7. ORTEP EXAMPLES

This section includes several example structures that illustrate a number of the capabilities found in ORTEP-III. The ORTEP input file for each example is provided.

7.1 CELL PACKING – 5-HYDROXY-5-PHENYLNORBORNANONE

Two illustrations of 5-hydroxy-5-phenylnorbornanone are provided here. The data were obtained from a neutron diffraction study at room temperature.[24] The first illustration shows one complete molecule, and the second shows the contents of the unit cell.

The input file of the first structure illustrates ORTEP's original format for the symmetry operators. The atom parameter lines were taken directly from the output of a least squares refinement, and information is included there that is not needed by ORTEP. The extra information lies in card fields that are not required for ORTEP's operation and is ignored by the program. Note that the atoms are individually labeled with 901 instructions.

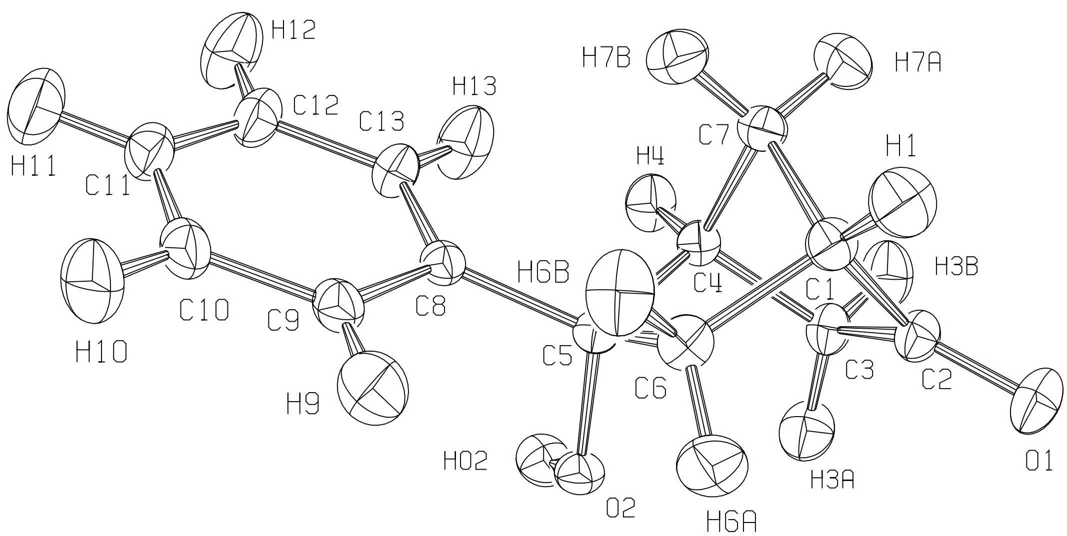

Fig. 7.1. Single molecule of 5-hydroxy-5-phenylnorbornanone.

```
 PHENYL HYDROXYL NORBORNANONE
   10.331   10.646   10.099      0.0 -.283810      0.0
             .0  1  0  0             .0  0  1  0             .0  0  0  1
             .0 -1  0  0             .0  0 -1  0             .0  0  0 -1
             .5 -1  0  0             .5  0  1  0             .5  0  0 -1
1            .5  1  0  0             .5  0 -1  0             .5  0  0  1
  C1      0.661000 1.000000 0.224802 0.001638 0.901515 0.0
 0.011930 0.006750 0.011647 0.000642 0.003989 0.000860               0  1  0
  C2      0.661000 1.000000 0.335043 0.050840 0.844329 0.0
 0.010432 0.007831 0.012112 0.001274 0.003947-0.000264               0  1  0
  C3      0.661000 1.000000 0.327553 0.192798 0.850375 0.0
 0.009129 0.007883 0.013469-0.000262 0.003784 0.000058               0  1  0
  C4      0.661000 1.000000 0.206609 0.213473 0.908171 0.0
 0.008568 0.006819 0.009641-0.000310 0.002118-0.001032               0  1  0
```

```
 C5      0.661000 1.000000 0.074610 0.177193 0.796977 0.0
0.008590 0.006732 0.008260-0.000670 0.002360 0.000103            0  1  0
 C6      0.661000 1.000000 0.091094 0.031659 0.790120 0.0
0.011368 0.006963 0.012116-0.001403 0.003143-0.001297            0  1  0
 C7      0.661000 1.000000 0.223679 0.102901 1.010406 0.0
0.011840 0.009377 0.008981 0.001423 0.002835 0.000648            0  1  0
 C8      0.661000 1.000000-0.053735 0.216149 0.834431 0.0
0.008328 0.007955 0.008995-0.000100 0.002374 0.001216            0  1  0
 C9      0.661000 1.000000-0.175896 0.157400 0.769638 0.0
0.008481 0.012396 0.011267-0.001406 0.001677 0.001394            0  1  0
 C10     0.661000 1.000000-0.296122 0.195813 0.795042 0.0
0.008526 0.016481 0.014906-0.000226 0.002743 0.004954            0  1  0
 C11     0.661000 1.000000-0.295600 0.294171 0.886394 0.0
0.011357 0.014259 0.016607 0.003003 0.006602 0.005712            0  1  0
 C12     0.661000 1.000000-0.175266 0.352517 0.950755 0.0
0.012936 0.012232 0.018491 0.002923 0.008046 0.001071            0  1  0
 C13     0.661000 1.000000-0.055392 0.314579 0.925104 0.0
0.010921 0.009871 0.014343 0.000394 0.005261-0.001410            0  1  0
 O1      0.577000 1.000000 0.414647-0.009305 0.801699 0.0
0.014915 0.010743 0.020270 0.002523 0.008903-0.001350            0  1  0
 O2      0.577000 1.000000 0.068052 0.227607 0.664516 0.0
0.010744 0.010771 0.008919-0.000196 0.003244 0.001269            0  1  0
 H1     -0.375000 1.000000 0.236869-0.096021 0.933996 0.0
0.020624 0.008781 0.019162 0.002373 0.007156 0.003208            0  1  0
 H3A    -0.375000 1.000000 0.318029 0.234292 0.749440 0.0
0.015989 0.012191 0.019604 0.000563 0.008507 0.003596            0  1  0
 H3B    -0.375000 1.000000 0.419746 0.227078 0.923493 0.0
0.011065 0.013144 0.022925-0.001035 0.003225-0.001808            0  1  0
 H4     -0.375000 1.000000 0.205933 0.307044 0.952030 0.0
