10
- Hybrid model, 525
- HYDRA*, 449
- Hydration, estimation of, 153
- Hydration surface, 714
- Hydrogen atoms  
 at atomic resolution, 491  
 in *PrimeX*, 535  
 neutron diffraction, 553
- Hydrogen-bond acceptors, 824
- Hydrogen bonding, 721  
 amino-aromatic, 728  
 analysis of in structure validation, 651, 655  
 and secondary structure, 723, 742  
 bidentate, 756  
 bifurcated, 721  
 C–H...O, 727, 742  
 C–H...X, 741  
 cooperative, 721, 755, 758  
*HBPLUS*, 722  
 in amino acids, 741  
 in helices, 723  
 in nucleic acids, 722, 726  
 in *PrimeX*, 535  
 in proteins, 721, 723  
 in  $\beta$ -sheets, 724  
 in side chains, 724  
 in turns, 724  
 in ubiquitin, simulation of, 635–637  
 involving sulfur, 727  
 local, 724  
 N–H...carbonyl, 741  
 N–H... $\pi$ , 742  
 O–H...O, 741  
 O–H... $\pi$ , 742  
 protein–water, 725  
 resonance-assisted, 741  
 resonance-induced, 741  
 short, in phosphate-binding protein, 763  
 transition metals as proton acceptors, 742  
 use of the CSD, 740
- Hydrogen-bonding criteria, 722
- Hydrogen-bonding motifs, 725, 743
- Hydrogen-bonding patterns, 721
- Hydrogen-bonding potential, 721–722  
 saturation of, 723
- Hydrogen/deuterium exchange, 556
- Hydrophobic effects in halogen interactions, 821
- Hydrophobic interaction chromatography, 86
- Hydrophobicity, 714–715
- Hydroxyapatite chromatography, 86
- Hyperglycosylation, 82
- I*/ $\sigma$ (*I*) ratio, 224–225, 228, 653
- Ice formation, 241–242, 249  
 nucleation, 241  
 prevention of, 241
- Icosahedral particles, 603
- Icosahedral point groups, 52
- Icosahedral symmetry, 47
- Image plates  
 for neutrons, 172  
 for X-rays, 180
- Image reconstruction, 620
- IMAGIC*, 630
- IMAGIC 4D*, 624
- Imaging of whole cells, 234
- Immersion microbalance, 154
- Immobilized metal affinity chromatography (IMAC), 95
- Immuno-affinity chromatography, 87
- Implicit solvation, 535
- Incoherent neutron scattering, 575
- Indexing, 274  
 alternative schemes, 221  
 autoindexing, 263, 283  
 basis vectors, 264

## SUBJECT INDEX

- Indexing  
 distribution of reciprocal-lattice vectors, 263  
 of crystal faces, 146
- Inelastic scattering, 52
- Infectious diseases, 16
- Information content of crystallographic data, 487–488
- Information measure, 487  
 quadratic, 487
- Input–output algorithm, 234
- Insect cell–virus expression systems, 83
- Insertion devices, 161, 190  
 multipole wigglers, 190  
 periodic magnet, 191  
 undulators, 190  
 wavelength shifters, 190
- Insertion fusion, 132
- Insight II*, 718
- Instrument errors, 67
- Insulin, 6, 9
- Integration of diffraction data, 266, 275  
 accuracy, 266  
 background determination, 267  
 by profile fitting, 266, 268  
 by summation, 266–267  
 from fibres, 586  
 standard profiles, 268
- Inteins, 77
- Intensity-based likelihood refinement, 489
- Intermolecular interactions  
 data from the CSD, 740  
 energies of, 45  
 weak, 742
- Intermolecular perturbation theory, 742
- Internal contrast, variation of, 577
- International Tables for Crystallography*, 5
- Internationale Tabellen zur Bestimmung von Kristallstrukturen*, 5
- Inverse-beam geometry, 375
- Inverse Fourier transformation, 60
- Inversion symmetry, 46
- Ion binding, 733–734
- Isoelectric focusing, 88
- Isomorphism, lack of, 330
- Isomorphous replacement, 7, 367  
 and fibre diffraction, 586  
 data-collection strategies, 226  
 height of peaks in a Patterson map, 62  
 location of heavy-atom sites, 327  
 noncrystallographic symmetry, 331  
 preparation of heavy-atom derivatives, 317  
 pseudosymmetry, 331
- IsoStar, 743–744
- Isosurface representations, 452
- Isotopic substitution  
 statistical labelling method, 580  
 triple, 578
- Iterative model building, 526
- Jaynes' maximum-entropy formalism, 434
- Jaynes' maximum-entropy principle, 434
- JIFFILOOP*, 699
- $K\alpha$  edge positions of different elements, 54
- KcsA, 95
- Kendrew, J. C., 7
- Kendrew models, 10
- Ketosteroid isomerase, 825
- Kinimages, 688, 694, 699
- KiNG*, 688, 694, 698–699
- Klug, A., 7
- Knowledge-based interaction potentials, 663
- Kramers–Kronig transform, 55
- $L_1$  norm, 460
- $L_2$  norm, 460
- Lack of closure error, 329, 370
- Lack of isomorphism, 330
- Lactate dehydrogenase, 9
- LALS* (linked-atom least squares), 587
- Langevin model, 730–731
- Lattice plane, 45
- Lattice point, 45
- Lattice pseudosymmetry in autoindexing, 284
- Lattice symmetry in autoindexing, 283
- Lattice-translocation disorder, 315
- Laue, M. von, 5
- Laue conditions, 56
- Laue diffraction, 205  
 radiation damage, 207  
 time-resolved studies, 205, 208  
 use of synchrotron radiation, 195, 205  
 wavelength normalization curve, 195, 206
- Laue equations, 272
- LaueView*, 207
- Layer-line splitting, 587
- Layer lines in fibre diffraction, 584
- LEAP*, 207
- Least-squares full matrix, variances and covariances  
 from, 499
- Least-squares methods, 460, 488, 500  
 in *SHELXL*, 531  
 normal equations, 500
- Legume lectins, solvent structure, 808
- Length distribution, 576
- Lennard–Jones 6–12 potential, 642
- Lewis acids, 823
- Lewis bases, 823
- Ligand fitting  
 in *Coot*, 444  
 in *PHENIX*, 541  
 in *PrimeX*, 537
- Ligands at atomic resolution, 494
- Ligation-independent cloning, 141
- Light-harvesting complex 2, 123
- Light-harvesting complex II, 123
- Likelihood-based selection of masks, 439
- Linderström–Lang, K. U., 8
- Linear absorption coefficient, 59
- Linear diffractometer, 848, 856
- Linear solvent dielectric models, 731
- Linked-atom least squares (*LALS*), 587
- Lipids, 96
- Lipson, H., 6
- Liquid helium, 244
- LLG-Z score, 71
- Local hydrogen bonds, 724
- Local intensity difference, 313
- Local minima, 466
- Local scaling, 381  
 in *TNT*, 522
- Locked rotation function, 343
- Locked translation function, 350
- Log-likelihood gain, 71
- Lonsdale, K., 5–6
- Loop refinement, in *PrimeX*, 537
- Lorentz factor, 59–60, 273  
 errors in, 285
- Low-abundance tRNAs, 79
- Low-resolution *ab initio* phasing, 437
- Low-resolution data  
 importance of, 228  
 in atomic resolution refinement, 488
- Low-resolution images, 437
- Low-resolution structures, coordinate uncertainty,  
 506
- LUDI*, 745
- Lunes, 214
- Luzzati distribution, 403
- Luzzati plot, 73, 404, 509, 658
- Lysozyme, 9, 845  
 absorption corrections, 860  
 at 2 Å resolution, 854, 863  
 at 6 Å resolution, 845, 852–853  
 biological function of, 866  
 calculation of phase values, 862  
 catalytic mechanism of, 868  
 crystal-type problem, 861  
 crystallization, 846  
 data processing, 850, 859  
 heavy-atom derivatives, 846, 855  
 hen egg-white, molecular-dynamics  
 simulation, 642, 645  
 intensity measurements at high resolution, 858  
 model in crystallization studies, 111, 113  
 refinement of heavy-atom parameters, 862  
 scaling intensity data, 851  
 T4, mutants, 824  
 T4, solvent structure, 812
- Machine emittance, 190
- Machine learning, 739
- Macromolecular crystallographic information file  
 (mmCIF), 663, 737, 833
- MAD. See Multiwavelength anomalous diffraction
- Maestro*, 534, 537
- MAGICSQUASH*, 361
- Magnesium sulfate, 319
- Maltoporin, 124
- Mammalian-cell expression systems, 84
- Mammalian-cell inducible promoters, 85
- Map connectivity, 438
- Marching-cube algorithm, 453, 714
- Masks, likelihood-based selection, 439
- Mass spectrometry, 88
- Matthews number, 152
- MAVE*, 361
- Maximum entropy, 433  
 and crystallography, 435  
 equations, 434  
 Jaynes' formalism, 434  
 Jaynes' principle, 434
- Maximum likelihood, 460, 489  
 estimation of phase errors, 403  
 in *CNS*, 517  
 structure refinement, 467
- Maximum-likelihood minimization, in *PrimeX*, 536
- MDIR (multidimensional isomorphous replacement)  
 in fibre diffraction, 587
- Mean anomalous signal-to-noise ratio, 68
- Mean signal-to-noise ratio, 67
- Mechanosensitive ion channel, 123
- Medicine and crystallography, 13  
 bacterial diseases, 16, 19  
 blindness, 23  
 cancers, 22  
 cardiovascular disorders, 23  
 diabetes, 23  
 fungi, 17, 21  
 genetic diseases, 14  
 helminths, 18, 21  
 infectious diseases, 16  
 neurological disorders, 23  
 protozoan infections, 16, 21  
 structure-based drug design, 15  
 viruses, 16–17
- Membrane proteins, 123  
 bacteriorhodopsin, 123  
 crystallization, 122–123  
 crystallization using additives, 123  
 crystallization using antibody Fv fragments, 126  
 crystallization using cubic bicontinuous  
 lipidic phases, 126  
 crystallization using detergents, 123, 125
- cyclooxygenase 1, 124
- cyclooxygenase 2, 124
- cytochrome  $bc_1$  complex, 123
- cytochrome *c* oxidase, 123, 126
- electron crystallography of, 561
- expression and purification of, 92
- FepA, 124
- FhuA, 124
- $\alpha$ -haemolysin, 124
- light-harvesting complex 2, 123
- light-harvesting complex II, 123
- maltoporin, 124
- mechanosensitive ion channel, 123
- OmpA, 124
- OmpF, 124
- PhoE, 124
- photosynthetic reaction centres, 9, 123
- porins, 124
- potassium channel, 123
- precipitants, 123
- prostaglandin  $H_2$  synthase, 124
- squalene cyclase, 124
- Merging *R* factors, 653  
 $R_{\text{meas}}$ , 66, 653  
 $R_{\text{merge}}$ , 66, 653  
 $R_{\text{p.i.m.}}$ , 66  
 $R_{\text{r.i.m.}}$ , 66
- Merohedral twinning, 311
- Metal coordination geometry, use of the CSD, 740
- Metal ions at atomic resolution, 494

