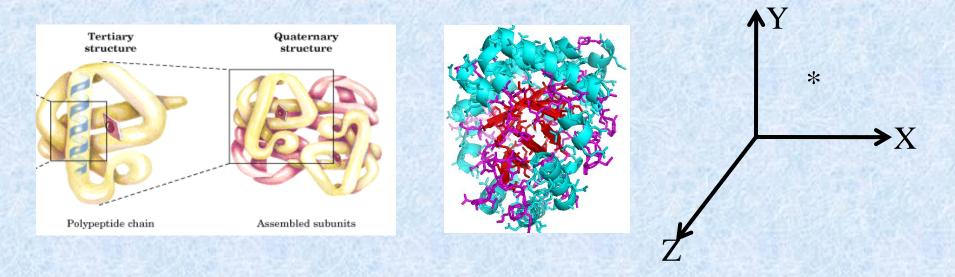
Tertiary and quaternary structures

Tertiary structure provides the information about the threedimensional structure of a protein with atomic details; the positions of each atom in Cartesian coordinate system.



3D structure of a protein contains the complete information.

3D structure determination Experiment

X-ray crystallography

Protein purification

Protein crystallization

Crystal mounting

Data collection

distribution of electrons in the molecule,

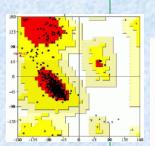
i.e. an electron density map.

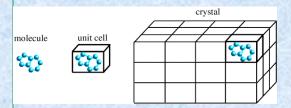
Data processing

Structure solution

Structure refinement

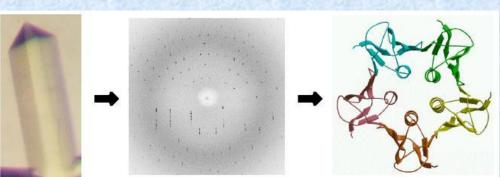
Structure analysis





NMR spectroscopy Electron microscopy

It is based on the quantum mechanical properties of atoms, particularly spin, and it determines information about atoms from the fact that their local environment influences how they respond to applied magnetic fields.

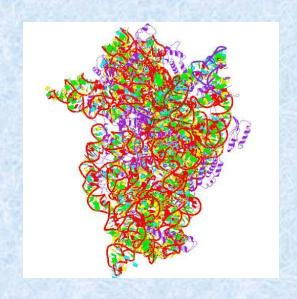


All available structures are stored in Protein Data Bank (PDB).

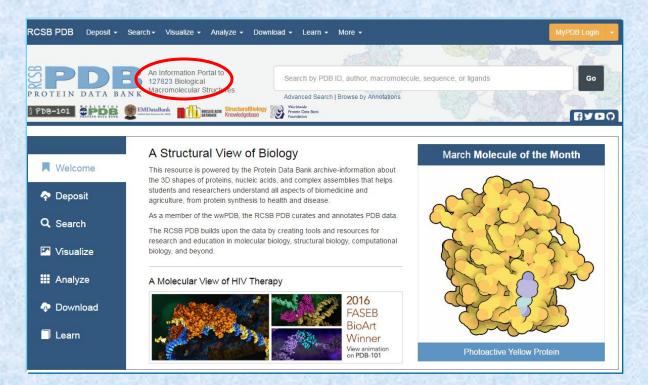
Myoglobin, Kendrew (1958)

PDB (USA), PDB (Europe) and PDB (Japan)

World wide Protein Data Bank: Organizations that act as deposition, data processing and distribution centers for PDB data.

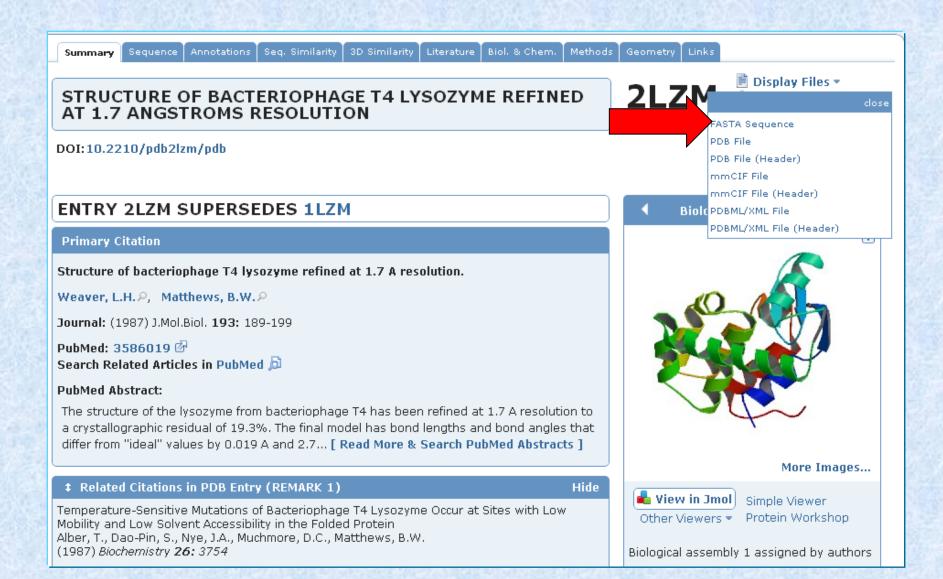


2009 Nobel Prize for Chemistry has been awarded to Venki Ramakrishnan (UK), Tom Steitz (USA) and Ada Yonath (Israel). These three crystallographers have contributed enormously to our understanding of how the protein production machinery works at the atomic level by determining the detailed three-dimensional structure of so-called <u>ribosomes</u>.



