```
REM  ------------------------------------------------------------------  2PHY
REM                                                                      2PHY
REM  STRIDE: Knowledge-based secondary structure assignment              2PHY
REM  Please cite: D.Frishman & P.Argos, Proteins XX, XXX-XXX, 1995       2PHY
REM                                                                      2PHY
REM  Residue accessible surface area calculation                         2PHY
REM  Please cite: F.Eisenhaber & P.Argos, J.Comp.Chem. 14, 1272-1280, 1993 2PHY
REM               F.Eisenhaber et al., J.Comp.Chem., 1994, submitted     2PHY
REM                                                                      2PHY
REM  ------------------------ General information ----------------------  2PHY
REM                                                                      2PHY
HDR  PHOTORECEPTOR                            12-APR-95   2PHY           2PHY
CMP  MOL_ID: 1;                                                          2PHY
CMP   MOLECULE: PHOTOACTIVE YELLOW PROTEIN;                              2PHY
CMP   CHAIN: A;                                                          2PHY
CMP   SYNONYM: PYP                                                       2PHY
SRC  MOL_ID: 1;                                                          2PHY
SRC   ORGANISM_SCIENTIFIC: HALORHODOSPIRA HALOPHILA;                     2PHY
SRC   ORGANISM_TAXID: 1053;                                              2PHY
SRC   STRAIN: BN9626                                                     2PHY
AUT  G.E.O.BORGSTAHL,E.D.GETZOFF                                         2PHY
REM                                                                      2PHY
REM  -------------------- Secondary structure summary -------------------  2PHY
REM                                                                      2PHY
CHN  /home/proj/stride/tmp/tmpR5MTpzpdb A                                2PHY
REM                                                                      2PHY
REM                .         .         .         .         .             2PHY
SEQ  1    MEHVAFGSEDIENTLAKMDDGQLDGLAFGAIQLDGDGNILQYNAAEGDIT   50        2PHY
STR           TTTT HHHHHHHH   HHHHH    EEEEEETTTEEEEE HHHHHHH            2PHY
REM                                                                      2PHY
REM                .         .         .         .         .             2PHY
SEQ  51   GRDPKQVIGKNFFKDVAPCTDSPEFYGKFKEGVASGNLNTMFEYTFDYQM  100        2PHY
STR          GGGTTTEEIIIII GGGTTTTTHHHHHHHHHH   EEEEEEEETTTT            2PHY
REM                                                                      2PHY
REM                .         .                                           2PHY
SEQ  101  TPTKVKVHMKKALSGDSYWVFVKRV                          125        2PHY
STR         EEEEEEEEE  TTTEEEEEEEE                                       2PHY
REM                                                                      2PHY
REM                                                                      2PHY
REM                                                                      2PHY
LOC  AlphaHelix   ASP    10 A      ALA     16 A                          2PHY
LOC  AlphaHelix   ASP    20 A      ASP     24 A                          2PHY
LOC  AlphaHelix   ALA    44 A      THR     50 A                          2PHY
LOC  AlphaHelix   TYR    76 A      SER     85 A                          2PHY
LOC  310Helix     PRO    54 A      GLN     56 A                          2PHY
LOC  310Helix     PRO    68 A      THR     70 A                          2PHY
LOC  PiHelix      PHE    62 A      VAL     66 A                          2PHY
LOC  Strand       GLY    29 A      ASP     34 A                          2PHY