## SUBJECT INDEX

- Metalloproteins, metal-ion replacement in, 324  
 Metcalf's law, 449  
 Methane monooxygenase hydrolase, 821  
 Methyl-group conformations from neutron diffraction, 554  
 2-Methylpentane-2,4-diol (MPD), 241, 249  
 Metropolis Monte Carlo simulation, 469  
 Micelles, 94–96, 122  
 Microfluidics, 109  
 Microfocus X-ray tubes, 160  
 Microgravity, 107, 113, 838  
   effect on crystallization, 102  
   gravity and hypergravity, 110  
   mimicking of, 107, 109–110  
 Microspectrophotometry, 259  
*MIDAS*, 449  
 Miller indices, reduced, 296  
 Minimal function, 69, 417  
 Minor-groove-binding drugs, 790  
 MIR. *See* Multiple isomorphous replacement  
 Mirror symmetry, 46  
 Misfolded proteins, 80  
 Misindexing, 284  
 Mis-setting angles, 297  
 Missing symmetry, 654  
 MLF target function, 468  
 MLHL target function, 468  
 MLI target function, 468  
 mmCIF (macromolecular crystallographic information file), 663, 737, 833  
*MMSX*, 449  
 Model bias, 401, 466, 472, 651  
   in combined phase maps, 404  
   in figure-of-merit weighted maps, 404  
 Model building  
   in *Coot*, 443  
   in *PHENIX*, 541, 544  
 Model evaluation, 464  
 Model/noise bias, 632  
 Model phases, figure-of-merit weighting, 404  
 Model rebuilding, 651  
 Moderators, 169  
   for cold neutrons, 169  
   for spallation sources, 173  
   for thermal neutrons, 169  
 Modified Fourier method for estimating coordinate uncertainty, 505  
 Modified Patterson functions, 329  
 Molecular biology, 75  
 Molecular-boundary identification by automated convolution method, 387  
 Molecular design, 39  
 Molecular dynamics, 633, 642  
   animation of trajectories, 454  
   average structures, 644  
   Cartesian, 469  
   effect of crystallographic resolution, 645  
   extended-atom parameters, 642  
   in fibre diffraction, 588  
   in simulated annealing, 463, 469  
   internal motions, 644  
   particle mesh Ewald method, 643  
   potential-energy functions, 642  
   relaxation periods, 634  
   restraints, 633, 643  
   simple point charge model, 633–634  
   torsion-angle, 469–470  
   united-atom approach, 633  
 Molecular-dynamics simulation  
   bovine pancreas ribonuclease A, 645  
   bovine  $\alpha$ -lactalbumin, 645  
   BPTI, 633, 645  
   hen egg-white lysozyme, 642, 645  
   trypsin, 645  
   ubiquitin, 633  
   ubiquitin, atomic mean-square position fluctuations, 636  
   ubiquitin, averaging period, 638  
   ubiquitin, dihedral-angle fluctuations, 639  
   ubiquitin, hydrogen bonding, 635–637  
   ubiquitin, internal motions, 639  
   ubiquitin, potential energy, 634  
   ubiquitin, root-mean-square atom-position deviation, 634  
   Molecular-dynamics simulation  
     ubiquitin, translational and rotational fitting, 636  
     ubiquitin, water diffusion, 640  
 Molecular envelopes, 352  
   determination of, 356  
 Molecular graphics, 448–449, 534, 688, 694  
   animation, 456  
   CPK models, 450  
   direct volume rendering, 453  
   geometric representation, 450  
   illustration, 455  
   ray tracing, 451  
   volumetric representation, 452  
 Molecular machines, 620  
 Molecular masks, 352  
 Molecular packing, 148  
   efficiency, 709  
   measurement of, 709  
 Molecular replacement, 9  
   combined, 349  
   data-collection strategies, 227  
   electron-density averaging, 352  
   in fibre diffraction, 587  
   noncrystallographic symmetry, 333  
   quality indicators for, 70  
   rotation functions, 340  
   translation functions, 347  
   using an NMR structure, 615  
   with *MOLREP*, 364  
   with twinning, 548  
 Molecular surface, 451, 707, 713  
 Molecular volumes, 703  
   Delaunay triangulation, 705  
   Voronoi construction, 703  
 Molecular weight  
   measurement using SANS, 579  
   measurement using SAXS, 567  
*Molkin*, 688, 692  
*MolProbity*, 689–690, 692, 694  
*MolProbity* score, 697  
*MolScript*, 450, 455  
 Monochromatic data collection, 211  
   data-collection geometries, 212  
   detectors, 212  
   exposure time, 224  
   fine slicing, 215  
   rotation range, 215–217, 219  
   still exposure, 213  
   wide slicing, 215  
 Monochromators  
   crystal, for neutrons, 170  
   crystal, for X-rays, 166  
   curved single-crystal, 196  
   double-crystal, 196  
   for synchrotron radiation, 196  
   multilayer, for neutrons, 170  
   polarizing multilayer, for neutrons, 171  
 Monoclinic crystal system, 47  
 Monte Carlo method, in *PrimeX*, 535  
 Monteath Robertson, J., 5–6  
 Moore's law, 449  
 Mosaic spread, 58, 163  
 Mosaicity, 58, 103, 113, 214, 288  
   and data integration, 266  
   anisotropic, 300  
   ideal, 59  
*MOSFLM*, 265, 269  
*MRC*, 630  
*MTZ2HKL*, 532  
 Multiconformer models, 472  
 Multi-copy search, in *MOLREP*, 365  
 Multidimensional isomorphous replacement (MDIR)  
   in fibre diffraction, 587  
 Multidimensional NMR, 616  
 Multidomain averaging, 360  
 Multifiltering cyclic phasing procedure, 438  
 Multilayer monochromators for neutrons, 170  
 Multiple-crystal-form averaging, 360  
   in *DM/DMMULTI*, 408, 412  
 Multiple isomorphous replacement (MIR), 368, 373  
   preparation of heavy-atom derivatives, 317  
   with twinning, 548  
 Multiplicity of a data set, 66  
 Multi-reference alignment, 626  
 Multistart refinement, 471  
 Multivariate statistical analysis, 601, 626, 739  
 Multiwavelength anomalous diffraction (MAD), 373  
   advantages of cryocrystallography, 376  
   and synchrotron radiation, 199  
   anomalous-scatterer labels, 377  
   automated structure solution, 379  
   conversion of data to a pseudo-SIRAS form, 379  
   data-collection strategies, 227  
   data handling, 376  
   design of experiments, 375  
   effect of errors, 376  
   phasing, 374, 376  
   phasing signal strength, 375  
 Multiwire proportional counters  
   for neutrons, 171  
   for X-rays, 180  
 Myoglobin, 6, 8, 756  
  
