約束事項

ATOM、HETATM、TER、END で始まる行以外は全てコメント行

ATOM または HETATM で始まる行は座標データ

```
HEADER    HYDROLASE                               13-OCT-06   2J7N       PDB ID: 座標データ ID 番号
TITLE     STRUCTURE OF THE RNAI POLYMERASE FROM NEUROSPORA CRASSA
COMPND    MOL_ID: 1;                                                    構造中に含まれる蛋白質の ID 番号
COMPND   2 MOLECULE: RNA-DEPENDENT RNA POLYMERASE;                  構造中に含まれる蛋白質の名前
COMPND   3 CHAIN: A, B;                                          独立な蛋白質分子 ID（ポリペプチド鎖 ID）
COMPND   4 FRAGMENT: RESIDUES 381-1402;
COMPND   5 SYNONYM: HYPOTHETICAL PROTEIN NCU07534.1;
COMPND   6 ENGINEERED: YES
SOURCE    MOL_ID: 1;
SOURCE   2 ORGANISM_SCIENTIFIC: NEUROSPORA CRASSA;
SOURCE   3 EXPRESSION_SYSTEM: SACCHAROMYCES CEREVISIAE;
SOURCE   4 EXPRESSION_SYSTEM_STRAIN: INVSC1;
SOURCE   5 EXPRESSION_SYSTEM_PLASMID: PEM69
KEYWDS    RNA DEPENDENT RNA POLYMERASE, RNAI RESPONSE, HYPOTHETICAL
KEYWDS   2 PROTEIN, RNA-DIRECTED RNA POLYMERASE, HYDROLASE
EXPDTA    X-RAY DIFFRACTION
AUTHOR    P.S.SALGADO,M.R.L.KOIVUNEN,E.V.MAKEYEV,D.H.BAMFORD,
AUTHOR   2 D.I.STUART,J.M.GRIMES
REVDAT   1   13-DEC-06 2J7N    0
JRNL        AUTH   P.S.SALGADO,M.R.KOIVUNEN,E.V.MAKEYEV,D.H.BAMFORD,
JRNL        AUTH 2 D.I.STUART,J.M.GRIMES
JRNL        TITL   THE STRUCTURE OF AN RNAI POLYMERASE LINKS RNA
JRNL        TITL 2 SILENCING AND TRANSCRIPTION.
JRNL        REF    PLOS BIOL.                    V.   4  E434 2006
JRNL        REFN   ASTM PBLIBG  US ISSN 1544-9173
REMARK   1
REMARK   1 REFERENCE 1
REMARK   1  AUTH   E.V.MAKEYEV,D.H.BAMFORD
REMARK   1  TITL   CELLULAR RNA-DEPENDENT RNA POLYMERASE INVOLVED IN
REMARK   1  TITL 2 POSTTRANSCRIPTIONAL GENE SILENCING HAS TWO
REMARK   1  TITL 3 DISTINCT ACTIVITY MODES.
REMARK   1  REF    MOL.CELL                      V.  10  1417 2002
REMARK   1  REFN   ASTM MOCEFL  US ISSN 1097-2765                    構造が発表された論文
REMARK   2
REMARK   2 RESOLUTION. 2.30 ANGSTROMS.                                                  分解能
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : REFMAC 5.2.0005
REMARK   3   AUTHORS     : MURSHUDOV,VAGIN,DODSON
REMARK   3
REMARK   3    REFINEMENT TARGET : MAXIMUM LIKELIHOOD
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) : 2.30
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) : 19.98
REMARK   3   DATA CUTOFF            (SIGMA(F)) : NULL
REMARK   3   COMPLETENESS FOR RANGE        (%) : 97.7
REMARK   3   NUMBER OF REFLECTIONS             : 108414
                                                X線回折データの統計値（データの質の評価）
```

