**Instructions for data in S01_Example_PC**

**Description:**

The data in S01_Example_PC is used for supporting the results "*3.1 Overview of the method for recognizing SSE packing clusters*" in this article, which gives the decomposition of a domain (d1atza_) into two SSE packing clusters (**Fig. 1B**).

| File name | Description |
|---|---|
| **d1atza_.ent** | The PDB structure file for d1atza_ |
| **d1atza_PC1.pdb** | The information and structure of SSE PC A |
| **d1atza_PC2.pdb** | The information structure of SSE PC B |

The file "d1atza_PC1.pdb" not only gives the intact structure of SSE packing cluster A, but also presents the corresponding information of SSE packing cluster in the header of the file.

```
REMARK 111  PDB Structure for a Packing Cluster.
REMARK 222  Sites in Packing Cluster:
REMARK 222  7,3,5,9,20,23,24,26,27,29,30,31,34,36,41,
REMARK 222  43,45,47,56,52,67,71,74,110,108,112,136,138,140,160,
REMARK 222  164,170,171,173,174,180,181,184,15,167,12,14,81,114,
REMARK 333  Packing Face 1: E 3,5,7,9,
REMARK 333  Packing Face 2: H 20,23,24,26,27,29,30,31,
REMARK 333  Packing Face 3: E 41,43,45,47,
REMARK 333  Packing Face 4: E 52,56,
REMARK 333  Packing Face 5: H 67,71,
REMARK 333  Packing Face 6: E 108,110,112,
REMARK 333  Packing Face 7: E 136,138,140,
REMARK 333  Packing Face 8: H 170,171,173,174,
REMARK 444  FaceInfor: SUM 8 H 3 E 5
ATOM     10  N   PRO A   2      17.204   6.905  41.225  1.00 19.54           N
ATOM     11  CA  PRO A   2      17.879   7.928  40.419  1.00 15.16           C
ATOM     12  C   PRO A   2      17.779   7.581  38.937  1.00 11.65           C
ATOM     13  O   PRO A   2      17.894   6.414  38.554  1.00 10.50           O
ATOM     14  CB  PRO A   2      19.323   7.844  40.903  1.00 16.80           C
ATOM     15  CG  PRO A   2      19.183   7.411  42.316  1.00 19.92           C
ATOM     16  CD  PRO A   2      18.124   6.341  42.225  1.00 19.12           C
ATOM     17  N   LEU A   3      17.545   8.596  38.118  1.00  7.55           N
ATOM     18  CA  LEU A   3      17.414   8.421  36.687  1.00  6.70           C
ATOM     19  C   LEU A   3      18.136   9.532  35.945  1.00  3.92           C
ATOM     20  O   LEU A   3      17.874  10.706  36.188  1.00  3.73           O
ATOM     21  CB  LEU A   3      15.928   8.457  36.276  1.00  7.28           C
ATOM     22  CG  LEU A   3      15.652   8.527  34.761  1.00  6.70           C
ATOM     23  CD1 LEU A   3      15.941   7.179  34.085  1.00  8.22           C
ATOM     24  CD2 LEU A   3      14.206   8.927  34.520  1.00  8.60           C
```

REMARK 222 contains the residues involved in an SSE packing cluster.
REMARK 333 contains the interfaces involved in an SSE packing cluster.