 N–H...carbonyl hydrogen bonding, 741  
 N–H... $\pi$  hydrogen bonding, 742  
 Nanobodies, 132  
 Nanocrystal analysis, 41  
 Nanomanipulator, 457  
 Nanotechnology, 41  
 NDB. *See* Nucleic Acid Database  
 Neurological disorders, 23  
 Neutron-beam collimators, 169  
 Neutron-beam filters, 169  
 Neutron beamline optics, 173  
 Neutron density maps, 553  
 Neutron detectors, 171  
   image plates, 172  
   multiwire proportional counters, 171  
 Neutron diffraction, 553  
   and solvent structure, 801  
   D<sub>2</sub>O – H<sub>2</sub>O difference maps, 554–555  
   geometries, 553  
   phasing, 554  
   quasi-Laue, 553  
   refinement, 555  
   time-of-flight, 174  
 Neutron guides, 171  
 Neutron instrument resolution functions, 172  
 Neutron scattering  
   coherent, 575  
   incoherent, 575  
 Neutron scattering lengths, 553  
 Neutron sources, 168  
   reactors, 168  
   spallation, 172  
*NEWHELIX*, 770  
 Nicol prism, 147  
 Nominal resolution, 64–65  
 Nonbonded interactions  
   IsoStar, 743–744  
   restraints, 482  
 Noncrystalline fibres, 583  
 Noncrystallographic asymmetric unit, 354  
 Noncrystallographic point-group symmetry, 333  
 Noncrystallographic redundancy, 354  
 Noncrystallographic symmetry, 333, 352  
   cross-rotation function, 335  
   cross-translation function, 335  
   determination of, 390  
   eigendensity functions, 337  
   electron-density averaging, 352, 391  
   electron-density averaging in *DM/DMMULTI*, 409, 411  
   generalized, 333  
   improper, 352–353  
   in *Coot*, 445  
   in isomorphous replacement, 331  
   in phasing, 354  
   in *PHENIX*, 540  
   in structure determination, 335, 337  
   in structure validation, 656, 658  
   overdetermination ratio, 336  
   proper, 352–353  
   refinement of, 391  
   restraints in *SHELXL*, 532  
   rotation functions, 333  
   self-rotation function, 334  
   standard, 333

## SUBJECT INDEX

- Noncrystallographic symmetry  
   subunits, 333  
   translation functions, 334  
   use of Patterson function, 333  
 Nonlinear constraints, 396  
 Non-merohedral twinning, 311  
 Non-primitive (centred) unit cell, 46  
 Normal equations, 463, 500  
 Normal-mode analysis, 474  
 Normal probability analysis, 68  
 Normalized structure factors, 57, 415  
*NUCheck*, 833  
 Nuclear magnetic resonance (NMR), 615  
   and single-crystal X-ray diffraction, 617  
   and solvent structure, 801  
   *cis-trans* isomerization of peptide bonds, 615  
   conformational equilibria, 618  
   dynamic processes, 615, 618  
   multidimensional, 616  
   Nucleic Acid Database, 833  
   Protein Data Bank, 827  
   proton exchange, 615  
   resonance assignments, 616  
   ring flipping, 615, 618  
   structure determination, 615  
   studies of solvation, 617  
   transient local conformational states, 615  
   triple-resonance experiments, 616  
   water-molecule location, 617  
   water-molecule residence times, 617  
 Nuclear Overhauser effect (NOE), 616  
   upper-distance constraints, 616  
 Nucleation, 99, 103, 111, 115  
 Nucleic Acid Database (NDB), 833  
   structure validation, 663  
 Nucleic acids, 766  
   A, B and Z helices, 773  
   A-DNA, 766  
   B-DNA, 766  
   backbone geometry, 766  
   base pairing, 767  
   crystallization of, 100–102, 115  
   DNA, 766  
   DNA/RNA hybrids, 766  
   duplex RNA, 766  
   duplexes, 766  
   glycosyl bond geometry, 773–774  
   helix parameters, 766, 770  
   Hoogsteen base pairing, 769  
   hydrogen bonding in, 722, 726  
   interactions with proteins, 757  
   Nucleic Acid Database, 833  
   stacking of base pairs, 776  
   structure validation, 662  
   sugar ring conformations, 766, 771, 775  
   Watson–Crick base pairing, 769  
   Z-DNA, 766  
 Nucleophilicity, 318–319  
 N-terminal heterogeneity, 88  
  
*O*, 464  
 O—H...O hydrogen bonding, 741  
 O—H... $\pi$  hydrogen bonding, 742  
 Obliquity correction for CCD detectors, 186  
 Observational equations, 462  
 Obsolete PDB entries, archive of, 680, 682  
 Occam's principle, 280  
 Oligonucleotides, 766  
 OmpA, 124  
 OmpF, 124  
*OOPS*, 651  
 Opening angle of synchrotron radiation, 190  
 OPLS force field, 535–537  
 Optical properties of crystals, 145–146  
 Optical resolution, 65  
 Optimization of crystallization conditions, 105–107,  
   110–111, 113, 115  
 Optimization methods, 460, 462  
   first-order, 462  
   Monte Carlo, 462  
   second-order, 462  
   simulated annealing, 462  
   zero-order, 462  
 Order–disorder phenomena, 315  
  
 Origin-removed Patterson refinement, 379  
*ORTEP*, 449, 455  
 Orthogonal molecular interactions in halogen bonds,  
   824  
 Orthogonalization matrix, 355  
 Orthorhombic crystal system, 47  
 Outliers  
   in data integration, 267, 270  
   in derivation of restraints, 477  
   in protein-structure models, 464, 650  
 Overdetermination ratio, 336  
 Overfitting, 466, 651  
 Overlap of electron density in noncrystallographic-  
   symmetry-related regions, 70  
 Overloads, 271  
 Oversampling phasing method, 234  
  