0.012786 0.009537 0.016431-0.000243 0.003014-0.003491            0  1  0
 H6A    -0.375000 1.000000 0.092339 0.004576 0.685888 0.0
0.019268 0.012340 0.014229-0.000125 0.002520-0.004920            0  1  0
 H6B    -0.375000 1.000000 0.009600-0.018900 0.814691 0.0
0.014224 0.009647 0.026857-0.003061 0.006299 0.000168            0  1  0
 H7A    -0.375000 1.000000 0.316741 0.107454 1.094270 0.0
0.016598 0.016936 0.012393 0.003607 0.001040 0.000321            0  1  0
 H7B    -0.375000 1.000000 0.138340 0.092052 1.052878 0.0
0.017074 0.014780 0.014417 0.001660 0.007380 0.002011            0  1  0
 H9     -0.375000 1.000000-0.177376 0.080634 0.699229 0.0
0.014017 0.019179 0.019187-0.004154 0.001724-0.005322            0  1  0
 H10    -0.375000 1.000000-0.389010 0.146805 0.746257 0.0
0.010867 0.027857 0.025083-0.003438 0.003403 0.001062            0  1  0
 H11    -0.375000 1.000000-0.387954 0.322178 0.907661 0.0
0.015401 0.023080 0.028789 0.005406 0.011698 0.006558            0  1  0
 H12    -0.375000 1.000000-0.172867 0.427707 1.023741 0.0
0.021232 0.019665 0.030399 0.002995 0.013356-0.006345            0  1  0
 H13    -0.375000 1.000000 0.036386 0.362903 0.977271 0.0
0.015325 0.017015 0.026705-0.002320 0.007502-0.010296            0  1  0
 HO2    -0.375000 1.000000 0.071033 0.317748 0.672629 0.0
10.013588 0.011864 0.013832-0.001003 0.004119 0.003274            0  1  0
```

```
     201
     301      7.2      5.4       12      1.0
     401   155501 -2955501
     501   555501   655501   255501   255501   355501                  0
     502        2       28        1      2.7
     604                                 1.00
     601      4.0      1.5
 2  1001
         1 29  1 29  3   .80   1.6   .05
     716
 2   812
         1 29  1 29  3   .80   1.6   .05
     901   155501                                  .10     -.05     -.22
     901   255501                                  .10     +.10     -.22
     901   355501                                  .10     +.17     -.22
     901   455501                                  .10     +.05    -.212
     901   555501                                  .10     -.20     -.12
     901   655501                                  .10     -.17     -.22
     901   755501                                  .10     -.25     -.03
     901   855501                                  .10    -.063     -.22
     901   955501                                  .10     -.27     -.07
     901  1055501                                  .10     +.05     -.30
     901  1155501                                  .10     -.25     -.17
     901  1255501                                  .10     +.27     +.07
     901  1355501                                  .10     -.12     +.27
     901  1455501                                  .10     +.02     -.30
     901  1555501                                  .10     +.22    -.185
     901  1655501                                  .10     0.00     +.27
     901  1755501                                  .10     +.10     -.27
     901  1855501                                  .10     +.35     +.05
     901  1955501                                  .10     0.00     +.27
     901  2055501                                  .10     +.05    -.265
     901  2155501                                  .10     -.40     +.10
     901  2255501                                  .10     +.35     0.00
     901  2355501                                  .10     -.40     0.00
     901  2455501                                  .10     -.33     -.07
     901  2555501                                  .10     0.00     -.33
     901  2655501                                  .10     -.05     -.30
     901  2755501                                  .10     +.30     +.12
     901  2855501                                  .10    +.012     +.32
     901  2955501                                  .10    -.475     0.00
     202
      -1
```