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LOC  Strand       ASN    38 A      TYR     42 A                          2PHY
LOC  Strand       LYS    60 A      ASN     61 A                          2PHY
LOC  Strand       ASN    89 A      PHE     96 A                          2PHY
LOC  Strand       THR   103 A      LYS    111 A                          2PHY
LOC  Strand       SER   117 A      ARG    124 A                          2PHY
LOC  TurnII       ALA     5 A      SER      8 A                          2PHY
LOC  TurnI        ASP    34 A      GLY     37 A                          2PHY
LOC  TurnII       VAL    57 A      LYS     60 A                          2PHY
LOC  TurnI        SER    72 A      PHE     75 A                          2PHY
LOC  TurnIV       PRO    73 A      TYR     76 A                          2PHY
LOC  TurnIV       ASP    97 A      MET    100 A                          2PHY
LOC  TurnIV       SER   114 A      SER    117 A                          2PHY
LOC  GammaInv     THR    70 A      SER     72 A                          2PHY
REM                                                                      2PHY
REM  --------------- Detailed secondary structure assignment-------------  2PHY
REM                                                                      2PHY
REM  |---Residue---|    |--Structure--|   |-Phi-|   |-Psi-|  |-Area-|      2PHY
ASG  MET A    1    1    C          Coil    360.00    146.81    190.6      2PHY
ASG  GLU A    2    2    C          Coil    -82.98    126.40     45.0      2PHY
ASG  HIS A    3    3    C          Coil    -90.49     85.97    169.8      2PHY
ASG  VAL A    4    4    C          Coil   -138.24    132.92     16.7      2PHY
ASG  ALA A    5    5    T          Turn    -91.24    137.96     60.6      2PHY
ASG  PHE A    6    6    T          Turn    -55.73    131.36     33.8      2PHY
ASG  GLY A    7    7    T          Turn     84.75      5.75     30.6      2PHY
ASG  SER A    8    8    T          Turn    -59.42    138.95     40.7      2PHY
ASG  GLU A    9    9    C          Coil    -59.57    -31.59    162.3      2PHY
ASG  ASP A   10   10    H    AlphaHelix   -109.87     26.30     94.3      2PHY
ASG  ILE A   11   11    H    AlphaHelix    -54.94    -38.42      0.4      2PHY
ASG  GLU A   12   12    H    AlphaHelix    -62.43    -33.37     37.6      2PHY
ASG  ASN A   13   13    H    AlphaHelix    -71.42    -42.81     91.8      2PHY
ASG  THR A   14   14    H    AlphaHelix    -63.86    -42.99     42.0      2PHY
ASG  LEU A   15   15    H    AlphaHelix    -77.88    -14.85      2.3      2PHY
ASG  ALA A   16   16    H    AlphaHelix    -61.52    -24.49     68.1      2PHY
ASG  LYS A   17   17    C          Coil    -88.83     -5.23    136.6      2PHY
ASG  MET A   18   18    C          Coil    -93.80    124.52     12.1      2PHY
ASG  ASP A   19   19    C          Coil    -76.47    170.85     84.2      2PHY
ASG  ASP A   20   20    H    AlphaHelix    -57.24    -32.22     76.9      2PHY
ASG  GLY A   21   21    H    AlphaHelix    -67.33    -37.22     39.4      2PHY
ASG  GLN A   22   22    H    AlphaHelix    -75.82    -33.38     67.3      2PHY
ASG  LEU A   23   23    H    AlphaHelix    -61.57    -32.44      1.6      2PHY
ASG  ASP A   24   24    H    AlphaHelix    -67.68    -15.73     67.4      2PHY
ASG  GLY A   25   25    C          Coil    -89.78      2.50     27.3      2PHY
ASG  LEU A   26   26    C          Coil    -72.79    151.36      8.4      2PHY
ASG  ALA A   27   27    C          Coil    -79.58     -1.84     65.8      2PHY
ASG  PHE A   28   28    C          Coil   -141.34    165.84      6.7      2PHY
ASG  GLY A   29   29    E        Strand    -71.86    141.94      0.0      2PHY
ASG  ALA A   30   30    E        Strand   -143.22    127.89      0.0      2PHY
ASG  ILE A   31   31    E        Strand   -128.84    132.59      0.2      2PHY