*p*-cell, 354  
 Packing coefficient, 709  
 Packing density, 709  
 Packing efficiency, 709  
 Papain, 9  
 Parallel-axis theorem, 578  
 Parallel processing, 309  
   in *EMAN*, 630  
 Parameter-shift method, 418  
 Parseval's theorem, 401  
 Partial occupancy, 485, 490  
   water-molecule sites, 493  
 Partial specific volume, 152  
 Partial spots, 273  
 Partial twinning, 312  
 Partiality, 289, 296  
 Partiality model, 301  
 Partially recorded reflections, 214  
   in data processing, 296  
   profile fitting, 271  
 Particle mesh Ewald method, 643  
 Patterson, A. L., 6  
 Patterson–correlation translation function, 348  
 Patterson functions, 62, 328  
   and noncrystallographic symmetry, 333  
   cross vectors, 328–329  
   cylindrically averaged, 586  
   modified, 329  
   origin peak, 328  
   self vectors, 329  
   use of, in *Shake-and-Bake*, 419  
 Patterson maps, 62  
   anomalous difference, 331  
   Bijvoet, 9  
   diffraction ripples in, 62  
   number of peaks in, 62  
   sharpening of, 62  
 Patterson minimum function, 330  
 Patterson synthesis, 6  
 Pauling, L., 6  
 PCR (polymerase chain reaction), 76–77  
 PDB Exchange Dictionary (PDBx), 827  
 PDB Japan (PDBj), 830  
*PDBeFold*, 830  
*PDBeMotif*, 830  
*PDBePISA*, 830  
*PDBeXplore*, 831  
 Peak picking, 418  
 Peaklist optimization, 418  
 Pearson correlation, 550  
 PEGs (polyethylene glycols), 86, 100–101, 123,  
   249  
 Penicillin, 5  
 Pepinsky, R., 6, 448  
 Pepsin, 6  
 Peptide flip, 650, 655  
 Peptides  
   *cis*, 654  
   *cis-trans* isomerization, NMR studies of, 615  
   *trans*, 654  
 Perfect twinning, 312  
 Perturbation- $\gamma$  correction, 395  
   in *DM/DMMULTI*, 409  
 Perutz, M. F., 6  
 pET vectors, 92  
 Phase averaging, 440  
 Phase circle, 549  
  
 Phase combination, 385, 394, 404  
   in *DM/DMMULTI*, 409  
 Phase contrast, 595, 599  
 Phase determination, quality indicators for, 69  
 Phase extension  
   and noncrystallographic symmetry, 359  
   by electron-density averaging, 352  
   in *DM/DMMULTI*, 409  
   in reciprocal space, 417  
 Phase improvement, 385  
   constraints, 396  
   in *DM/DMMULTI*, 407  
   quality indicators for, 69  
 Phase probability, 330  
 Phase probability distributions, 369  
   Bayesian calculation of, 379  
   for anomalous scattering, 370  
 Phase problem, 40, 327  
 Phase refinement  
   by electron-density averaging, 352  
   in reciprocal space, 417  
 Phase retrieval, from single-particle diffraction data,  
   235  
 Phase retrieval transfer function, 235  
 Phase sets  
   alignment of, 440  
   cluster analysis of, 441  
   comparison of, 439  
   generation of, 438  
 Phased translation function, 347, 349  
*PHASES*, 361  
 Phasing  
   *ab initio*, 413  
   *ab initio*, in molecular replacement, 360  
   in neutron diffraction, 554  
   in *PHENIX*, 540  
   MAD, 376  
   multisolution methods, 417  
   power of, 360  
   using anomalous scattering, 367  
   using noncrystallographic symmetry, 354  
 Phasing figure of merit, 330, 369, 381  
 Phasing power, 69, 330  
   anomalous, 69  
*PHENIX*, 539, 701  
   graphical user interface, 539  
 Phenotypic selection methods, 130  
 PhoE, 124  
 Phong shading, 451  
 Phosphate-binding protein, 761  
   short hydrogen bond to phosphate, 763  
 Photographic film, 594, 599–600  
 Photon-counting X-ray detectors, 179  
 Photon-integrating X-ray detectors, 179–180  
 Photosynthetic reaction centres, 123  
 Planarity restraints, 481  
 Plasma X-ray sources, 159  
*Pluto*, 455  
 Point groups, 47  
   centrosymmetric, 50  
   enantiomorphous, 47–48  
   icosahedral, 52  
 Point inducible dipole, 730  
 Point X-ray detectors, 179  
 Poisson–Boltzmann equation, 731  
 Polarity, 731  
 Polarizability, 730–731  
   hard and soft metals, 756  
 Polarization factor, 59–60  
 Polarization of electron density, 823  
 Polarization of synchrotron radiation, 189  
 Polarizing multilayer monochromators for neutrons,  
   171  
 Polycrystalline fibres, 583  
 Polyethylene glycols (PEGs), 86, 100–101, 123, 249  
 Polymerase chain reaction (PCR), 76–77  
 Polymorphism, 146, 333  
 Polymorphs, 113, 115  
 Polynucleotide chain tracing, 527  
 Pooled coefficient of variation, 67, 653  
 Porins, 124  
 Position error, 507  
 Positional search, in *MOLREP*, 365  
 Positional shifts, 509



## SUBJECT INDEX

- Post refinement, partially recorded reflections, 296  
 Post-translational modifications, 75–76, 82, 89  
   removal of, 133  
 Potassium channel, 123  
 Potential-energy functions, 642  
 Power of phase determination, 360  
 Precipitants, 123, 319  
   ammonium sulfate, 86, 319  
   magnesium sulfate, 319  
   sodium/potassium phosphate, 319  
 Precision, 499  
   full-matrix estimates of, 505  
   relative, 665  
 Preconditioned conjugate-gradient method, 463, 523  
   in *TNT*, 522  
 Prenucleation, 111  
*Prime*, 534, 537  
*PrimeX*, 534  
 Primitive unit cell, 46  
 Principal component analysis, 739  
*Probe*, 688, 690–692, 694–695, 698–699  
 Probe radius, 709  
 Probe sphere, 707  
*PROCHECK*, 464, 662–663, 677, 684  
*PROCHECK-NMR*, 684  
 Profile fitting, 266, 268  
   in fibre diffraction, 586  
   partially recorded reflections, 271  
   strong reflections, 270  
   systematic errors, 271  
   weak reflections, 270  
 Project MAC, 449  
*cis*-Prolines, frequency of, 474  
*PROLS*, 463  
*PROSA II*, 664  
 Prostaglandin H<sub>2</sub> synthase, 124  
*PROTEIN*, 330  
 Protein–carbohydrate recognition, 755  
 Protein chain tracing, 526  
 Protein crystallization, 129  
 Protein Data Bank (PDB), 827  
   deposition sites, 827  
   IsoStar, 743–744  
 Protein Data Bank in Europe (PDBe), 830  
 Protein–DNA recognition, water molecules in, 816  
 Protein domains, 752  
   boundaries, 752  
   discontinuous, 752  
   identification, 749, 752  
 Protein engineering, 75, 129, 140  
 Protein expression, 75–77, 142  
   baculoviruses, 83  
   constitutive, 78  
   constructs, 76  
   fermentation, 80  
   growth media, 80  
   in *E. coli*, 77, 79, 142  
   in yeasts, 82  
   inducible, 78  
   insect cell–virus, 83  
   mammalian cells, 84  
   misfolded proteins, 80  
   plasmids, 78  
   post-translational modifications, 75–76, 82, 89  
   preparation of cDNA clones, 76  
   T7 polymerase, 78  
 Protein families, 749  
 Protein folding, 81  
   hydrogen bonding in, 723  
   *in vivo*, 81  
   misfolded proteins, 80  
   refolding, 87  
   role of water molecules, 800  
   studied by SAXS, 572  
   use of chaperones, 81  
 Protein function  
   role of metal ions, 756  
   role of water molecules, 800  
 Protein heterogeneity, conformational, 104  
 Protein kinase A, solvent structure, 814  
 Protein–ligand docking programs, 745  
 Protein–ligand interactions, 755  
   carbohydrates, 755  
   IsoStar, 743  
 Protein–ligand interactions  
   metals, 756  
   phosphate, 761  
   role of water molecules, 800, 807  
   sulfate, 761  
   use of the CSD, 740, 743  
 Protein–nucleic acid interactions, 757  
   DNA, 757, 759  
   RNA, 759–760  
   transfer RNA, 759  
 Protein purification, 85  
   chromatography, 86  
   isoelectric focusing, 88  
   mass spectrometry, 88  
   N-terminal heterogeneity, 88  
   sample heterogeneity, 89  
   SDS–PAGE, 88  
 Protein refolding, 87  
 Protein stability  
   effect of hydrogen bonding, 723  
   role of metal ions, 756  
 Protein structure classification, 749, 752  
   CATH, 749–751  
   DALI, 749–751  
   DALI domain dictionary, 751, 753  
   3Dee, 749–750  
   ENTREZ, 749, 751  
   HOMSTRAD, 749–750  
   SCOP, 749–750  
   SSAP, 749  
   STAMP, 749  
   VAST, 751  
 Protein superfamilies, 750  
 Protein targets, stabilization of, 134  
 Protein–water interactions  
   database analysis, 802  
   effect of secondary structure, 805  
   effect of tertiary structure, 806  
*ProteinCCD* server, 136  
 Proteins, storage of, 89  
 Proteolysis, 131  
   in *E. coli*, 81  
   N-end rule, 79  
   of recombinant proteins, 81  
 Proton exchange, NMR studies of, 615  
 Protozoan infections, 16, 21  
*PROVE*, 664  
*PS79*, 587  
 Pseudo-crystallographic symmetry, 333  
 Pseudo-merohedral twinning, 312  
 Pseudosymmetry, 654  
   in isomorphous replacement, 331  
 Pump–probe studies, 42  
 Pycnometry, 154  
 Python, 630  
  