CODE 2LZMA

| Exp.Method | Proteins | Nucleic Acids | Protein/NA Complexes | Other | Total |
|---------------------|----------|---------------|----------------------|-------|--------|
| X-RAY | 107061 | 1820 | 5471 | 4 | 114356 |
| NMR | 10300 | 1190 | 241 | 8 | 11739 |
| ELECTRON MICROSCOPY | 1022 | 30 | 367 | 0 | 1419 |
| HYBRID | 99 | 3 | 2 | 1 | 105 |
| other | 181 | 4 | 6 | 13 | 204 |
| Total | 118663 | 3047 | 6087 | 26 | 127823 |



>2LZM: A| PDBID| CHAIN| SEQUENCE

MNIFEMLRIDEGLRLKIYKDTEGYYTIGIGHLLTKSPSLNAAKSELDKAIGRNCNGVITKDEAEKLFNQDVDAAVRGILR NAKLKPVYDSLDAVRRCALINMVFQMGETGVAGFTNSLRMLQQKRWDEAAVNLAKSRWYNQTPNRAKRVITTFRTGTWDA YKNL

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REMARK
                                                     REMARK
                                                               2 RESOLUTION.
                                                                                  1.70 ANGSTROMS.
HEADER
         HYDROLASE (O-GLYCOSYL)
                                                     REMARK
         STRUCTURE OF BACTERIOPHAGE T4 LYSOZYME REFI
TITLE
                                                     REMARK
                                                               3 REFINEMENT.
TITLE
        2 RESOLUTION
                                                     REMARK
                                                               3
                                                                    PROGRAM
                                                                                  : TNT
COMPND
         MOL ID: 1;
                                                     REMARK
                                                               3
                                                                    AUTHORS
                                                                                   TRONRUD, TEN EYCK, MATTHEWS
        2 MOLECULE: T4 LYSOZYME;
COMPND
                                                     DEMADE
COMPND
        3 CHAIN: A:
COMPND
        4 EC: 3.2.1.17;
COMPND
        5 ENGINEERED: YES
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                                                        1 A
                                                             164
SOURCE
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                                                              164
                                                                    ARG LEU LYS ILE TYR LYS ASP THR GLU GLY TYR TYR THR
SOURCE
        2 ORGANISM SCIENTIFIC: ENTEROBACTERIA
                                              SEORES
                                                                    ILE GLY ILE GLY HIS LEU LEU THR LYS SER PRO SER LEU
        3 ORGANISM TAXID: 10665;
SOURCE
                                              SEQRES
                                                        4 A
                                                              164
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SOURCE
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                                                              164
                                                                    ASN CYS ASN GLY VAL ILE THR LYS ASP GLU ALA GLU LYS
KEYWDS
         HYDROLASE (O-GLYCOSYL)
                                              SEORES
                                                                            ASN GLN ASP VAL ASP ALA ALA VAL ARG GLY ILE
EXPDTA
         X-RAY DIFFRACTION
                                              SEQRES
                                                                    LEU ARG ASN ALA LYS LEU LYS PRO VAL TYR ASP SER LEU
AUTHOR
         L.H. WEAVER, B.W. MATTHEWS
                                                              164
REVDAT
            13-JUL-11 2LZM
                                      VERSN
                                              SEORES
                                                              164
                                                                    ASP ALA VAL ARG ARG CYS ALA LEU ILE ASN MET VAL PHE
REVDAT
            24-FEB-09 2LZM
                              1
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                                                                        MET GLY GLU THR GLY VAL ALA GLY PHE THR ASN SER
REVDAT
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            01-APR-03 2LZM
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                                      JRNL
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                                                       10 A
                                                              164
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REVDAT
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                                      REMARK
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                                                              164
                                                                   VAL ASN LEU ALA LYS SER ARG TRP TYR ASN GLN THR PRO
REVDAT
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REVDAT
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                                                                    THR TRP ASP ALA TYR LYS ASN LEU
                                              SEQRES
                                                       13 A
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REVDAT
            24-OCT-86 2LZM
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SPRSDE
          24-OCT-86 2LZM
                                              FORMUL
                                                           HOH
                                                                   *118 (H2 O)
                              1LZM
JRNL
           AUTH
                  L.H.WEAVER, B.W.MATTHEWS
                                                                                                                                   9
                                              HELIX
                                                           H1 ILE A
                                                                             GLU A
                                                                                      11
JRNL
                  STRUCTURE OF BACTERIOPHAGE
                                              HELIX
                                                           H2 LEU A
                                                                             ILE A
                                                                                      50
                                                                                          1
                                                                                                                                  12
JRNL
           TITL 2 RESOLUTION.
                                              HELIX
                                                           H3 LYS A
                                                                             ARG A
                                                                                      80
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                                                                                                                                  21
JRNL
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                                                           H4 ALA A
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                                              HELIX
                                                                             SER A
                                                                                      90
JRNL.
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                                              HELIX
                                                           H5 ALA A
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                                                                             MET A
                                                                                     106
                                                                                                                                  14
JRNL
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                  10.1016/0022-2836(87)90636-X HELIX
                                                           H6 GLU A
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JRNL
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REMARK
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                                              HELIX
                                                           H7 THR A
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                                                                             GLN A
                                                                                                                                   9
REMARK
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                                                                                                                                   9
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                                                            H8 TRP A
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                                                                                     134
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REMARK
        1 AUTH
                  T.ALBER, S.DAO-PIN, J.A.NYE, D
                                                                                                                                   5
                                              HELIX
                                                           Н9
                                                               ARG A
                                                                       137
                                                                             GLN A
                                                                                     141
REMARK
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                                              HELIX
                                                       10 H10
                                                               PRO A
                                                                             THR A
                                                                                                                                  13
           TITL 2 OCCUR AT SITES WITH LOW MOB
REMARK
                                              SHEET
                                                           S1 4 GLY A
                                                                         56
                                                                              ILE A
                                                                                      58
REMARK
           TITL
                3 ACCESSIBILITY IN THE FOLDED
                                              SHEET
                                                           S1 4 ARG A
                                                                         14
                                                                              ASP A
                                                                                      20
                                                                                              0
                                                                                                                  ILE A
                                                                                         -1
                                                                                                 LEU A
                                                                                                         15
REMARK
        1
           REF
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                                                                              ILE A
                                  ISSN 0006-29 SHEET
                                                            S1 4 TYR A
                                                                         24
                                                                                      27 - 1
                                                                                              0
                                                                                                 TYR A
                                                                                                               Ν
                                                                                                                  ASP A
REMARK
           REFN
                                              SHEET
                                                           S1 4 HIS A
                                                                         31
                                                                              THR A
                                                                                     34 -1
                                                                                            N
                                                                                                 HIS A
                                                                                                                  ILE A
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1TOM 32308 P