This second example shows the packing of the norbornanone molecules in a unit cell. The unit cell contains four molecules, but six have been drawn. The hydrogen atoms have been omitted for clarity, and the carbon and oxygen atoms have been drawn with different representations for easier visual identification. (The oxygen atoms are the ellipsoids with the shaded octant.) The input shows the new format for the symmetry operators that is available in ORTEP-III. In the atom parameters, dummy atoms have been provided for a corner of the unit cell (atom #16 at 0.,0.,0.) and one for its center (atom #17 at .5,.5,.5).

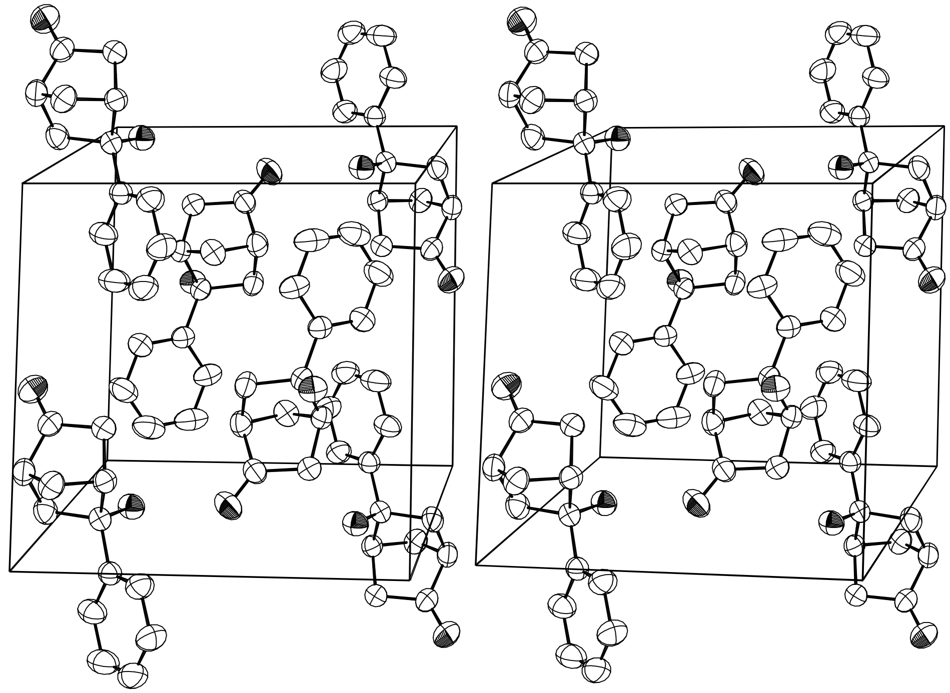

Fig. 7.2. Packing diagram of 5-hydroxy-5-phenylnorbornanone.

```
 PHENYL HYDROXYL NORBORNANONE
1  10.331   10.646   10.099      0.0 -.283810      0.0
  x,y,z
  -x,-y,-z
  1/2-x,1/2+y,1/2-z
1 1/2+x,1/2-y,1/2+z
  C1       0.661000 1.000000 0.224802 0.001638 0.901515 0.0
 0.011930 0.006750 0.011647 0.000642 0.003989 0.000860          0  1  0
  C2       0.661000 1.000000 0.335043 0.050840 0.844329 0.0
 0.010432 0.007831 0.012112 0.001274 0.003947-0.000264          0  1  0
  C3       0.661000 1.000000 0.327553 0.192798 0.850375 0.0
 0.009129 0.007883 0.013469-0.000262 0.003784 0.000058          0  1  0
  C4       0.661000 1.000000 0.206609 0.213473 0.908171 0.0
 0.008568 0.006819 0.009641-0.000310 0.002118-0.001032          0  1  0
  C5       0.661000 1.000000 0.074610 0.177193 0.796977 0.0
 0.008590 0.006732 0.008260-0.000670 0.002360 0.000103          0  1  0
  C6       0.661000 1.000000 0.091094 0.031659 0.790120 0.0
 0.011368 0.006963 0.012116-0.001403 0.003143-0.001297          0  1  0
  C7       0.661000 1.000000 0.223679 0.102901 1.010406 0.0
 0.011840 0.009377 0.008981 0.001423 0.002835 0.000648          0  1  0
  C8       0.661000 1.000000-0.053735 0.216149 0.834431 0.0
 0.008328 0.007955 0.008995-0.000100 0.002374 0.001216          0  1  0
  C9       0.661000 1.000000-0.175896 0.157400 0.769638 0.0
 0.008481 0.012396 0.011267-0.001406 0.001677 0.001394          0  1  0
  C10      0.661000 1.000000-0.296122 0.195813 0.795042 0.0
 0.008526 0.016481 0.014906-0.000226 0.002743 0.004954          0  1  0
  C11      0.661000 1.000000-0.295600 0.294171 0.886394 0.0
```

```
 0.011357 0.014259 0.016607 0.003003 0.006602 0.005712           0  1  0
  C12     0.661000 1.000000-0.175266 0.352517 0.950755 0.0
 0.012936 0.012232 0.018491 0.002923 0.008046 0.001071           0  1  0
  C13     0.661000 1.000000-0.055392 0.314579 0.925104 0.0
 0.010921 0.009871 0.014343 0.000394 0.005261-0.001410           0  1  0
  O1      0.577000 1.000000 0.414647-0.009305 0.801699 0.0
 0.014915 0.010743 0.020270 0.002523 0.008903-0.001350           0  1  0
  O2      0.577000 1.000000 0.068052 0.227607 0.664516 0.0
 0.010744 0.010771 0.008919-0.000196 0.003244 0.001269           0  1  0
ORIGIN                           0.0      0.0      0.0
      .01
CENTER                           0.5      0.5      0.5
1
      201
      301      5.4      5.4       12      1.0
# Store unit cell corners for cell outline
      401  1655501 -1666601
# Find and store all atoms within 5.5 A of unit cell center
      402  1755501       17        1       15      5.5
# Reiterative convolution around found atoms to complete molecules
      406        1       15        1       15       2.
      501  1655501  1655501  1656501  1655501  1655601                 0
      502        3      180        1       10        2      -10
      604
      503        2      2.7
     1101
  2  1001        1
  2        1 15  1 15  3   .80   1.6   .03
          16 16 16 16  1   10.   11.   .01
# Different representations for carbons (1-13) and oxygens (14-15)
  1   702
                                   1       13
  1   701
                                  14       15
  2   802
  2        1 15  1 15  3   .80   1.6   .03
          16 16 16 16  1   10.   11.   .01
     1102
      202    2.375
      503        2     -2.7
     1103
      202
       -1
```

7.2 HELICAL STRUCTURE – POLY-L-ALANINE

The structure of poly-L-alanine was published by Elliott and Malcolm in 1959.[25] The Pauling and Corey right-handed alpha helix repeats after 13 turns and 47 residues and can be represented in ORTEP by 47 symmetry cards with $N = 47$; $M = 13$; $L = 0, 1, \ldots, 46$; $T_1, T_2, T_3 = 0$. The input atom list then contains the contents of one residue. In this example there are 48 symmetry cards with operator 1 and operator 48 related by one cell translation along c.