*Q* factor, 601  
 Quadratic information measure, 487  
 Quality indicators, 650, 652  
   *G* factors, 656  
   merging *R* factors, 653  
   pooled coefficient of variation, 653  
 Quality of data, 65  
 Quasi-Laue neutron diffraction, 553  
  
*R* factors, 464  
   crystallographic, 71, 651, 657, 665  
   for density modification, 70  
   in fibre diffraction, 588  
   *R*<sub>anom</sub>, 67  
   *R*<sub>Cullis</sub>, 69, 330  
   *R*<sub>Cullis,ano</sub>, 69  
   *R*<sub>d</sub>, 68  
   *R*<sub>free</sub>, 70, 71, 464, 466, 506, 651, 657, 665  
   *R*<sub>Kraut</sub>, 330  
   *R*<sub>meas</sub>, 66  
   *R*<sub>merge</sub>, 66, 224, 228, 298, 559  
   *R*<sub>mrgd-F</sub>, 66  
   *R*<sub>mrgd-I</sub>, 66  
   *R*<sub>p.i.m.</sub>, 66  
   *R*<sub>r.i.m.</sub>, 66  
   *R*<sub>scale</sub>, 68  
   *R*<sub>sym</sub>, 559  
   real-space, 657, 666  
  
*R*-factor translation function, 347  
*RADDOSE*, 258  
 Radiation damage, 68, 225, 249, 256  
   and cryogenic vitrification, 225  
   and Laue diffraction, 207  
   free radicals, 243  
   in electron diffraction, 558  
   in electron microscopy, 593–594  
   in single-particle diffraction, 236  
   suppression of, 242  
 Radiation-damage-induced phasing (RIP), 260  
 Radiation dose, 256  
 Radiation dose limit, 258  
 Radiation-induced shrinkage, 236  
 Radicals, 259  
 Radioactive X-ray sources, 159  
 Radius of convergence, 459  
 Radius of gyration, 565, 567, 576  
 Ramachandran plot, 454, 650, 654, 678, 685, 739  
   analysis, 695  
   multiple-model, 656  
 Ramachandran restraints, in *Coot*, 444  
 Random-atom model, 435  
 Random-conical reconstruction, 620  
 Random omit maps, 419  
*RasMol*, 450  
*Raster3D*, 717  
*RAVE*, 361  
 Ray tracing, 451  
 Rayleigh scattering, 59  
 Reaction potential, 731  
 Real-space calculations, in *PrimeX*, 537  
 Real-space constraints, 418  
 Real-space fit, 650, 657  
 Real-space *R* factor, 657, 666  
 Real-space refinement, in *Coot*, 444  
 Real-space residual, 71  
 Real-space search, in *MOLREP*, 366  
 Recentring, 435  
 Reciprocal lattice, 57  
 Reciprocal-lattice points, non-integral, 354  
 Reciprocal-lattice vectors, distribution of, 263  
 Reciprocal space, 57  
 Reciprocal-space calculations, in *PrimeX*, 536  
 Recombinant proteins, 75  
   incorporation of selenomethionine, 76  
   minimizing proteolysis of, 81  
   toxicity of, to host, 81  
 Recombination cloning, 141  
 Reconstruction engine, 620  
 Reduced cell, 264, 279  
 Reduced Miller indices, 296  
 Redundancy, 66, 206–207, 217, 227, 376, 653  
   noncrystallographic, 354  
 Re-entrant surface, 707, 713  
 Reference bias, 626  
 Refinement, 459  
   against intensities, 460  
   atomic resolution, 485  
   bias, 405  
   block-matrix approximation, 488  
   conjugate-gradient method, 397, 463, 488  
   conjugate-gradient method, preconditioned, 463, 522  
   coordinate uncertainty, 499  
   data quality, 460  
   diagonal-approximation method, 488  
   difference-Fourier method, 459  
   global minimum, 466  
   in electron diffraction, 560  
   in fibre diffraction, 587  
   in *SHELX*, 529  
   in *SHELXL*, 531  
   intensity-based likelihood, 489  
   least-squares, 459–460, 488, 500  
   local minima, 466  
   maximum-likelihood, 460, 467, 489  
   modelling of solvent, 462, 464  
   models, 461  
   neutron diffraction data, 555  
   normal equations, 463, 500  
   observational equations, 462