Sample entry in PDB

X Y Z

| | | ATOM | 32308 P | A A1531 | -35.808 111.810 71.195 1.00149 | 9.38 P |
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| | | ATOM | 32309 OP | 1 A A1531 | -36.543 110.930 70.262 1.00 80 | 0.60 |
| | | ATOM | 32310 OP | 2 A A1531 | -34.421 112.237 70.863 1.00 79 | 9.54 0 |
| | | ATOM | 32311 05 | | -36.706 113.117 71.371 1.0013 | |
| | | | | | -36.782 114.102 70.307 1.00140 | |
| VIDEO DE LA COMPANION DE LA CO | | ATOM | 32313 C4 | | -37.439 115.378 70.797 1.00142 | |
| HETATM 1311 O HOH A 166 39.473 -8.320 | 18.352 1.00 12.66 0 | ОМ | 32314 04 | | -36.965 115.684 72.133 1.00142 | |
| METATM 1312 O HOH A 167 40.661 -1.625 | 3.146 1.00 26.18 O | OM | 32315 C3 | | -37.122 116.620 69.973 1.00143 | |
| HETATM 1313 O HOH A 168 45.808 -7.180 | 1.965 1.00 6.69 0 | OM | 32316 03 | | -37.665 116.753 68.649 1.0014 | |
| HETATM 1314 O HOH A 169 48.014 -0.84 | 0.963 1.00 20.51 0 | MC MC | 32317 C2 32318 O2 | | -37.276 117.753 70.980 1.00143 -38.623 118.161 71.132 1.00142 | |
| | | OM | 32310 C2 | | -36.782 117.083 72.272 1.00142 | |
| HETATM 1315 O HOH A 170 37.070 -18.992 | | OM | 32320 N9 | | -35.360 117.309 72.554 1.00 9 | |
| HETATM 1316 O HOH A 171 47.674 0.600 | 28.073 1.00 24.92 0 | OM | 32321 C8 | | -34.295 116.513 72.186 1.00 9 | |
| HETATM 1317 O HOH A 172 24.914 -23.325 | 4.060 1.00 27.79 0 | OM | 32322 N7 | | -33.129 116.984 72.551 1.00 9 | |
| HETATM 1318 O HOH A 173 37.436 1.541 | -8.076 1.00 25.60 O | ом | 32323 C5 | A A1531 | -33.440 118.165 73.210 1.00 9 | 7.00 C |
| HETATM 1319 O HOH A 175 21.473 0.044 | | OM | 32324 C6 | A A1531 | -32.639 119.138 73.829 1.00 9 | 7.05 C |
| | | OM | 32325 N6 | A A1531 | -31.306 119.075 73.874 1.00 9 | 7.96 N |
| HETATM 1320 O HOH A 176 41.618 -8.847 | | OM | 32326 N1 | | -33.260 120.195 74.404 1.00 9 | |
| ■ HETATM 1321 O HOH A 177 55.648 -1.163 | 27.564 1.00 50.85 O | ом | 32327 C2 | | -34.600 120.258 74.349 1.00 98 | |
| HETATM 1322 O HOH A 178 44.310 -13.062 | -1.772 1.00 28.63 0 | OM | 32328 N3 | | -35.463 119.409 73.792 1.00 9 | |
| HETATM 1323 O HOH A 179 21.105 -20.149 | 4.804 1.00 22.47 0 | ом | 32329 C4 32330 | | -34.812 118.372 73.231 1.00 9 | 5.66 C |
| HETATM 1324 O HOH A 180 35.498 -5.517 | | М | | A A1531 VAL B 7 | -19.397 100.525 10.485 1.00200 | 0.65 N |
| | | OM | 32332 CA | | -20.293 99.359 10.728 1.00200 | |
| HETATM 1325 O HOH A 181 35.182 -7.197 | | OM | 32333 C | VAL B 7 | -20.301 98.977 12.206 1.00200 | |
| HETATM 1326 O HOH A 182 47.378 -15.737 | 28.584 1.00 43.98 0 | ом | 32334 0 | | -21.119 99.472 12.983 1.00200 | |
| HETATM 1327 O HOH A 184 29.866 -10.719 | 23.430 1.00 39.76 0 | ом | 32335 CB | VAL B 7 | -19.848 98.133 9.890 1.00200 | 0.65 C |
| HETATM 1328 O HOH A 185 38.214 -15.827 | 20.622 1.00 33.83 0 | OM | 32336 CG | | -20.768 96.948 10.160 1.00200 | 0.65 C |
| HETATM 1329 O HOH A 186 40.794 -19.490 | 20.666 1.00 29.74 0 | OM | 32337 CG | | -19.859 98.485 8.409 1.00200 | |
| | | ОМ | 32338 N | | -19.385 98.097 12.593 1.00150 | |
| HETATM 1330 O HOH A 187 45.407 0.094 | | OM | 32339 CA | | -19.304 97.656 13.974 1.00150 | |
| HETATM 1331 O HOH A 188 53.213 -9.478 | 19.700 1.00 37.14 0 | OM OM | 32340 C 32341 O | LYSB8 LYSB8 | -18.666 98.735 14.847 1.00150 -19.366 99.574 15.413 1.00150 | |
| HETATM 1332 O HOH A 190 45.016 5.850 | 15.793 1.00 29.76 0 | | 32341 CB | | -18.499 96.360 14.059 1.00 9° | |
| HETATM 1333 O HOH A 191 46.234 7.935 | 13.619 1.00 47.62 0 | OM | 32343 CG | | -18.979 95.269 13.102 1.00 9 | |
| HETATM 1334 O HOH A 192 50.975 0.435 | 9.753 1.00 42.44 0 | ом | 32344 CD | | -20.427 94.863 13.355 1.00 9 | |
| | -3.124 1.00 21.98 O | OM | 32345 CE | LYS B 8 | -20.836 93.721 12.432 1.00 9 | 7.02 C |
| neikim 1335 O non k 194 50.670 -10.434 | -3.124 1.00 21.90 | OM | 32346 NZ | LYS B 8 | -22.236 93.250 12.662 1.00 9 | 7.02 N |
| | | ATOM | 32347 N | | -17.339 98.717 14.942 1.00169 | |
| | | | | | -16.600 99.684 15.754 1.00169 | |
| | | ATOM | 32349 C | GLU B 9 | -16.730 101.138 15.292 1.00169 | |
| | | | | | -16.709 102.060 16.113 1.00169 | |
| | | ATOM | 32351 CB | GLU B 9 | -15.118 99.288 15.808 1.0019 | 7.29 C |
| | | | | | | |

Occupancy

Macromolecular crystals are composed of many individual molecules packed into a symmetrical arrangement.

