

## 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  
 Beevers, C. A., 6  
 Beevers–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- $\theta$ , 285  
     data, 284  
 Coordinate uncertainty, 499  
     approximate methods, 505  
     block-matrix calculations, 505  
     low-resolution structures, 506  
     modified Fourier method, 505  
*Coot*, 443  
 $\text{CorA}$ , 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  
*CRYSTOL*, 567  
 Crystal-density measurement, 152  
     Archimedes' method, 154  
     by flotation, 154  
     by pycnometry, 154  
     by tomographic crystal-volume measurement, 155  
     by volumenometry, 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  
 $D_{m,m'}^{\ell}$  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–Scherre 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  
 Detective 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  
 Detectors  
     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  
 Enantiomeric 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  
     polyptides, 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  
*FLEXS*, 745  
*FLEXX*, 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 wiggler, 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  
 Kinemages, 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  
     maltoxin, 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*<sub>meas</sub>, 66, 653  
     *R*<sub>merge</sub>, 66, 653  
     *R*<sub>p.i.m.</sub>, 66  
     *R*<sub>r.i.m.</sub>, 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  
*Molikin*, 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  
  enantiomorphic, 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  
 mean anomalous, 68
- 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  
 $F_1$  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 wiggler, 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  
 wiggler, 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  
 in fibre 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
- United-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