## SUBJECT INDEX

- Refinement  
 partial occupancy, 490  
 quality indicators for, 71  
 radius of convergence, 459  
 restrained, 501, 504  
 restraints, 474–475  
 rigid groups, 461  
 simulated annealing, 463, 466  
 singularity in, 463  
 target functions, 466–467  
 torsion-angle, 466  
 weighting, 460, 500  
 with twinning, 549
- Reflection intensity, integrated, 58
- Reflection-omit method, 395  
 in *DM/DMMULTI*, 409
- Reflection profiles, 223
- REFMAC*, 489
- Refraction, 146
- Refractive index, 146, 148
- Register error, 649
- Remote data collection, 231
- Representation of information, 454
- Representation of structures, 448–449  
 animation, 456  
 CPK models, 450  
 direct volume rendering, 453  
 geometric, 450  
 illustration, 455  
 isosurfaces, 452  
 physical models, 456  
 ray tracing, 451  
 stereolithography, 456  
 three-dimensional printing, 456  
 volumetric, 452
- Representation of surfaces, 450, 713, 717  
 colour coding, 451  
 Gouraud shading, 451  
 Phong shading, 451  
 photorealistic rendering, 717  
 roadmaps, 719  
 shaded backbone, 717  
 texture mapping, 451
- Research Collaboratory for Structural Bioinformatics (RCSB PDB), 829
- Residual function, 501
- Resolution, 243  
 effective, 66  
 in single-particle reconstruction, 632  
 nominal, 64–65  
 optical, 65  
 true, 65
- Resonance-assisted hydrogen bonding, 741
- Resonance-induced hydrogen bonding, 741
- RESTRAIN*, 488
- Restrained full-matrix inversion for concanavalin A, 502
- Restrained refinement, 501, 504  
 in fibre diffraction, 587  
 residual function, 501  
 two-atom model, 501
- Restraints, 71, 461, 474–475, 535  
 atomic displacement parameter, 490  
 bond-angle, 474, 477, 479  
 bond-length, 474, 476–477  
 choice of, 475  
 coordinate, 490  
 effect on error estimates, 488  
 ensemble-averaged, 633  
 geometrical, 461  
 in molecular dynamics, 633, 643  
 in *PHENIX*, 543  
 in *SHELXL*, 531  
 in *TNT*, 520  
 nonbonded interactions, 482  
 planarity, 481  
 special geometries, 482  
 target parameters, 474  
 time-averaged, 633  
 torsion-angle, 482  
 use of the CSD, 474  
 weighting of, 502
- Reticular twinning, 312
- Rhodopsin tag, 93
- Ribonuclease, 9  
 A, solvent structure, 813  
 T1, solvent structure, 813
- Ribose-pucker outliers, 697
- Ribosome, synchrotron-radiation studies of, 198
- Ribulose-1,5-bisphosphate carboxylase/oxygenase (RuBisCO), structure validation, 679
- Richards box, 10, 449
- Rigid-body superposition, 749
- Rigid-group refinement, 461  
 in *TNT*, 522
- Ring flipping, NMR studies of, 615, 618
- RIP (radiation-damage-induced phasing), 260
- RNA  
 duplex RNA, 766  
 hydrogen bonding in, 726  
 interactions with proteins, 759–760  
 Nucleic Acid Database, 833  
 treatment in *PHENIX*, 541
- RNA backbone suite outliers, 699
- RNA dimerization initiation site, 825
- RNABC*, 699
- Robertson sorting board, 6
- Robotic crystal loading, 231
- Robotics, in crystallization, 107
- Robots, 247
- Rocking curve, 214
- Rocking width, 197
- Root-mean-square correlation ratio, 68
- Root-mean-square deviation from crystallographic symmetry, 73
- Root-mean-square *Z* score, 73
- Rossmann, M. G., 9
- Rotamer conformations, 655
- Rotamer side-chain fit, 651
- Rotating-anode X-ray tubes, 159
- Rotation axes, 46–47
- Rotation functions, 340  
 and noncrystallographic symmetry, 333  
 computation of, 342  
 cross-rotation, 341  
 fast, 342  
 locked, 343  
 quality indicators for, 70  
 sampling of, 342  
 self-rotation, 341  
 symmetry properties of, 343
- Rotation group, 342  
 metric of, 341
- Rotation method, 213, 272
- Rotation range, 215–217, 219
- Rotational disorder in fibre diffraction, 584
- Rotational search, in *MOLREP*, 365
- Rotational symmetry, 46
- Rotations in three-dimensional Euclidean space, 340
- Royal Institution, The, 845
- Rusticyanin, structure validation, 667
- RvR calculation, 549
- $\sigma$  holes, 823, 825  
 $\sigma_A$  plot, 73, 404, 658  
 $\sigma_A$  values, estimation of, 403  
 $\sigma_A$  weighting, 394
- Saddlepoint method, 435
- Sample acceptance, 191
- SANS. *See* Small-angle neutron scattering
- SAXS. *See* Small-angle X-ray scattering
- Sayre's equation  
 application to macromolecules at non-atomic resolution, 392  
 for phase refinement and extension, 392  
 in real and reciprocal space, 392  
 shape function, 392
- Scale factor, 286, 290–291
- Scaling, 68, 277  
 anisotropic, 488  
 Hamilton, Rollett and Sparks method, 296  
 in density modification, 390  
 in *DM/DMMULTI*, 410  
 in *MOLREP*, 365  
 in *SFCHECK*, 666  
 local, 381  
 of intensity data for lysozyme, 851  
 of structure factors, 57
- Scaling  
 partially recorded reflections, 296  
*R* factors, 68, 298  
 restraints and constraints, 297  
 selection of reflections for, 297
- SCALEPACK*, 282
- Scattering, 59  
 Compton, 59  
 elastic, 52  
 electron, 557  
 inelastic, 52  
 Rayleigh, 59  
 Thomson, 53
- Scattering factors  
 anomalous, 373  
 atomic, 54, 373  
 atomic, solvent-corrected, 587
- Scattering lengths, neutron, 553
- Scavengers, 259
- SCOP, 749–750
- Screening potential, 731
- Screenless rotation method, 212
- Screw axes, 46, 61
- Screw disorder in fibre diffraction, 584
- SDS–PAGE, 88
- Search model, in *MOLREP*, 364
- SEC (size-exclusion chromatography), 95
- Secondary structure  
 and hydrogen bonding, 723, 742  
 effect on protein–water interactions, 805  
 from NMR studies, 615  
 of RNA, 759
- Selection rule in fibre diffraction, 584
- Selenocysteine, 325
- Selenomethionine, 76, 317, 325, 377
- Self-potential, 731
- Self-rotation function, 334, 341
- Self vectors, 329
- Sequence tags, 77
- Serine proteases, solvent structure, 808
- SFCHECK*, 657, 666, 834  
 global quality indicators, 666, 668  
 local quality indicators, 667, 670
- Shake-and-Bake*, 423
- 'Shaking', 417
- Shannon's sampling theorem, 358
- Shape function, 392
- $\beta$ -Sheets, 6  
 hydrogen bonding in, 724
- SHELX*, 529
- SHELXL*, 487, 665
- SHELXL98*, 463–464
- SHELXPRO*, 532
- Shine–Dalgarno sequence, 78–79
- Shutterless detector systems, 41
- Side-chain hydrogen bonding, 724
- Side-chain placement, in *PrimeX*, 537
- Side-chain rotamers, 695
- Side-chain torsion angles, 655
- SIFTS, 831
- SIGMAA*, 403, 405
- Signal sequence, 93
- Signal strength and structure validation, 653
- Signal-to-noise ratio, 64  
 highest possible, 67  
 mean, 67
- Sim distribution, 402, 467
- Sim weighting, 394  
 in *DM/DMMULTI*, 409
- Simple point charge (SPC) model, 633–634
- Simulated annealing, 463, 466  
 annealing schedules, 470  
 comparison with conjugate-gradient method, 471  
 in *CNS*, 517  
 in fibre diffraction, 588  
 in *PrimeX*, 536–537  
 molecular dynamics, 469  
 multistart refinement, 471  
 searching conformational space, 468  
 temperature, 469
- Single isomorphous replacement (SIR), 371
- Single-particle diffraction, 42, 235
- Single-particle electron cryomicroscopy, 42, 624