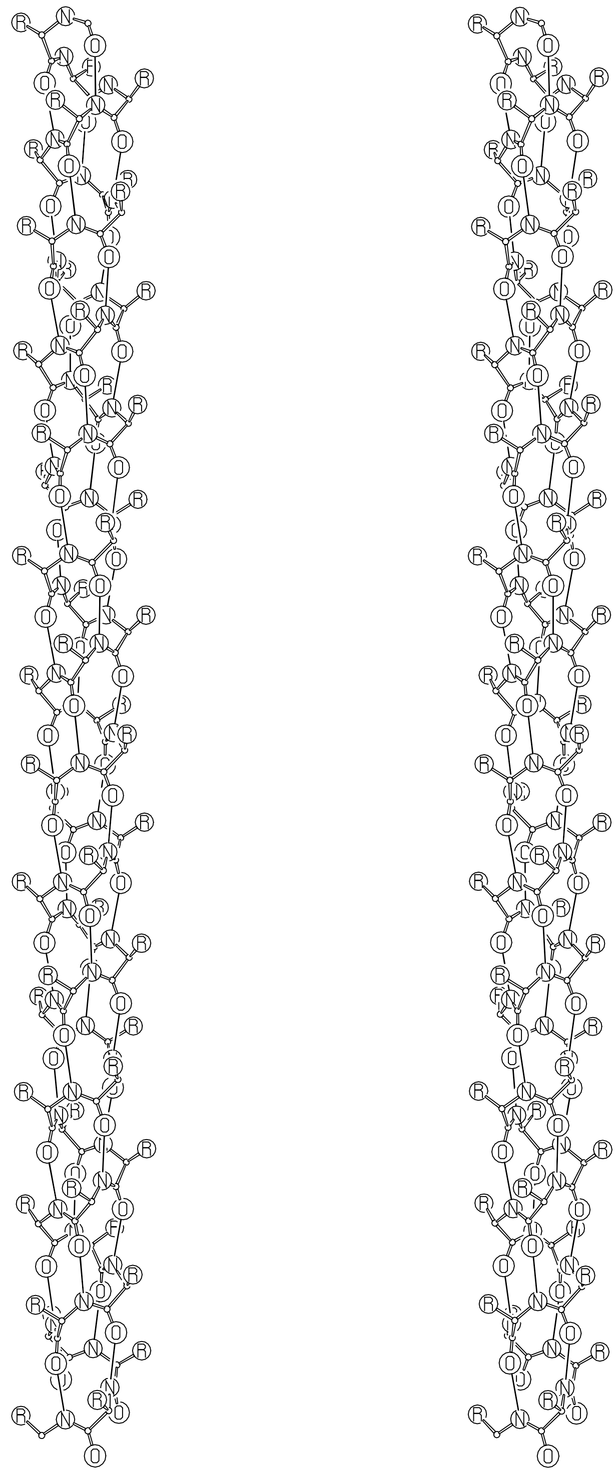

Fig. 7.3. 47/13 α-Helix of poly-L-alanine. The thin "vertical" lines between nitrogen and oxygen atoms indicate a hydrogen bond path.

```
POLY-L-ALANINE  47/13 HELIX      ELLIOTT AND MALCOLM (1959)
    8.55     8.55     70.3      90.      90.     120.
                                                              0 13 47
                                                              1 13 47
                                                              2 13 47
                                                              3 13 47
                                                              4 13 47
                                                              5 13 47
                                                              6 13 47
                                                              7 13 47
                                                              8 13 47
                                                              9 13 47
                                                             10 13 47
                                                             11 13 47
                                                             12 13 47
                                                             13 13 47
                                                             14 13 47
                                                             15 13 47
                                                             16 13 47
                                                             17 13 47
                                                             18 13 47
                                                             19 13 47
                                                             20 13 47
                                                             21 13 47
                                                             22 13 47
                                                             23 13 47
                                                             24 13 47
                                                             25 13 47
                                                             26 13 47
                                                             27 13 47
                                                             28 13 47
                                                             29 13 47
                                                             30 13 47
                                                             31 13 47
                                                             32 13 47
                                                             33 13 47
                                                             34 13 47
                                                             35 13 47
                                                             36 13 47
                                                             37 13 47
                                                             38 13 47
                                                             39 13 47
                                                             40 13 47
                                                             41 13 47
                                                             42 13 47
                                                             43 13 47
                                                             44 13 47
                                                             45 13 47
                                                             46 13 47
1                                                            47 13 47
                                1.63     94.9     -.40      3
       .1                                                   7
```

```
                              2.29     20.7     -.81        3
     .1                                                     7
 R                            3.17       0.       0.        3
     .3                                                     7
 N                            1.49     49.7      .06        3
     .3                                                     7
 0                            1.98     104.    -1.58        3
    .35                                                     7
ORGN                            .0        0       .5
1
# Initialize plotting
     201
# Landscape drawing orientation
     301      8.5      2.0       15      0.5
# Rotate lettering for landscape orientation
     302      -90
# Store atoms to be drawn
     401   155501  -555548
# Define coordinate system
     501   655501   155501   155601   155501   165501
# Rotate structure for landscape orientation
     502        1      90.
# Automatic position and scale
     604
# Shift plot origin for left eye view
     202        0       5
# Stereo rotation for left eye view
     503        1      2.5
# Start save sequence
    1101
# Calculate overlap
 2  1001
 2        1  5  1  5  1   1.1   1.6  .050
          4  4  5  5  1   2.7   3.0  .010
# Draw atoms and labels
     714                                         .07      .03
# Draw covalent bonds and inter-residue hydrogen bonds
 2   812
 2        1  5  1  5  1   1.1   1.6  .050
          4  4  5  5  1   2.7   3.0  .010
# End save sequence
    1102
# Stereo rotation for right eye view
     503        1     -2.5
# Shift plot origin for right eye view (view separation = 2.375 in.)
     202        0    2.625
# Repeat save sequence
    1103
# Terminate plotting
     202
# Terminate ORTEP
      -1
```

7.3 COORDINATION POLYHEDRA – POTASSIUM PERXENATE NONAHYDRATE

The crystal structure of this hydrated ionic material was published by Zalkin *et al*. in 1964.[26] The only covalent bonds are between the xenon and oxygen atoms in the perxenate anions (the darker bonds in Fig. 7.4). To see better how the oxygens of the perxenate anions and water molecules coordinate around the potassium and atoms, lines have been drawn from the potassiums to all oxygens within a distance of 3.3 Å.