ASG  GLN A   32   32    E        Strand   -110.50    128.64     26.9      2PHY
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ASG  LEU A   33   33    E        Strand   -118.83    152.07      0.0      2PHY
ASG  ASP A   34   34    E        Strand    -89.38   -178.19     38.5      2PHY
ASG  GLY A   35   35    T          Turn    -60.60    -21.22     19.9      2PHY
ASG  ASP A   36   36    T          Turn    -92.97     -1.48    120.7      2PHY
ASG  GLY A   37   37    T          Turn     92.47     10.11      0.0      2PHY
ASG  ASN A   38   38    E        Strand    -79.87    139.92     48.7      2PHY
ASG  ILE A   39   39    E        Strand    -81.21    121.13      1.7      2PHY
ASG  LEU A   40   40    E        Strand   -100.36    -35.39     78.8      2PHY
ASG  GLN A   41   41    E        Strand   -142.44    149.95     33.1      2PHY
ASG  TYR A   42   42    E        Strand   -157.65    112.67     12.5      2PHY
ASG  ASN A   43   43    C          Coil    -85.53    169.75      0.4      2PHY
ASG  ALA A   44   44    H    AlphaHelix    -61.61    -40.64     35.0      2PHY
ASG  ALA A   45   45    H    AlphaHelix    -61.22    -35.09     17.2      2PHY
ASG  GLU A   46   46    H    AlphaHelix    -67.82    -41.96      2.0      2PHY
ASG  GLY A   47   47    H    AlphaHelix    -63.44    -33.23      8.6      2PHY
ASG  ASP A   48   48    H    AlphaHelix    -66.96    -38.26    142.0      2PHY
ASG  ILE A   49   49    H    AlphaHelix    -73.47    -39.47     41.9      2PHY
ASG  THR A   50   50    H    AlphaHelix   -102.85    -17.57     13.2      2PHY
ASG  GLY A   51   51    C          Coil     91.01    -12.64     67.6      2PHY
ASG  ARG A   52   52    C          Coil    -71.90    147.71     45.3      2PHY
ASG  ASP A   53   53    C          Coil    -89.56    119.88     84.6      2PHY
ASG  PRO A   54   54    G      310Helix    -47.42    -52.51     31.7      2PHY
ASG  LYS A   55   55    G      310Helix    -61.81    -27.56    133.8      2PHY
ASG  GLN A   56   56    G      310Helix    -79.86    -23.23    133.9      2PHY
ASG  VAL A   57   57    T          Turn    -94.06    -14.84      9.8      2PHY
ASG  ILE A   58   58    T          Turn    -63.96    129.23     66.4      2PHY
ASG  GLY A   59   59    T          Turn     99.42    -16.02     58.3      2PHY
ASG  LYS A   60   60    E        Strand    -83.39    158.43     92.9      2PHY
ASG  ASN A   61   61    E        Strand    -86.42    123.37     25.4      2PHY
ASG  PHE A   62   62    I       PiHelix    -60.08    -46.31      7.0      2PHY
ASG  PHE A   63   63    I       PiHelix    -78.87    -30.37      2.7      2PHY
ASG  LYS A   64   64    I       PiHelix    -92.89    -43.82    163.7      2PHY
ASG  ASP A   65   65    I       PiHelix    -95.54    -57.28     80.7      2PHY
ASG  VAL A   66   66    I       PiHelix    -79.91    -42.77     16.3      2PHY
ASG  ALA A   67   67    C          Coil   -129.57     66.76     11.5      2PHY
ASG  PRO A   68   68    G      310Helix    -59.50    -25.75     47.0      2PHY
ASG  CYS A   69   69    G      310Helix    -66.34    -17.47     31.2      2PHY
ASG  THR A   70   70    G      310Helix    -91.32     -6.20      0.2      2PHY
ASG  ASP A   71   71    T          Turn    -80.70     85.03     93.9      2PHY
ASG  SER A   72   72    T          Turn   -161.02    165.37     31.6      2PHY
ASG  PRO A   73   73    T          Turn    -62.54    -27.21    111.6      2PHY
ASG  GLU A   74   74    T          Turn    -75.49    -13.94    125.7      2PHY
ASG  PHE A   75   75    T          Turn   -130.59    -74.27      0.0      2PHY
ASG  TYR A   76   76    H    AlphaHelix    -55.56    -39.15     83.8      2PHY
ASG  GLY A   77   77    H    AlphaHelix    -59.77    -38.15     12.5      2PHY
ASG  LYS A   78   78    H    AlphaHelix    -71.78    -38.16     60.8      2PHY