## SUBJECT INDEX

- Single-particle imaging, 41
- Single-particle reconstruction, 620, 629  
resolution of, 43
- Single-wavelength anomalous scattering (dispersion),  
data-collection strategies, 227
- Singularity in refinement, 463
- Site-directed mutagenesis, 130, 317, 325
- Size-exclusion chromatography (SEC), 86, 95
- Skeletonization, 392  
in *DM/DMMULTI*, 407, 409
- Skewness of electron density, 70
- Small amphiphile concept, 125
- Small-angle neutron scattering (SANS), 575  
crystallization studies, 111  
Debye equation, 575  
distance measurements, 579–580  
length distribution, 576  
molecular weights, 579
- Small-angle X-ray scattering (SAXS), 563  
computer programs, 571  
crystallization studies, 111  
data collection, 570  
data processing, 571  
experiment design, 570  
instrumentation for conventional sources, 568  
low-resolution model determination, 567  
sample handling, 569  
sample preparation, 569  
single-crystal, 563  
solution, 564  
synchrotron instrumentation, 568
- SnB*, 421
- Sodium/potassium phosphate, 319
- Soft ligands, 318
- Soft metals, 757
- Solubility of proteins, 99, 101, 114–115, 130  
solubility enhancers, 103  
solubilizing agents, 103
- Solution X-ray scattering, 564  
and crystal structures, 567  
computer programs, 571  
data collection, 570  
data processing, 571  
Debye formula, 567  
Debye function, 565  
electron pair distribution function, 565–566  
experiment design, 570  
Guinier plot, 565  
instrumentation for conventional sources, 568  
low-resolution model determination, 567  
molecular weights, 567  
radius of gyration, 565, 567  
sample handling, 569  
sample preparation, 569  
synchrotron instrumentation, 568
- Solvation, NMR studies of, 617
- Solvation free energies, 822
- Solvation potential, 731
- Solve*, 330, 379, 382  
scoring trial heavy-atom solutions, 380
- Solvent  
bound, 153  
bulk, modelling of, 462, 464, 493  
in structure validation, 656  
modelling in *SHELXL*, 532  
ordered, at atomic resolution, 493  
variation of density, 577
- Solvent-accessible surface, 451, 707, 713
- Solvent-corrected atomic scattering factor, 587
- Solvent density, 156
- Solvent-excluding surface, 451, 713
- Solvent flattening, 386  
in *DM/DMMULTI*, 407–408  
in fibre diffraction, 587
- Solvent flipping, 388, 395
- Solvent masks, in *DM/DMMULTI*, 407, 411
- Solvent modification, 241
- Solvent structure, 800  
D<sub>2</sub>O – H<sub>2</sub>O difference maps, 555  
neutron diffraction, 554, 801  
NMR studies, 801  
simulation of, 801  
solution X-ray scattering, 567
- Source entropy, 433
- Space-group assignment, 278, 654
- Space groups, 46  
common, for protein crystals, 47
- Spallation neutron sources, 172
- Special positions, 47
- Spectral brightness of synchrotron radiation, 189
- Sphere of influence algorithm, in *SHELXE*, 530
- Sphere refinement, in *Coot*, 444
- Spherical aberration, 599
- Spherical Bessel functions, 345
- Spherical harmonics, 345
- SPIDER*, 620, 630
- Spin contrast variation, 578, 580
- SPIRE*, 620
- Squalene cyclase, 124
- SQUASH*, 361
- SSAP, 749
- STAMP*, 749
- Standard atomic radii, 708
- Standard atomic volumes, 710  
in structure validation, 664
- Standard basis vectors, 46
- Standard profiles, 268
- Standard residue volumes, 710
- Standard spot shape, 273
- Standard uncertainty (s.u.), 65, 499, 501, 665  
estimation in *SHELXL*, 531
- Stanley, W., 7
- Stanley factor, 313
- Staphylococcal nuclease, 757
- Static disorder, 462, 485
- Stationary-target X-ray tubes, 159
- Stereolithography, 456
- Stereoscopic viewing, 237
- Still exposure, 213
- Storage of crystals at low temperature, 253
- Storage of proteins, 89
- Structural genomics, 13, 199
- Structure-based drug design, 15  
use of the CSD, 745
- Structure determination  
by fibre diffraction, 586  
by NMR, 615  
by single-crystal X-ray diffraction and NMR, 617  
in *CNS*, 512  
in *SHELX*, 529  
using noncrystallographic symmetry, 335, 337
- Structure-factor averaging, 471
- Structure-factor probability distributions, 401  
general treatment, 403  
Luzzati, 403  
Sim, 402, 467  
Wilson, 402  
Woolfson, 402
- Structure factors, 55–56  
centrosymmetric structures, 56  
Fourier–Bessel, 584  
in electron diffraction, 559  
in fibre diffraction, 584  
noncentrosymmetric structures, 56  
normalized, 57, 415  
placing on an absolute scale, 57
- Structure invariants, 416
- Structure refinement, in *PHENIX*, 543
- Structure representation, 448–449  
animation, 456  
CPK models, 450  
direct volume rendering, 453  
geometric, 450  
illustration, 455  
isosurfaces, 452  
physical models, 456  
ray tracing, 451  
stereolithography, 456  
three-dimensional printing, 456  
volumetric, 452
- Structure solution  
automated, for MAD and MIR, 379  
in *PHENIX*, 539
- Structure validation, 649, 662, 677  
agreement of model with experimental data, 662, 665  
at the NDB, 663  
Balasubramanian plot, 655
- Structure validation  
bond angles, 654, 662, 685  
bond lengths, 654, 662, 685  
C<sup>α</sup>-only models, 655  
choice of reference structures, 679  
data completeness, 653  
data resolution, 653  
detection of outliers, 650  
difference density quality, 658  
diphtheria toxin, 681  
directional atomic contact analysis, 655  
environment profiles, 663  
geometric parameters, 654, 662  
hetero groups, 663  
hydrogen-bonding analysis, 651, 655  
in *MolProbity*, 694  
knowledge-based interaction potentials, 663  
main-chain torsion angles, 677  
nonbonded interactions, 677  
nonbonded parameters, 663  
noncrystallographic symmetry, 656, 658  
nucleic acids, 662  
packing, 677  
pep-flip value, 650  
planarity, 654  
*PROCHECK*, 684  
quality indicators, 650  
Ramachandran plot, 650, 654, 678, 685  
real-space fit, 650, 657  
rotamer side-chain fit, 651  
RuBisCO, 679  
rusticyanin, 667  
*SFCHECK*, 666  
side-chain torsion angles, 655  
signal strength, 653  
solvent, 656  
standard atomic volumes, 664  
standard values, 662–663  
stereochemical parameters, 654, 662–663  
torsion angles, 654  
triacylglycerol lipase, 681  
unit-cell parameters, 653  
use of the CSD, 662, 737
- Stuhrmann equation, 577
- Substituent effects in halogen interactions, 821
- Substructure determination, 68  
in *PHENIX*, 540
- Substructure solution, with *SHELXD*, 529
- Subtilisin, 9
- Sugar ring conformations, 766, 771, 775  
C2'-endo, 767  
C3'-endo, 767  
envelope (E), 766
- Sulfate-binding protein, 761
- Summation integration, 266–267
- Supermirrors for neutrons, 170
- Supersaturation, 99
- SuperStar*, 745
- Support film, 597, 599, 603–604
- Supramolecular synthons, 743
- Surface-area calculation, 713–714  
analytical, 715  
complete rolling algorithm, 714  
connected rolling algorithm, 714  
Connolly dot surface algorithm, 714  
extended atoms, 715  
Gauss–Bonnet theorem, 715  
Lee & Richards planar slices, 714  
marching-cube algorithm, 714
- Surface areas, 703
- Surface-entropy reduction, 134
- Surface-entropy reduction server, 136
- Surfaces, 713  
Connolly surface, 451, 717  
contact surface, 707, 713  
convex hull, 706  
definitions of, 706  
*GRASP* surfaces, 718  
hydration surface, 714  
molecular surface, 451, 707, 713  
occluded molecular surface, 713  
probe sphere, 707  
re-entrant surface, 707, 713  
solid polyhedral surfaces, 717