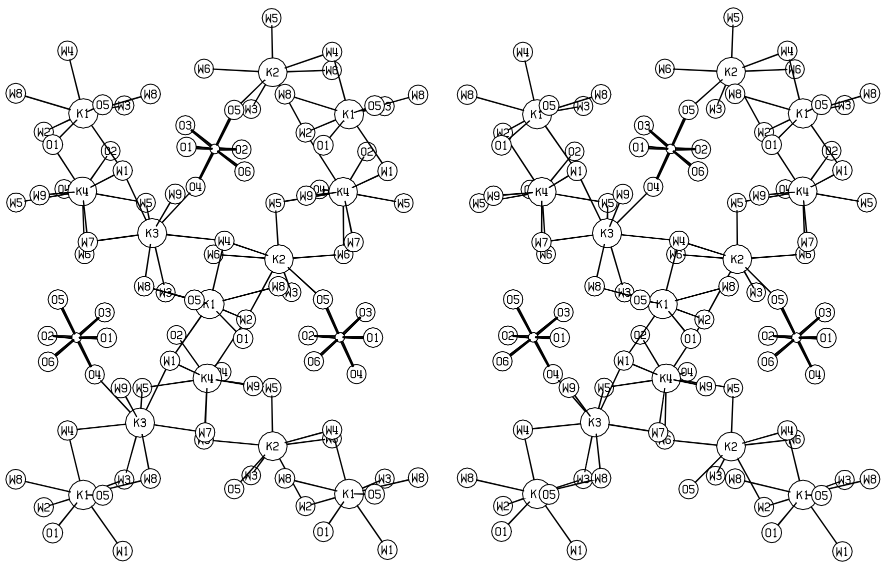

Fig. 7.4. Coordination polyhedra in potassium perxenate nonahydrate.

```
 POTASSIUM PERXENATE 9-HYDRATE/A.ZALKIN ET AL (1964) JACS 86,3569
1   9.049   10.924   15.606      90.      90.      90.
   x,y,z
  -x,-y,1/2+z
  -x,1/2+y,z
1  x,1/2-y,1/2+z
  XE                            .249     .988     .250
      .10                                                 7
  K1                            .628     .987     .339
      .30                                                 7
  K2                            .846     .238     .958
      .30                                                 7
  K3                            .307     .227     .026
      .30                                                 7
  K4                            .877     .989     .139
      .30                                                 7
  O1                            .403     .101     .251
      .20                                                 7
  O2                            .094     .878     .253
      .20                                                 7
  O3                            .138     .096     .316
      .20                                                 7
  O4                            .176     .058     .151
```

```
     .20                                                   7
  O5                         .323     .918     .351
     .20                                                   7
  O6                         .360     .881     .188
     .20                                                   7
  W1                         .654     .839     .190
     .20                                                   7
  W2                         .850     .136     .297
     .20                                                   7
  W3                         .873     .829     .369
     .20                                                   7
  W4                         .692     .046     .506
     .20                                                   7
  W5                         .997     .243     .111
     .20                                                   7
  W6                         .967     .980     .972
     .20                                                   7
  W7                         .376     .470     .002
     .20                                                   7
  W8                         .493     .262     .886
     .20                                                   7
  W9                         .606     .150     .124
     .20                                                   7
 ORGN                        .250     .500     .400
     .10                                                   7
                             .000     .000     .000
1    .03                                                   7
     201
     301      2.6      3.6       15     0.25
# Locate and store K and Xe atoms
     404       21       21        1        5      .13      .52      .57
# Convolute sphere of enclosure with each central atom
     405        1        5        1       20     3.30
# B axix horizontal, C axis vertical, viewed along -A axis
     501  2155501  2155501  2156501  2155501  2155601                 1
     604                                   2.
     503        2        3
    1101
  2  1001       1
  2         1  1  6 11  3   1.8   1.9   .04
            2  5  6 20  1   2.6   3.3   .01
  1   714                                       .04
                                2        20
# Xe not labeled
  1   714
                                1         1
  2   812
  2         1  1  6 11  3   1.8   1.9   .04
            2  5  6 20  1   2.6   3.3   .01
    1102
     202    2.375
     503        2       -3
```

```
    1103
     202
      -1
```

In the following representation of the same structure shown in Fig. 7.4, only the xenon and potassium atoms have been explicitly drawn. (The xenon atoms are the smaller circles.) The oxygen atoms are shown implicitly as the vertices of polyhedra centered on the potassium and xenon atoms. As in the previous case, oxygens within 3.3 Å of the potassium are treated as making up the coordination polyhedron. Only the instruction portion of the input file is provided. The input lines that precede these are the same as those in the previous case.

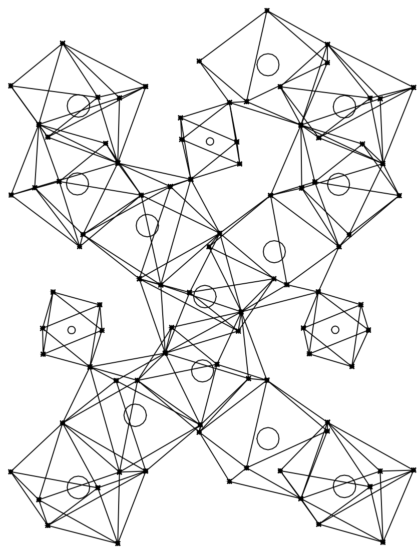

Fig. 7.5. Coordination polyhedra in potassium perxenate nonahydrate.

```
     201
     301      2.6      3.6       15     0.25
# Locate and store K and Xe atoms
     404       21       21        1        5      .13      .52      .57
# Convolute sphere of enclosure with each central atom
     405        1        5        1       20     3.30
# B axix horizontal, C axis vertical, viewed along -A axis
     501  2155501  2155501  2156501  2155501  2155601                 1
     604
     503        2        3
    1101
# Draw xenon and potassium atoms only
  1   714
                                  1        5
# Use polygon radii to limit bonds drawn
  2   813
  2        6 11   6 11      2.5   2.8          -1      1   1.8   1.9
           6 20   6 20      2.6   4.6          -2      5   2.6   3.3
    1102
     202    2.375
     503        2       -3
```

```
1103
 202
  -1
```

7.4 ATOM FEATURES – LYSOSOME MUTANT POLYPEPTIDE

The data for this example were taken from the Protein Data Bank #216L. The header information from that file is provided below.

```
HEADER    HYDROLASE(O-GLYCOSYL)                   10-MAY-94   216L
COMPND    LYSOZYME (E.C.3.2.1.17) MUTANT WITH SER 44 REPLACED BY TRP,
COMPND   2 CYS 54 REPLACED BY THR, CYS 97 REPLACED BY ALA (S44W,
COMPND   3 C54T, C97A)
SOURCE    BACTERIOPHAGE T4 (MUTANT GENE DERIVED FROM THE M13
SOURCE   2 PLASMID BY CLONING THE T4 LYSOZYME GENE)
AUTHOR    M.BLABER,B.W.MATTHEWS
REVDAT   1   31-JUL-94 216L    0
SPRSDE     31-JUL-94 216L      116L
JRNL        AUTH   M.BLABER,X.-J.ZHANG,B.W.MATTHEWS
JRNL        TITL   STRUCTURAL BASIS OF ALPHA-HELIX PROPENSITY AT TWO
JRNL        TITL 2 SITES IN T4 LYSOZYME
JRNL        REF    SCIENCE                          V. 260  1637 1993
JRNL        REFN   ASTM SCIEAS  US ISSN 0036-8075                0038
```

Only the first 63 amino acids (500 atoms) of the protein were used for this example since that is the size used in the dimension statements in ORTEP-III. The first 500 ATOM lines were extracted from the PDB file and placed unaltered in a file named ATOMS.DAT. A few of the lines are shown below.

```
ATOM      1  N   MET A   1      82.486  23.405  25.378  1.00 29.06      216L 127
ATOM      2  CA  MET A   1      81.291  22.758  24.885  1.00 15.78      216L 128
ATOM      3  C   MET A   1      80.495  23.789  24.150  1.00 33.32      216L 129
ATOM      4  O   MET A   1      80.951  24.925  24.017  1.00 29.09      216L 130
ATOM      5  CB  MET A   1      80.556  22.168  26.090  1.00 14.87      216L 131
ATOM      6  CG  MET A   1      79.353  21.283  25.811  1.00 44.92      216L 132
ATOM      7  SD  MET A   1      78.906  20.301  27.306  1.00 34.12      216L 133
ATOM      8  CE  MET A   1      80.536  19.686  27.844  1.00  7.96      216L 134
ATOM      9  N   ASN A   2      79.348  23.416  23.650  1.00  7.39      216L 135
ATOM     10  CA  ASN A   2      78.619  24.379  22.897  1.00 14.21      216L 136
  .            .            .            .            .            .
  .            .            .            .            .            .
  .            .            .            .            .            .
ATOM    491  CB  GLU A  62      69.880  12.430   7.589  1.00  6.64      216L 617
ATOM    492  CG  GLU A  62      70.251  11.994   6.135  1.00  1.34      216L 618
ATOM    493  CD  GLU A  62      69.487  10.795   5.671  1.00 27.84      216L 619
ATOM    494  OE1 GLU A  62      68.805  10.091   6.416  1.00 19.47      216L 620
ATOM    495  OE2 GLU A  62      69.547  10.652   4.368  1.00 34.69      216L 621
ATOM    496  N   ALA A  63      70.531  13.275  10.600  1.00 32.33      216L 622
ATOM    497  CA  ALA A  63      70.126  13.774  11.873  1.00  6.04      216L 623
ATOM    498  C   ALA A  63      70.877  15.054  12.241  1.00 55.04      216L 624
ATOM    499  O   ALA A  63      70.278  16.027  12.662  1.00 13.24      216L 625
ATOM    500  CB  ALA A  63      70.323  12.701  12.964  1.00 18.46      216L 626
```