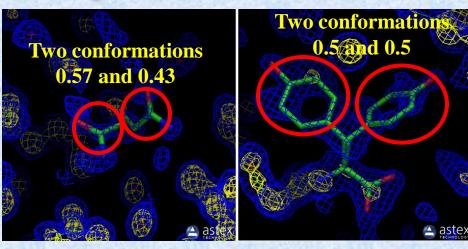
A sidechain on the surface may wag back and forth between several conformations, or a substrate may bind in two orientations in an active site, or a metal ion may be bound to only a few of the molecules.

When building the atomic model of these portions, the occupancy can be used to estimate the amount of each conformation that is observed in the crystal.

For most atoms, the occupancy is given a value of 1, indicating that the atom is found in all of the molecules in the same place in the crystal.

However, if a metal ion binds to only half of the molecules in the crystal, the researcher will see a weak image of the ion in the electron density map, and can assign an occupancy of 0.5 in the PDB structure file for this atom.

The occupancy value is used to indicate the fraction of molecules that have each of the conformations. Two (or more) atom records are included for each atom, with occupancies like 0.5 and 0.5, or 0.4 and 0.6, or other fractional occupancies that sum to a total of 1.



Gln8 (0.57 and 0.43) and Tyr151 in 1A6M

| _ | | • | , | | |
|---|----------------|----------|-----------|-----|---|
| | ATOM | 63 | N GLN A | 8 | 5,404 13,203 22,532 1,00 8,42 N |
| | ANISOU | 63 | N GLN A | 8 | 991 1372 837 -55 _ 112 -21 N |
| | ATOM | 64 | CA GLN A | . 8 | 6.475 12.812 23.418 100 8.84 C |
| | ANISOU | 64 | CA GLN A | 8 | 1086 1404 868 36 13 60 C |
| | ATOM | 65 | C GLN A | . 8 | 7.602 12.149 22.631 .00 8.08 C |
| | ANISOU | 65 | C GLN A | 8 | 1159 1168 744 -7 |
| | ATOM | 66 | O GLN A | | 8.769 12.399 22.918 1.00 .39 0 |
| | ANISOU | 66 | O GLN A | | 1114 1262 812 🐉 7 -3 0 |
| | ATOM | 67 | CB AGLN A | | 5.987 11.822 24.520 0.57 1 03 C |
| | ANISOU | 67 | CB AGLN A | | 1886 2182 884 - 4 38. 376 C |
| | ATOM | 68 | CB BGLN A | | 5.948 11.968 24.580 0.43 9 68 C |
| | ANISOU | 68 | CB BGLN A | | 765 1824 1090 1 5 188 255 C |
| | ATOM | 69 69 | CG AGLN A | | 7.030 11.303 25.500 0.57 16 30 C |
| | ANISOU ATOM | 70 | CG AGLN A | | 2914 1636 1644 87 -429 642 C 6.967 12.094 25.68 0.43 12 07 C |
| | ANISOU | 70 | CG BGLN A | | 1548 1875 1164 - 03 -193 395 C |
| | ATOM | 71 | CD AGLN A | | 7,981 10,227 25,06 0,57 15 61 C |
| | ANISOU | 71 | CD AGLN A | | 2461 1432 2038 - 28 -802 629 C |
| | ATOM | 72 | CD BGLN A | | 6.439 11.470 26.95 0.43 14 43 C |
| | ANISOU | 72 | CD BGLN A | | 2356 2084 1045 - 00 -11 87 C |
| | ATOM | 73 | OE1AGLN A | | 7.688 9.392 24.21 0.57 19 54 0 |
| | ANISOU | 73 | OE1AGLN A | | 3567 1731 2125 -186 -831 300 0 |
| | ATOM | 74 | OE1BGLN A | | 5.419 10.767 26.918 0.43 17 46 0 |
| | ANISOU | 74 | OE1BGLN A | 8 | 2786 2908 939 -12 3 -341 822 0 |
| | ATOM | 75 | NE2AGLN A | 8 | 9.219 10.114 25.607 0.57 21 38 N |
| | ANISOU | 75 | NE2AGLN A | 8 | 2518 2791 2813 -5 8 -105 1739 N |
| | ATOM | 76 | NE2BGLN A | . 8 | 7.067 11.762 28.084 0.43 1 03 N |
| | ANISOU | 76 | NE2BGLN A | 8 | 2245 1968 1117 -5 -7 225 N |
| | ATOM | 77 | N LEU A | | 7.271 11.269 21.697 1.00 .05 N |
| | ANISOU | 77 | N LEU A | | 1062 1121 877 - 81 N |
| | ATOM | 78 | CA LEU A | | 8.296 10.604 20.915 .00 8.31 C |
| | ANISOU | 78 | CA LEU A | | 1085 1164 907 41 84 206 C |
| | ATOM | 79 | C LEU A | | 9.080 11.630 20.080 1 7.19 C |
| | ANISOU | 79 | C LEU A | | 1008 1038 685 70 41 2 C |
| | ATOM | 80 80 | O LEU A | | 10.311 11.526 19.962 1.00 7.98 0 1019 1097 915 232 143 83 0 |
| | ANISOU ATOM | 81 | CB LEU A | | 7.677 9.576 19.969 1.00 9.04 C |
| | ANISOU | 81 | CB LEU A | | 1440 983 1012 -45 222 79 C |
| | ATOM | 82 | CG LEU A | | 7,090 8,338 20,698 1,00 10,56 C |
| | ANISOU | 82 | CG LEU A | | 1658 982 1370 -49 291 80 C |
| | ATOM | 83 | CD1 LEU A | | 6,290 7,498 19,721 1,00 12,91 C |
| | ANISOU | 83 | CD1 LEU A | | 2111 1030 1763 -292 327 -155 C |
| | ATOM | 84 | CD2 LEU A | | 8.189 7.510 21.315 1.00 16.75 C |
| | ANISOU | 84 | CD2 LEU A | | 2279 1349 2735 -8 -215 792 C |
| | ATOM | 85 | N VAL A | | 8.391 12.589 19.483 1.00 6.70 N |
| | ANISOU | 85 | N VAL A | 10 | 931 934 681 29 49 12 N |
| | ATOM | 86 | CA VAL A | 10 | 9.019 13.628 18.670 1.00 6.25 C |
| | ANISOU | 86 | CA VAL A | 10 | 822 859 692 15 113 1 C |

Temperature factor

If we were able to hold an atom rigidly fixed in one place, we could observe its distribution of electrons in an ideal situation.