## SUBJECT INDEX

- Surfaces  
 solvent-accessible surface, 451, 707, 713  
 solvent-excluding surface, 451, 713  
 van der Waals surface, 707, 713  
 Voronoi polyhedra, 706
- Surfaces, representation of, 450, 713, 717  
 colour coding, 451  
 Gouraud shading, 451  
 Phong shading, 451  
 photorealistic rendering, 717  
 roadmaps, 719  
 shaded backbone, 717  
 texture mapping, 451
- SurVol*, 664
- Symmetry, 46  
 helical, 333, 584  
 icosahedral, 47  
 in diffraction patterns, 60  
 inversion, 46  
 mirror, 46  
 missing, 654  
 rotational, 46  
 translational, 46
- Symmetry correction, 336–337
- Synchrotron radiation, 189, 212  
 and Laue diffraction, 195, 205  
 and MAD, 199  
 and SAXS, 568  
 angular brightness, 189  
 area detectors, 195, 198  
 atomic resolution studies, 198  
 beamlines for macromolecular crystallography, 192  
 bending magnets, 161  
 collimation, 189  
 critical wavelength, 161, 190  
 detectors, 195  
 F<sub>1</sub> ATPase, 198  
 flux, 189  
 in protein crystallography, 197  
 insertion devices, 161, 190–191  
 instrumentation, 189, 194  
 intensity, 192  
 machine emittance, 190  
 monochromatic, 196  
 monochromators, 196  
 multipole wigglers, 190  
 opening angle, 190  
 polarization, 189  
 production of, 189  
 properties of, 189  
 sample acceptance, 191  
 sources, 160  
 sources, first-generation, 192  
 sources, second-generation, 193  
 sources, third-generation, 193  
 spectral brightness, 189  
 studies of multi-macromolecular complexes, 198  
 studies of small crystals, 198  
 studies of the ribosome, 198  
 time-resolved studies, 198  
 total radiated power, 190  
 tunability, 189  
 undulators, 161, 190  
 universal curve, 190  
 wavelength shifters, 190  
 wigglers, 161
- Synthetic biology, 824
- Systematic absences, 61
- $\pi$  systems in halogen bonds, 824–825
- T4 lysozyme, solvent structure, 812
- T7 polymerase expression system, 78
- Tags, 77, 131  
 removal of, 77
- Tangent formula, 417
- Target constructs, optimization of, 131
- Target functions, 466–467  
 in *CNS*, 512, 514  
 MLF, 468  
 MLHL, 468  
 MLI, 468
- Target parameters, 474
- Telluromethionine, 317
- Temperature (in simulated annealing), 469
- Temperature factors (atomic displacement parameters), 56–57, 485  
 anisotropic, 56, 485  
 anisotropic, at atomic resolution, 492  
 anisotropic, refinement in *SHELXL*, 531  
 constraints, 490  
 effect of coordinate errors, 461  
 effect on coordinate uncertainty, 499  
 group *B* factors, 461  
 in structure validation, 656  
 isotropic, 56  
 refinement of, 461  
 restraints, 490, 522
- Tertiary structure  
 effect on protein–water interactions, 806  
 of RNA, 759
- Tetartohedral twinning, 315
- Tetragonal crystal system, 52
- Texture mapping, 451
- Thermostability, 134
- Thomson scattering, 53
- Thon rings, 42
- Three-dimensional image reconstruction, 596–597,  
 601–602
- Three-dimensional printing, 456
- Three-dimensional reconstruction, 42, 626  
 in electron diffraction, 558  
 software, 43
- Thyroxine, 821
- Time-resolved crystallography, 41
- Time-resolved imaging, 42
- Time-resolved studies, 198, 205, 208
- Time-resolved diffraction, 585  
 using SAXS, 572
- TNT*, 463
- Tobacco mosaic virus (TMV), 6  
 fibre diffraction, 587
- Tomographic crystal-volume measurement, 155
- Torsion-angle molecular dynamics, 469–470
- Torsion-angle refinement, 466
- Torsion-angle restraints, 482
- Torsion angles  
 in DNA, 771  
 in nucleic acid backbone chains, 766
- Transfection, 84
- Transfer RNA  
 interactions with proteins, 759  
 low-abundance, 79
- Translation functions, 347  
 and noncrystallographic symmetry, 334  
 correlation-coefficient, 347  
 locked, 350  
 packing analysis, 349  
 Patterson-correlation, 348  
 phased, 347, 349  
 quality indicators for, 70  
*R*-factor, 347
- Translation, libration and screw tensor, 462, 485, 488,  
 492
- Translational cross-correlation, 621
- Translational disorder in fibre diffraction, 584
- Translational symmetry, 46
- Transmission factor, 59
- Transverse relaxation-optimized spectroscopy  
 (TROSY), 616
- Triacylglycerol lipase, structure validation, 681
- Triangulation number, 47
- Triclinic crystal system, 47
- Trigonal crystal system, 52
- Triple isotopic substitution, 578
- Triplet invariants, 416
- Tris buffer, 319
- True resolution, 65
- Trueblood, K. N., 5
- Truncation, 131
- Trypsin, molecular-dynamics simulation, 645
- Tubulin, electron-diffraction studies, 560–561
- Tunability of synchrotron radiation, 189
- Turns, hydrogen bonding in, 724
- Twin fraction, 312, 548
- Twinning, 146  
 by hemihedry, 312  
 by merohedry, 311  
 by non-merohedry, 311
- Twinning  
 by pseudo-merohedry, 312  
 by tetartohedry, 315  
 epitaxial, 311  
 hemihedral, 146  
 in autoindexing, 284  
 indications of, 312  
 partial, 312  
 perfect, 312  
 reticular, 312  
 tests for, 313  
 treatment in *SHELXL*, 532
- Two-dimensional crystals, 558, 561, 603
- Ubiquitin, molecular-dynamics simulation, 633
- Undulators, 161, 190
- Uneven crystal rotation, 290
- Uneven exposure, 290
- Uniaxial crystals, 147
- Unified-atom parameters, 708
- Unit cell, 45  
 non-primitive (centred), 46  
 origin choice, 46  
 primitive, 46
- Unit-cell parameters, accuracy of, 266, 653
- Unified-atom approach, 633
- Universal curve, 190
- Unrestrained full-matrix inversion  
 for an immunoglobulin, 504  
 for concanavalin A, 502
- Vaccines, 26
- Validation  
 in *Coot*, 445  
 in *PHENIX*, 542  
 Protein Data Bank, 827  
 van der Waals radii, 708, 713, 740, 821–822  
 from the CSD, 709  
 van der Waals surface, 707
- Vapour-diffusion methods of crystallization, 104, 106
- Variable virtual bond method, 587
- Variances, 499
- VAST, 751
- Velocity selectors, 171
- VERIFY3D*, 678
- Vertex error, 705
- Virtual reality, 449
- Viruses, 16–17  
 crystallization of, 108, 110, 112, 115  
 early studies, 9  
 helical, 589  
 icosahedral symmetry, 47
- Visualization, 40  
 of information, 454
- Vitamin B<sub>12</sub>, 5
- Vitrification of specimens for cryoTEM, 597, 599
- Volume *Z* score, 664
- Volumenometry, 154
- Voronoi construction, 664, 703
- Voronoi polyhedra, 703  
 and surfaces, 706  
 chopping-down method, 705  
 for proteins, 704  
 method B, 704  
 radical-plane method, 705  
 ratio method, 704  
 vertex error, 705
- Water molecules  
 as mediators in complex formation, 815  
 automatic location of, 493  
 buried, 726, 810  
 channel sites, 810  
 criteria for placing in electron-density maps, 801  
 crystal-contact sites, 810  
 D<sub>2</sub>O – H<sub>2</sub>O difference maps, 555  
 determining position of, 801  
 distribution around amino acids, 802  
 in antigen–antibody association, 815  
 in dimeric haemoglobin, 816  
 in protein–DNA recognition, 816  
 interactions with proteins, 802  
 location by NMR, 617  
 NMR studies, 801

## SUBJECT INDEX

- Water molecules  
 orientation of, from neutron diffraction, 554–555  
 partially occupied sites, 493  
 residence times, 617  
 role in protein folding, 800  
 role in protein structure and function, 800  
 surface sites, 810
- Watson, J. D., 6
- Watson–Crick base pairing, 769
- Watson–Crick Z-DNA, 778
- Wavelength bandpass, 214
- Wavelength normalization curve, 195, 206
- Wavelength shifters, 190
- Wavevector, 272
- Weak intensity data, inclusion in refinement, 460
- Weak intermolecular interactions, 742
- Weak-phase-object approximation, 599
- Weighting, 500  
 in *MOLREP*, 365  
 of data in refinement, 460  
 of diffraction data and restraints, 502  
 $\sigma_A$ , 394  
 Sim, 394
- WHAT IF*, 464, 662–663, 678
- Wide slicing, 215
- Wiener filtering, 621
- Wigglers, 161  
 multipole, 190
- Wilson distribution, 402
- Wilson plot, 57  
*B* factor, 68
- Woolfson distribution, 402
- XDS*, 272, 304
- XDSCONV*, 309
- X-PLOR*, 463, 644  
 for fibre diffraction, 588  
 restraints, 662
- X-RAC, 448
- X-ray detectors, 177, 183  
 accuracy, 177  
 and synchrotron radiation, 195  
 area, 179  
 dynamic range, 178  
 film, 180  
 flat-field corrections, 178  
 gas discharge (wire) counters, 180  
 geometric distortion, 178  
 image plates, 180  
 line spread function, 177  
 multiwire proportional counters, 180  
 photon counters, 179  
 photon integrators, 179–180  
 pixel array, 181  
 point, 179  
 point spread function, 177  
 reverse-biased semiconductor, 180  
 scintillator/photomultiplier, 179  
 signal-to-noise ratio, 177  
 spatial resolution, 177  
 stopping power, 178  
 storage phosphors, 180  
 television, 181
- X-ray free-electron lasers, 41, 194
- X-ray generation, 159
- X-ray mirrors, 164
- X-ray sources, 39, 159  
 channelling radiation, 159  
 for monochromatic data collection, 211  
 microfocus X-ray tubes, 160  
 plasmas, 159  
 radioactive sources, 159  
 rotating-anode X-ray tubes, 159  
 stationary-target X-ray tubes, 159  
 X-ray free-electron lasers, 41, 194
- X-ray topography, crystallization studies, 113
- X-ray tubes  
 characteristic radiation, 160  
 microfocus, 160  
 rotating-anode, 159  
 stationary-target, 159
- X-ray wavelength, choice of, 162, 222
- XSCALE*, 277, 308
- XtalPred* server, 136
- XtalView*, 330, 464
- Yeast, high-resolution imaging of, 235
- Yeasts as expression systems, 82
- z*-buffer, 450
- Z* score, 71  
 root-mean-square, 73
- Z-DNA, 766
- Zingers, 185