Since these atom data are not in the standard format used by ORTEP, subroutine READIN was written to read this particular format. It is shown below. As each atom is read by READIN, the subroutine sets the value of FEATURE #2 (id2) for the atom to the sequence number of the amino acid containing the atom. FEATURE #1 (id1) is set to a value that indicates the type of atom:

1	peptide link N
2	alpha carbon
3	carbon of C=O in peptide link
4	oxygen of C=O in peptide link
9	all other atoms

```
      subroutine readin(iu,chem,id1,id2,x1,x2,x3,it,is,b1,b2,b3,b4,
     1                 b5,b6,btype)
      integer*2 id1,id2
      character*1 chain
      character*3 res
      character*4 atom
      character*6 rec
      character*8 chem
      b1=.1
      b2=0
      b3=0
      b4=0
      b5=0
      b6=0
      btype=7.
      id1=0
      id2=0
      it=2
      read (iu,201) rec,iserno,atom,res,chain,id2,x1,x2,x3,occ,tf
  201 format(a6,i5,1x,a4,1x,a3,1x,a1,i4,4x,3f8.0,2f6.0)
      id1=9
      if (atom.eq.' N  ') id1=1
      if (atom.eq.' CA ') id1=2
      if (atom.eq.' C  ') id1=3
      if (atom.eq.' O  ') then
         id1=4
         b1=.15
      end if
      chem=atom(2:4)//res
      is=0
c *** check if another data record is available
      read (iu,202,end=203) rec
  202 format(a6)
      backspace(iu)
      return
  203 is=1
      return
      end
```

The ORTEP input file contains the instructions for producing three different illustrations. Each begins with a 201 instruction and ends with a 202. The second and third sets make use of the assigned atom features to select particular atoms for drawing. In the input file, a "2" in column 1 of the final symmetry card tells ORTEP (1) that the atom data are in a separate file and (2) to use subroutine READIN to read the data.

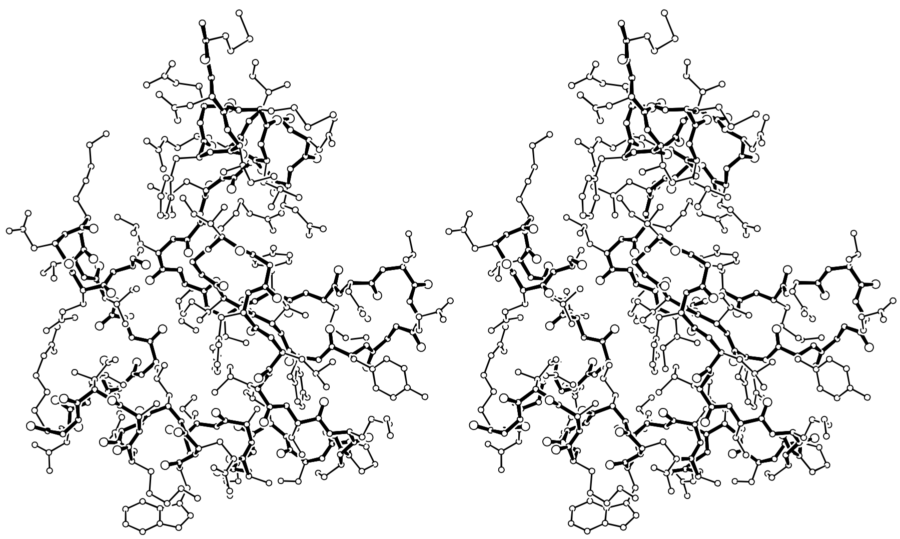

Fig. 7.6. First 63 amino acids of lysosome mutant protein.

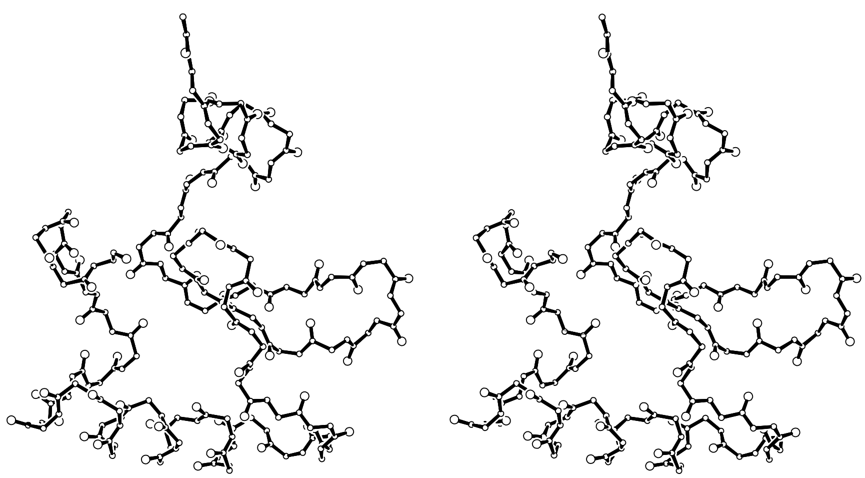

Fig. 7.7. First 63 amino acids of lysosome mutant protein with side chains eliminated.