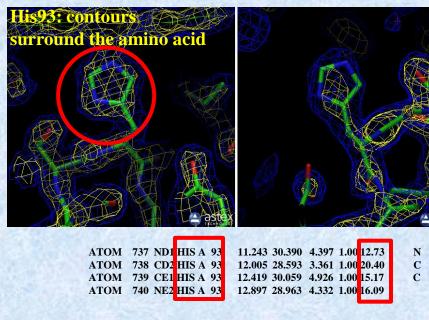
The image would be dense towards the center with the density falling off further from the nucleus.

The electrons usually have a wider distribution than this ideal. This may be due to vibration of the atoms, or differences between the many different molecules in the crystal lattice. The observed electron density will include an average of all these small motions, yielding a slightly smeared image of the molecule.

These motions, and the resultant smearing of the electron density, are incorporated into the atomic model by a B-value or temperature factor.

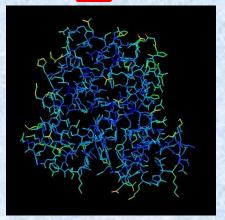
Values under 10 create a model of the atom that is very sharp, indicating that the atom is not moving much and is in the same position in all of the molecules in the crystal.

Values greater than 50 or so indicate that the atom is moving so much that it can barely been seen. This is often the case for atoms at the surface of proteins, where long sidechains are free to wag in the surrounding water.



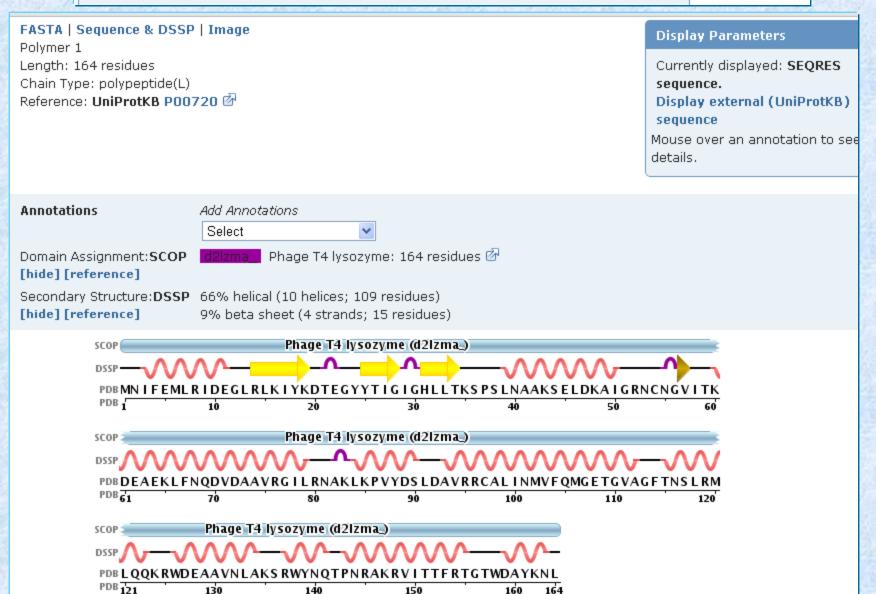
ATOM 642 ND1 HIS A 81 -2.541 24.541 20.570 1.00 72.63 ATOM 643 CD2 HIS A 81 -0.874 23.158 20.970 1.00 54.37 ATOM 644 CE1 HIS A 81 -3.006 23.416 21.159 1.00 53.46 ATOM 645 NE2 HIS A 81 -2.022 22.561 21.396 1.00 73.87

High values, indicating lots of motion, are in red and yellow, and low values are in blue.



N

2LZM



2LZM

| 🕠 Domain A | nnotation: SCOP C | assification (version | n 1.75) 🚰 | | | Hide | |
|---|---------------------------------|--|---------------------|---|---------------------|--------------------------------------|--|
| Domain Info | n Info Class Fold | | Superfamily | Family | Domain | Species | |
| d2lzma_ | Alpha and beta proteins (a+b) 🔎 | Lysozyme-like 🔎 | Lysozyme-like 🔎 | Phage lysozyme 🔎 | Phage T4 lysozyme 🔎 | Bacteriophage T4 [TaxId: 10665] 🔎 | |
| Domain A | nnotation: CATH Cl | assification (version | 3.4.0) 🗗 | | | Hide | |
| Domain | Class | | Architecture | Topology | Homolo | ogy | |
| 2lzmA00 | Mainly | / Alpha | Orthogonal Bundle 🔎 | Lysozyme 🔎 | ۵ | | |
| Protein Fa | amily Annotation: P | FAM Classification [| ₹ | | | Hide | |
| Chain PFAM A | Accession | PFAM ID | Description | Туре | Clan ID | , | |
| A PF0095 | 9 🚱 | Phage_lysozyme | Phage lysozyme | Domair | n | | |
| Gene Pro | duct Annotation: G(|) Terms 🚰 | | | | Hide | |
| Polymer | | Molecular Function | Biolog | gical Process | Cellular Compo | nent | |
| T4 LYSOZYME (2LZM:A) • lysozyme activity • catalytic activity • hydrolase activity • hydrolase activity, acting on glycosyl bonds • lysozyme activity • catalytic activity • hydrolase activity, acting on glycosyl bonds • lysozyme activity • hydrolase activity • hydrolase activity, acting on glycosyl bonds • lysozyme activity • hydrolase • | | | | etabolic process P eptidoglycan catabolic pro ell wall macromolecule cat rocess P rtolysis P efense response to bacter | abolic | | |
| Structura | l Biology Knowledg | ebase Data | | | | Hide | |
| Information fr | om the Structural B | iology Knowledgeba | se ਔ | | | | |
| Related BioRelated Clo | | > 21 annotations 🔗 y Materials Repositor | | | | | |