以下、結晶学的構造精密化データ等（中略）

```
SEQADV 2J7N ALA A  559  UNP  Q9Y7G6    GLY   559 CONFLICT
```

```
SEQADV 2J7N ALA B  559  UNP  Q9Y7G6    GLY   559 CONFLICT
SEQRES   1 A 1022  GLU SER ALA ARG SER GLN VAL GLN VAL HIS ALA PRO VAL
SEQRES   2 A 1022  VAL ALA ALA ARG LEU ARG ASN ILE TRP PRO LYS PHE PRO
```

蛋白質（A鎖ポリペプチド分）アミノ酸配列情報（中略）

```
SEQRES  77 A 1022  ARG LEU GLU GLY ASP GLY SER GLU TYR PRO ASP PRO GLU
SEQRES  78 A 1022  VAL TYR GLU VAL LEU GLY ASP ASP ASP PHE ASP GLY ILE
SEQRES  79 A 1022  GLY PHE THR GLY ASN GLY ASP TYR
SEQRES   1 B 1022  GLU SER ALA ARG SER GLN VAL GLN VAL HIS ALA PRO VAL
SEQRES   2 B 1022  VAL ALA ALA ARG LEU ARG ASN ILE TRP PRO LYS PHE PRO
```

蛋白質（B鎖ポリペプチド分）アミノ酸配列情報（中略）

```
SEQRES  77 B 1022  ARG LEU GLU GLY ASP GLY SER GLU TYR PRO ASP PRO GLU
SEQRES  78 B 1022  VAL TYR GLU VAL LEU GLY ASP ASP ASP PHE ASP GLY ILE
SEQRES  79 B 1022  GLY PHE THR GLY ASN GLY ASP TYR
HET     MG  A2374       1                                       蛋白質以外の分子（水分子は除く）
HET     MG  B2374       1                                       蛋白質以外の分子（水分子は除く）
HET    GOL  B2375       5                                       蛋白質以外の分子（水分子は除く）
HETNAM      MG MAGNESIUM ION                                    蛋白質以外の分子（水分子は除く）
HETNAM     GOL GLYCEROL                                         蛋白質以外の分子（水分子は除く）
FORMUL   3   MG    2(MG 2+)
FORMUL   5  GOL    C3 H8 O3
FORMUL   6  HOH   *920(H2 O)
HELIX    1   1 PRO A  406  HIS A  410  5                                    5
HELIX    2   2 PRO A  413  LYS A  428  1                                   16
```

二次構造（αヘリックス）形成残基（以下略）

```
SHEET    1  AA 3 GLU A 486  SER A 487  0
SHEET    2  AA 3 SER A 490  TYR A 500 -1  O  SER A 490   N  SER A 487
SHEET    3  AA 3 MET A 519  GLN A 522 -1  O  MET A 519   N  VAL A 493
SHEET    1  AB 6 GLU A 486  SER A 487  0
SHEET    2  AB 6 SER A 490  TYR A 500 -1  O  SER A 490   N  SER A 487
SHEET    3  AB 6 PHE A 535  PRO A 541  1  O  PHE A 535   N  LEU A 494
SHEET    4  AB 6 LYS A 609  GLY A 619 -1  O  GLU A 610   N  ILE A 540
SHEET    5  AB 6 ARG A 578  ASP A 587 -1  O  GLN A 579   N  GLU A 617
SHEET    6  AB 6 HIS A 573  LEU A 575 -1  O  HIS A 573   N  TRP A 580
SHEET    1  AC 5 TYR A 680  THR A 684  0
SHEET    2  AC 5 THR A 779  VAL A 785 -1  O  LEU A 780   N  ILE A 682
SHEET    3  AC 5 ALA A 734  PHE A 739 -1  O  GLN A 736   N  ARG A 783
SHEET    4  AC 5 ALA A 742  ILE A 748 -1  O  ALA A 742   N  PHE A 739
SHEET    5  AC 5 VAL A 711  MET A 714  1  O  GLY A 712   N  VAL A 747
SHEET    1  AD 2 ILE A 690  HIS A 692  0
```