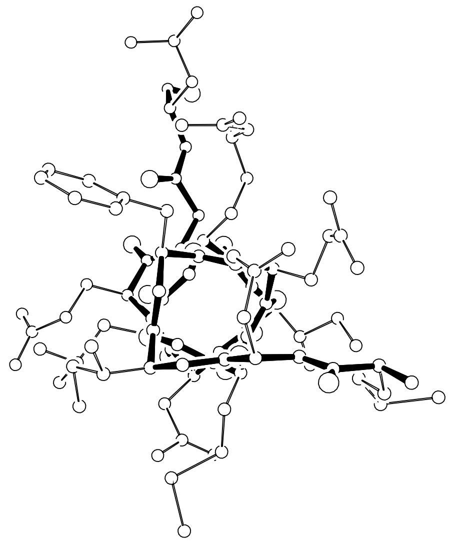

Fig. 7.8. First 13 amino acids of lysosome mutant protein, looking through α-helix.

```
 LYSOZYME MUTANT PROTEIN DATA BANK #216L - BLABER AND MATTHEWS
1 116.500   54.400   59.500    90.00   102.30    90.00
     X,Y,Z
     -X,Y,-Z
     X+1/2,Y+1/2,Z
2    -X+1/2,Y+1/2,-Z
# Polypeptide containing first 63 amino acids of protein.
      201
      301      5.0      3.5      15.       .4
      401   155501-50055501
      506
      502        3       90        1       35
      604                                  2.
      503        2      2.7
     1101
  2  1001                1
  2        1  4  1  4  5   0.9   2.0   .08
  2        1  4  5  9  1   0.9   2.0   .02
           5  9  5  9  1   0.9   2.0   .02
  1   714
                                 1        9        1
  2   812                1
  2        1  4  1  4  5   0.9   2.0   .08
  2        1  4  5  9  1   0.9   2.0   .02
           5  9  5  9  1   0.9   2.0   .02
     1102
      202      2.3
      503        2    -2.7
     1103
      202
# 63 amino acid polypeptide with side chains eliminated.
```

```
# The origin, axes, and scale are unchanged from above.
     201
     301      5.0      3.5      15.       .4
     410
  2  402   155501      500        1      500      2.0
                1  4  1
     503        2      2.7
    1101
  2 1001                 1
         1  4  1  4  5   0.9   2.0   .08
  1  714
                                  1        4        1
  2  812                 1
         1  4  1  4  5   0.9   2.0   .08
    1102
     202      2.3
     503        2     -2.7
    1103
     202
# First 13 amino acids looking through alpha helix.
     201
     301      5.0      3.5      15.       .4
     410
  2  402   155501      500        1      500      2.0
         1 13  1 13  2
     506
     502        2      100        1       15
     604                                  2.
     503        2      2.7
    1101
  2 1001                 1
  2      1  4  1  4  5   0.9   2.0   .08
  2      1  4  5  9  1   0.9   2.0   .02
         5  9  5  9  1   0.9   2.0   .02
  1  714
                                  1       13        2
  2  812                 1
  2      1  4  1  4  5   0.9   2.0   .08
  2      1  4  5  9  1   0.9   2.0   .02
         5  9  5  9  1   0.9   2.0   .02
    1102
     503        2     -2.7
     202      2.3
    1103
     202
      -1
```

7.5 CRITICAL NET – SODIUM CHLORIDE

ORTEP-III can produce “critical net” illustrations that depict some canonical topological characteristics of the global ensemble of overlapping atomic-thermal-motion Gaussian density functions in a crystal. Non-degenerate critical points occur where the first derivative of the global density is zero and the second derivative is a 3×3 symmetric matrix with a non-zero determinant. The signs of the three eigenvalues of the second derivative matrix specify the types of critical points, which are termed peak (–,–,–), pass (+,–,–), pale (+,+,–) and pit (+,+,+). Peaks correspond to density maxima, pits to density minima, and passes and pales to saddle points in the density function. The four types of critical points represent 0 (e.g., vertex), 1 (e.g., edge), 2 (e.g., face), and 3 (e.g., body) dimensional cells in the topological Morse function CW complex (i.e., C for closure finite, W for weak topology), simply called a critical net, and correspond with the number of + signs in the sign signature for each critical point. The most gradual up-density path from a pit to a peak follows the sequence pit $\rightarrow$ pale $\rightarrow$ pass $\rightarrow$ peak. A discussion of critical nets can be found on the World Wide Web at http://www.ornl.gov/ortep/topology/critnet.html.

Fig. 7.9 illustrates the critical net for NaCl with the larger corner spheres representing Cl peaks; the smaller corner spheres, Na peaks; the elongated "cigar-shaped" ellipsoids, passes; the flattened "pancake-shaped" ellipsoids, pales; and the smallest sphere in the center, a pit. The paths connecting the critical points, shown by the connection "bonds" in Fig. 7,9, are topologically unique.

New in ORTEP-III is the method for specifying the orientations and sizes of the elongated and flattened ellipsoids without giving their quadratic form coefficients. The temperature factor card following the atom parameter card for a pass or pale has the format:

Columns	
1	A sentinel $\neq 0$ if last atom
2-9	Unique axis length (Å)
10-18	Second (and third) axis length (Å)
19-27	VDC_1 (from)
28-36	VDC_1 (to)
37-45	[VDC_2 (from)
46-54	VDC_2 (to)]
55-63	7

VDC_1 is a vector parallel with the unique axis of the cigar-shaped pass or pancake-shaped pale and VDC_2 is a second vector *not* parallel with VDC_1 such that $VDC_1 \times VDC_2$ is a second principal axis of that ellipsoid. If VDC_1 and VDC_2 are parallel, VDC_2 is replaced by a suitable lattice translation vector. VDC_2 may be omitted from the input if desired, and the program will choose one of the three lattice vectors for VDC_2.

This example illustrates an important point about the relationship between the symmetry operators and atom input data unrelated to the fact that this is a critical net drawing. Sodium chloride crystallizes in space group $Fm\overline{3}m$, which has 192 symmetry operators. Of these, 48 are "unique", and the others may be obtained from these by adding the centering translations. The centering translations in this space group are (0,0,0), (0,.5,.5), (.5,0,.5), and (.5,.5,0). As discussed earlier (see 3.2.3), if all the symmetry operators are not provided in the ORTEP input file, each unique atom will require multiple entries with those centering translations added that are not provided in the symmetry cards. In this case only 48 symmetry operators have been included (although ORTEP-III allows a maximum of 96). As a consequence, each atom has four entries, obtained by adding the centering translation values to the atom's positional coordinates. If 96 operators had been included, each atom would have required two entries. The symmetry operators are provided in ORTEP's original format.