ASG  PHE A   79   79    H    AlphaHelix    -63.34    -49.53      2.4      2PHY
ASG  LYS A   80   80    H    AlphaHelix    -66.27    -30.48    125.4      2PHY
ASG  GLU A   81   81    H    AlphaHelix    -68.32    -41.07    128.8      2PHY
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ASG  GLY A   82   82    H    AlphaHelix    -67.59    -41.24      4.3      2PHY
ASG  VAL A   83   83    H    AlphaHelix    -63.19    -43.51     32.3      2PHY
ASG  ALA A   84   84    H    AlphaHelix    -66.34    -36.01     90.9      2PHY
ASG  SER A   85   85    H    AlphaHelix    -79.83    -21.94     96.0      2PHY
ASG  GLY A   86   86    C          Coil     81.59     14.79     37.4      2PHY
ASG  ASN A   87   87    C          Coil   -151.34    138.01    118.0      2PHY
ASG  LEU A   88   88    C          Coil   -159.21    128.29     12.7      2PHY
ASG  ASN A   89   89    E        Strand   -163.00     94.56     97.6      2PHY
ASG  THR A   90   90    E        Strand   -145.12    147.14     42.9      2PHY
ASG  MET A   91   91    E        Strand   -131.41    134.71     76.4      2PHY
ASG  PHE A   92   92    E        Strand   -159.91    159.51     28.1      2PHY
ASG  GLU A   93   93    E        Strand    -89.54    150.12    123.7      2PHY
ASG  TYR A   94   94    E        Strand   -152.42    160.51     34.3      2PHY
ASG  THR A   95   95    E        Strand   -115.61    121.51     56.9      2PHY
ASG  PHE A   96   96    E        Strand    -91.03    123.74     11.6      2PHY
ASG  ASP A   97   97    T          Turn   -141.79     18.54     86.7      2PHY
ASG  TYR A   98   98    T          Turn    -92.02    116.57     94.7      2PHY
ASG  GLN A   99   99    T          Turn     56.98     33.56    156.0      2PHY
ASG  MET A  100  100    T          Turn   -159.39    165.73     42.7      2PHY
ASG  THR A  101  101    C          Coil    -67.90    131.38    115.3      2PHY
ASG  PRO A  102  102    C          Coil    -52.09    122.51     91.6      2PHY
ASG  THR A  103  103    E        Strand   -124.57    121.80     16.5      2PHY
ASG  LYS A  104  104    E        Strand    -80.16    129.34    131.2      2PHY
ASG  VAL A  105  105    E        Strand   -136.69    162.96      0.0      2PHY
ASG  LYS A  106  106    E        Strand   -106.67    128.82     68.1      2PHY
ASG  VAL A  107  107    E        Strand   -114.79    135.25      0.0      2PHY
ASG  HIS A  108  108    E        Strand   -124.85    116.58      4.0      2PHY
ASG  MET A  109  109    E        Strand   -106.04    129.90      0.0      2PHY
ASG  LYS A  110  110    E        Strand   -147.61    138.72     21.2      2PHY
ASG  LYS A  111  111    E        Strand    -64.70    135.54     57.8      2PHY
ASG  ALA A  112  112    C          Coil    -74.85    167.78      5.6      2PHY
ASG  LEU A  113  113    C          Coil    -67.87    -34.52    100.7      2PHY
ASG  SER A  114  114    T          Turn    -63.01    162.77     76.8      2PHY
ASG  GLY A  115  115    T          Turn    -57.32    -74.29     51.8      2PHY
ASG  ASP A  116  116    T          Turn   -107.86     58.81    114.4      2PHY
ASG  SER A  117  117    E        Strand   -141.28    147.95      4.2      2PHY
ASG  TYR A  118  118    E        Strand   -137.62    144.12      2.4      2PHY
ASG  TRP A  119  119    E        Strand   -101.33    146.83      5.9      2PHY
ASG  VAL A  120  120    E        Strand   -127.19    115.18      0.2      2PHY
ASG  PHE A  121  121    E        Strand   -107.74    143.29      0.2      2PHY
ASG  VAL A  122  122    E        Strand   -140.35    137.11      0.2      2PHY
ASG  LYS A  123  123    E        Strand   -143.37    153.53     84.2      2PHY
ASG  ARG A  124  124    E        Strand    -71.17    148.60    183.9      2PHY
ASG  VAL A  125  125    C          Coil   -130.63    360.00    102.2      2PHY
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