二次構造（βシート）形成残基（以下略）

その他（中略）

```
CRYST1  101.021  122.553  114.701  90.00 108.90  90.00 P 1 21 1      4
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.009899  0.000000  0.003389        0.00000
SCALE2      0.000000  0.008160  0.000000        0.00000
SCALE3      0.000000  0.000000  0.009215        0.00000
```

結晶格子情報

以下、蛋白質座標データ（ATOM で始まる行）

```
識別子 原子通し番号 原子名 残基名 鎖 ID 残基番号 X 座標 Y 座標 Z 座標 占有率 温度因子
ATOM      1  N   HIS A 390      26.541  71.474  41.819  1.00 69.66           N
ATOM      2  CA  HIS A 390      25.822  72.575  41.113  1.00 69.69           C
ATOM      3  C   HIS A 390      24.527  72.938  41.831  1.00 69.47           C
ATOM      4  O   HIS A 390      23.484  72.328  41.598  1.00 69.31           O
ATOM      5  CB  HIS A 390      25.554  72.202  39.650  1.00 69.84           C
```

蛋白質（A 鎖）の座標データ（約 7000 原子分）（中略）

```
ATOM   7519  O   GLY A1372      79.239  84.159 104.461  1.00 60.47           O
ATOM   7520  N   ASP A1373      78.874  83.354 106.391  1.00 60.59           N
TER    7521      ASP A1373                                                  A 鎖蛋白質の末端を示す識別子
ATOM   7522  N   HIS B 390     124.290  71.909 126.512  1.00 56.05           N
ATOM   7523  CA  HIS B 390     123.321  72.141 125.405  1.00 56.09           C
ATOM   7524  C   HIS B 390     123.975  72.861 124.227  1.00 56.07           C
```

蛋白質（A 鎖）の座標データ（約 7000 原子分）（中略）

```
ATOM  15018  O   GLY B1372      69.931  81.136  58.065  1.00 54.74           O
ATOM  15019  N   ASP B1373      69.772  80.569  56.046  1.00 55.21           N
TER   15020      ASP B1373                                                  A 鎖蛋白質の末端を示す識別子
```

```
HETATM15021 MG    MG A2374      52.465  56.771  65.955  1.00 50.74          MG
HETATM15022 MG    MG B2374      96.102  57.234  99.946  1.00 31.56          MG
```

マグネシウムイオン（MG）の座標データ

```
HETATM15023  C1  GOL B2375      73.308 108.248  80.328  1.00 67.59           C
HETATM15024  O1  GOL B2375      72.077 108.269  79.630  1.00 67.09           O
HETATM15025  C2  GOL B2375      73.376 109.496  81.203  1.00 67.91           C
HETATM15026  O2  GOL B2375      73.431 110.643  80.381  1.00 67.64           O
HETATM15027  C3  GOL B2375      74.572 109.459  82.147  1.00 66.80           C
```

グリセロール（GOL）の座標データ

```
HETATM15028  O   HOH Y   1     121.225  71.655 122.868  1.00 77.52           O
HETATM15029  O   HOH Y   2      90.880 102.999 128.166  1.00 76.76           O
```

水分子（HOH）の座標データ（数百分子分、後略）

```
CONECT 476415021
CONECT 478415021
CONECT 479615021
CONECT1226315022
CONECT1228315022
CONECT1229515022
CONECT15021 4764 4784 479615787
CONECT1502115791
CONECT150221226312283122951530O
CONECT150221530115304
CONECT150231502415025
CONECT1502415023
CONECT150251502315026150 27
CONECT1502615025
CONECT1502715025
CONECT1530015022
CONECT1530115022
```

```
CONECT1530415022
CONECT1578715021
CONECT1579115021
                                                                原子間の結合情報
MASTER      972    0    3   85   78    0    6    615945    2   20  158
END                                                                                 PDB ファイルの終了の識別子
```