2LZM

| Rank 🕕 | PDB id | Entity id | Chains | Descriptio | n Details | Taxonomy | EC Number | | | | |
|----------------------------|---------------|---------------|--|-----------------|-------------------------------------|----------|---------------|--|--|--|--|
| Select for d | ownload / vie | w details OR: | Select two chair | ns for comparis | son | | | | | | |
| □ <u></u> Download Details | | | | | Select Comparison Method V Submit ① | | | | | | |
| 1 | 3FA0 | 1 | А | Lysozyme | | 10665 🗗 | 3.2.1.17 🔎 | | | | |
| 2 | 3LZM | 1 | А | T4 LYSOZY | ME | 10665 🗗 | 3.2.1.17 🔎 | | | | |
| 3 | 4LZM | 1 | Α | T4 LYSOZY | ME | 10665 🗗 | 3.2.1.17 👂 | | | | |
| <u> </u> | 7LZM | 1 | Α | T4 LYSOZY | ME | 10665 🗗 | 3.2.1.17 🔎 | | | | |
| 5 | 5LZM | 1 | А | T4 LYSOZY | ME | 10665 🗗 | 3.2.1.17 🔎 | | | | |
| <u> </u> 6 | 6LZM | 1 | Α | T4 LYSOZY | ME | 10665 🗗 | 3.2.1.17 2 | | | | |
| 7 | 2LZM | 1 | Α | T4 LYSOZY | ME | 10665 🗗 | 3.2.1.17 👂 | | | | |
| 8 | 1T6H | 1 | Α | Lysozyme | | 10665 🗗 | 3.2.1.17 👂 | | | | |
| 9 | 1LYD | 1 | А | T4 LYSOZY | ME | 10665 🗗 | | | | | |
| | | | ntities in PDB 2L otein, length: 16 | | | | | | | | |
| Cluster Seq | uence Similar | ity Cutoff | | Rank 🕕 | Nr. of chains in Clus | ter | Cluster Nr. 🕕 | | | | |
| LOO% | | | | 7 | 9 | | 3648 | | | | |
| 95% | | | | 199 | 522 | | 2 | | | | |
| 90% | | | | 200 | 530 | | 2 | | | | |
| 70% | | | | 200 | 530 | | 6 | | | | |
| 50% | | | | 200 | 530 | | 8 | | | | |
| 10% | | | | 200 | 530 | | 9 | | | | |
| 30% | | | | 200 | 530 | | 14 | | | | |



iii Display Files ▼ iii Download Files ▼ iii Share this Page ▼

Structural Similarities for the Entities in PDB 2LZM

The following structural similarities have been found using the jFATCAT-rigid algorithm. In order to reduce the number of hits, a 40% sequence identity clustering has been applied and a representative chain is taken from each cluster.

Entity #1: Chains: A

Description: T4 LYSOZYME protein

Length: 164

No structure alignment results are available for 2LZM.A explicitly.

It is represented by chain ${f 1SX7.A}$ which has more than 95% sequence similarity.

Click here to hide the structure comparison results for representative 1SX7.A

Results options

Hide

Currently viewing only significant results (P-value < 0.001).

Show all available results

Update Status

Hide

The data on this page are up to date as of:

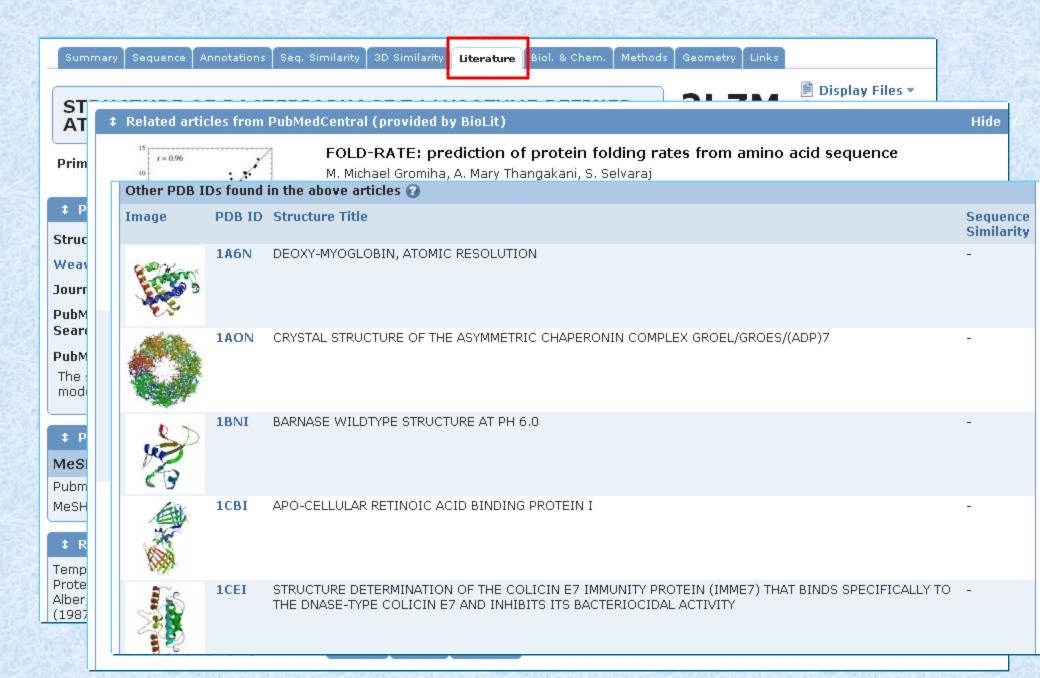


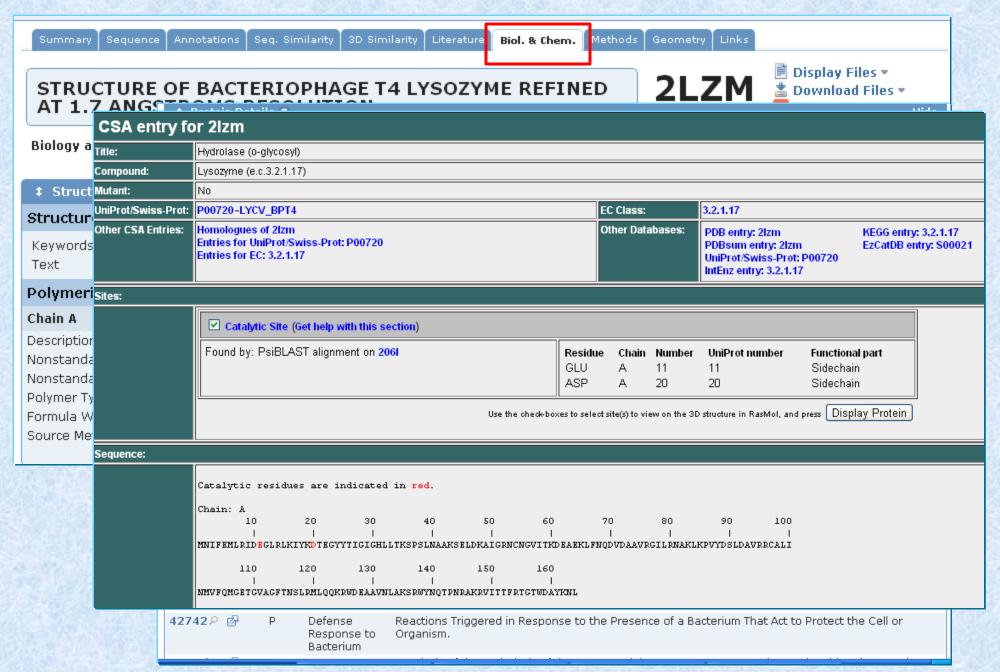
| 1SX7.A (chain 1) vs. representatives of other sequence clusters (chain 2) | | | | | | | | | | | | |
|---|---------|---------|--------------------------|----------|--------|------|------|------|-----|-------|-------|--|
| Rank | Results | Chain 2 | Title | P-value | Score | Rmsd | Len1 | Len2 | %ID | %Cov1 | %Cov2 | |
| 1 | view | 2QB0.B | TELSAM domain - Lysozym | 0.0 | 477.58 | 1.29 | 164 | 241 | 96 | 98 | 67 | |
| 2 | view | 207A.A | Lysozyme | 0.0 | 301.62 | 0.47 | 164 | 116 | 97 | 59 | 83 | |
| 3 | view | 3SN6.R | Lysozyme, Beta-2 adrene | 1.14E-10 | 457.36 | 1.62 | 443 | 164 | 97 | 36 | 97 | |
| 4 | view | 1WTH.A | Tail-associated lysozyme | 5.0E-10 | 442,54 | 1.16 | 164 | 571 | 43 | 99 | 28 | |
| 5 | view | 2RH1.A | beta-2-adrenergic recept | 1.55E-9 | 471.90 | 2.22 | 164 | 443 | 96 | 100 | 37 | |
| 6 | view | 3HDE.A | Lysozyme | 2.48E-8 | 270.98 | 2.99 | 164 | 165 | 17 | 83 | 82 | |

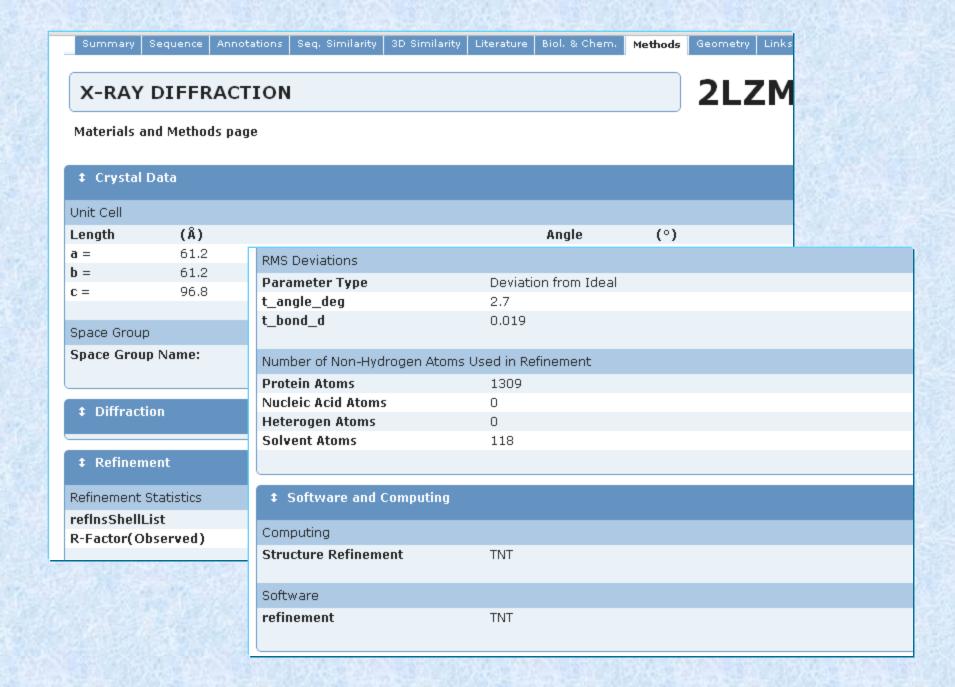
Table Legend

Hide

- Rank: current row position.
 Changes with different sorting orders and filter rules
- · Chain 2: PDB chain name
- · Title: Protein chain description
- P-value: P-value of this alignment (FATCAT) (default sorted by this)
- Score: Raw alignment score (FATCAT)
- · RMSD: RMSD value of the







| Bond Length | | | | | | | | |
|--------------|----------|---------|---------|------------|---------|------------|---------|---------|
| Bond Type | Chain Id | Tot Num | Cal Ave | Cal StdDev | Std Val | Std StdDev | Minimum | Maximum |
| C-N | Α | 160 | 1.33 | 0.020 | 1.329 | 0.014 | 1.27 | 1.38 |
| C-N(P) | Α | 3 | 1.33 | 0.014 | 1.341 | 0.016 | 1.31 | 1.34 |
| C-O | Α | 164 | 1.23 | 0.017 | 1.231 | 0.02 | 1.19 | 1.27 |
| CA-C | Α | 153 | 1.53 | 0.020 | 1.525 | 0.021 | 1.47 | 1.58 |
| CA-C(G) | Α | 11 | 1.53 | 0.014 | 1.516 | 0.018 | 1.51 | 1.56 |
| CA-CB | Α | 108 | 1.53 | 0.025 | 1.53 | 0.02 | 1.43 | 1.61 |
| CA-CB(A) | Α | 15 | 1.53 | 0.010 | 1.521 | 0.033 | 1.51 | 1.55 |
| CA-CB(I,T,V) | Α | 30 | 1.55 | 0.021 | 1.54 | 0.027 | 1.51 | 1.61 |
| N-CA | Α | 150 | 1.45 | 0.018 | 1.458 | 0.019 | 1.40 | 1.50 |