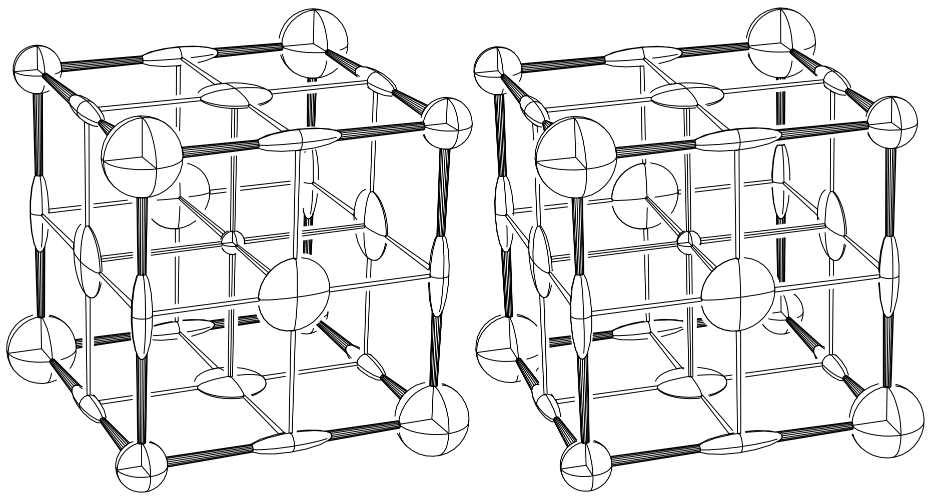

Fig. 7.9. Sodium chloride critical net.

```
NaCl Fm3m peak-a,b=m3m; pit c=4bar3m; pale-d=mmm; pass-e=4mm
  10.0000  10.0000  10.0000       0.        .0       0.
             0.  1  0  0             0.  0  1  0             0.  0  0  1
                 0  0  1                 1  0  0                 0  1  0
                 0  1  0                 0  0  1                 1  0  0
                 1  0  0                 0  0  1                 0  1  0
                 0  1  0                 1  0  0                 0  0  1
                 0  0  1                 0  1  0                 1  0  0
             0.  1  0  0             0.  0 -1  0             0.  0  0 -1
                 0  0 -1                 1  0  0                 0 -1  0
                 0 -1  0                 0  0 -1                 1  0  0
                 1  0  0                 0  0 -1                 0 -1  0
                 0 -1  0                 1  0  0                 0  0 -1
                 0  0 -1                 0 -1  0                 1  0  0
             0. -1  0  0             0.  0  1  0             0.  0  0 -1
                 0  0 -1                -1  0  0                 0  1  0
                 0  1  0                 0  0 -1                -1  0  0
                -1  0  0                 0  0 -1                 0  1  0
                 0  1  0                -1  0  0                 0  0 -1
                 0  0 -1                 0  1  0                -1  0  0
             0. -1  0  0             0.  0 -1  0             0.  0  0  1
                 0  0  1                -1  0  0                 0 -1  0
                 0 -1  0                 0  0  1                -1  0  0
                -1  0  0                 0  0  1                 0 -1  0
                 0 -1  0                -1  0  0                 0  0  1
                 0  0  1                 0 -1  0                -1  0  0
             0. -1  0  0             0.  0 -1  0             0.  0  0 -1
                 0  0 -1                -1  0  0                 0 -1  0
                 0 -1  0                 0  0 -1                -1  0  0
```

```
                 -1  0  0                  0  0 -1                  0 -1  0
                  0 -1  0                 -1  0  0                  0  0 -1
                  0  0 -1                  0 -1  0                 -1  0  0
              0. -1  0  0              0.  0  1  0              0.  0  0  1
                  0  0  1                 -1  0  0                  0  1  0
                  0  1  0                  0  0  1                 -1  0  0
                 -1  0  0                  0  0  1                  0  1  0
                  0  1  0                 -1  0  0                  0  0  1
                  0  0  1                  0  1  0                 -1  0  0
              0.  1  0  0              0.  0 -1  0              0.  0  0  1
                  0  0  1                  1  0  0                  0 -1  0
                  0 -1  0                  0  0  1                  1  0  0
                  1  0  0                  0  0  1                  0 -1  0
                  0 -1  0                  1  0  0                  0  0  1
                  0  0  1                  0 -1  0                  1  0  0
              0.  1  0  0              0.  0  1  0              0.  0  0 -1
                  0  0 -1                  1  0  0                  0  1  0
                  0  1  0                  0  0 -1                  1  0  0
                  1  0  0                  0  0 -1                  0  1  0
                  0  1  0                  1  0  0                  0  0 -1
1                 0  0 -1                  0  1  0                  1  0  0
  Na                              .0        .0        .0
      .10                                                      7
  Na                              .0        .5        .5
      .10                                                      7
  Na                              .5        .0        .5
      .10                                                      7
  Na                              .5        .5        .0
      .10                                                      7
b Cl                              .5        .0        .0
      .15                                                      7
b Cl                              .5        .5        .5
      .15                                                      7
b Cl                              .0        .5        .0
      .15                                                      7
b Cl                              .0        .0        .5
      .15                                                      7
c Pit                            .25       .25       .25
      .05                                                      7
c Pit                            .25       .75       .75
      .05                                                      7
c Pit                            .75       .25       .75
      .05                                                      7
c Pit                            .75       .75       .25
      .05                                                      7
  Pass                           .25       .00       .00
      .18      .04   155501   555501                           7
  Pass                           .75       .50       .00
      .18      .04   155501   555501                           7
  Pass                           .75       .00       .50
      .18      .04   155501   555501                           7
  Pass                           .25       .50       .50
```

```
      .18       .04   155501   555501                            7
  Pale                           .250     .250     .000
      .03       .15   155501   155601                            7
  Pale                           .750     .750     .000
      .03       .15   155501   155601                            7
  Pale                           .750     .250     .500
      .03       .15   155501   155601                            7
  Pale                           .250     .750     .500
      .03       .15   155501   155601                            7
center                           .250     .250     .250
1     .02                                                        7
      201
      301       3.2       3.2       12      0.5
      404  2155501  2155501        1       20      .26      .26      .26
      501  2155501   155501   165501   155501   156501                 1
      502         2       20        1       20
      503         2      2.5
      604        0.        0.       0.     4.00
     1101
  2  1001
  2        1  8 13 16  4   2.0   3.6   .07
  2        9 12 17 20  2   2.0   2.6   .04
          13 16 17 20  1   2.0   2.6   .03
  1   716
                                    1       12
  1   712
                                   13       20
  2   812
  2        1  8 13 16  4   2.0   3.6   .07
  2        9 12 17 20  2   2.0   2.6   .04
          13 16 17 20  1   2.0   2.6   .03
     1102
      503         2     -2.5
      202     2.375
     1103
      202
       -1
```