| Dihedral Angle | | | | | | | | |
|--|----------|---------|---------|------------|---------|------------|---------|---------|
| Dihedral Angle | Chain Id | Tot Num | Cal Ave | Cal StdDev | Std Val | Std StdDev | Minimum | Maximum |
| Chi1 g(+) | А | 78 | -71.67 | 18.724 | -66.7 | 15.0 | -115.50 | -3.60 |
| Chi1 g(-) | Α | 18 | 60.64 | 29.323 | 64.1 | 15.7 | 0.70 | 116.10 |
| Chi1 trans | Α | 42 | 184.84 | 16.233 | 183.6 | 16.8 | 144.40 | 237.90 |
| Omega | Α | 163 | 179.68 | 3.595 | 180 | 5.8 | 169.30 | 189.80 |
| Phi | Α | 53 | -71.51 | 72.347 | -65.3 | 11.9 | -157.70 | 88.50 |
| Phi helix | Α | 109 | -63.55 | 17.101 | -65.3 | 11.9 | -106.90 | 77.20 |
| Phi(P) | Α | 1 | -69.50 | 0.000 | -65.4 | 11.2 | -69.50 | -69.50 |
| Psi | Α | 46 | 94.20 | 72.308 | -39.4 | 11.3 | -48.60 | 175.00 |
| Psi helix | Α | 109 | -38.07 | 21.279 | -39.4 | 11.3 | -61.30 | 157.70 |
| Psi(G) | А | 8 | -26.81 | 76.181 | -39.4 | 11.3 | -177.40 | 31.70 |
| Save Dihedral Angle Summary CSV (Excel) Format in: | | | | | | | | |

STRUCTURE OF BACTERIOF AT 1.7 ANGSTROMS RESOL

External Links

STRUCTURE SUMMARY

- Protein Databank in Europe (PDBe)
- Protein Data Bank Japan (wwPDB Partn
- PSI Structural Biology Knowledgebase (
- Protein Interfaces, Surfaces and Assemb
- Molecular Modeling DataBase (NCBI/Ent
- PDBsum
- Jena Library
- PDBWiki
- Proteopedia
- OCA Browser (OCA)

STRUCTURE FEATURES

- Homology derived Secondary Structure (
- Analysis of Ligand-Protein Contacts (LPC)
- . Analysis of interatomic Contacts of Struc
- Computed Atlas of Surface Topography o
- Guassian Network Model (GNM)
- HIV Sequence/Structure Function Analyzer

LIGAND FEATURES

- BindinaDB: No external link available
- Ligand-Expo
- Chem-BLAST
- PubChem
- DrugBank

STRUCTURE CLASSIFICATION AND COMPARISON

- Structural Classification of Proteins (SCOP)
- Protein Structure Classification (CATH)
- Vector Alignment Search Tool (VAST)
- Flexible structure AlignmenT by Chaining Aligned fragment pairs allowing Twists (FATCAT)
- DALI
- SUPERFAMILY

SECONDARY STRUCTURE

Secondary Structure Assignments (DSSP)

EXPERIMENTAL DATA

NO EXTERNAL LINK IN EXPERIMENTAL DATA

BIOLOGICAL DETAILS

- CSA
- IEDB: No external link available

PATHWAYS

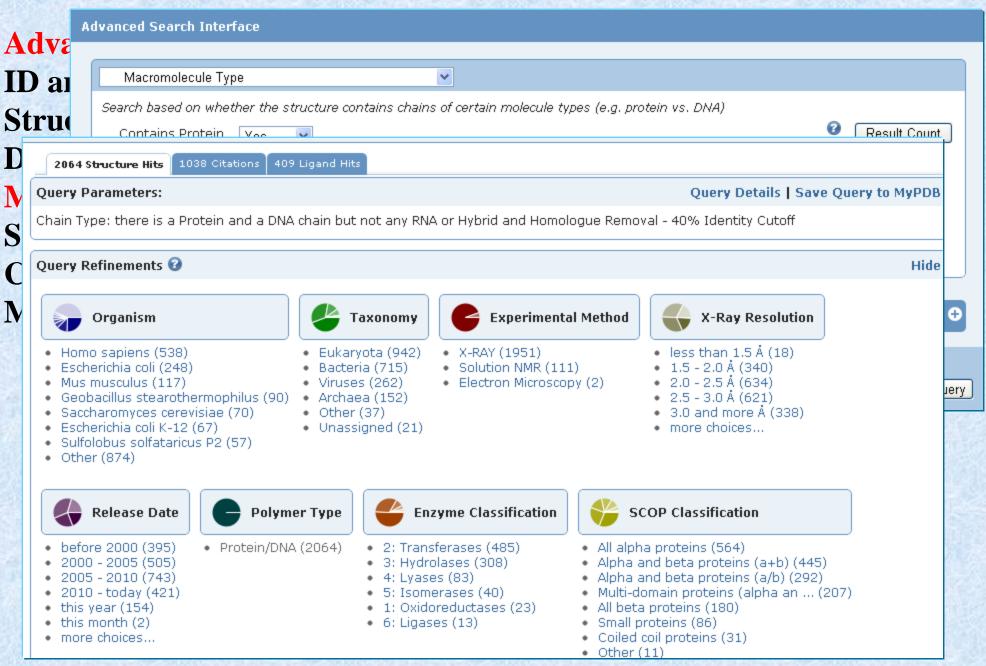
METACYC: No external link available

PROTEIN MOTIONS

Molecular Movements Database (MMD)

STEREOCHEMICAL QUALITY

- WHAT_CHECK (WHAT IF)



Protein visualization

Pymol

Rasmol

Jmol

KING

Webmol

SWISS-PDB viewer