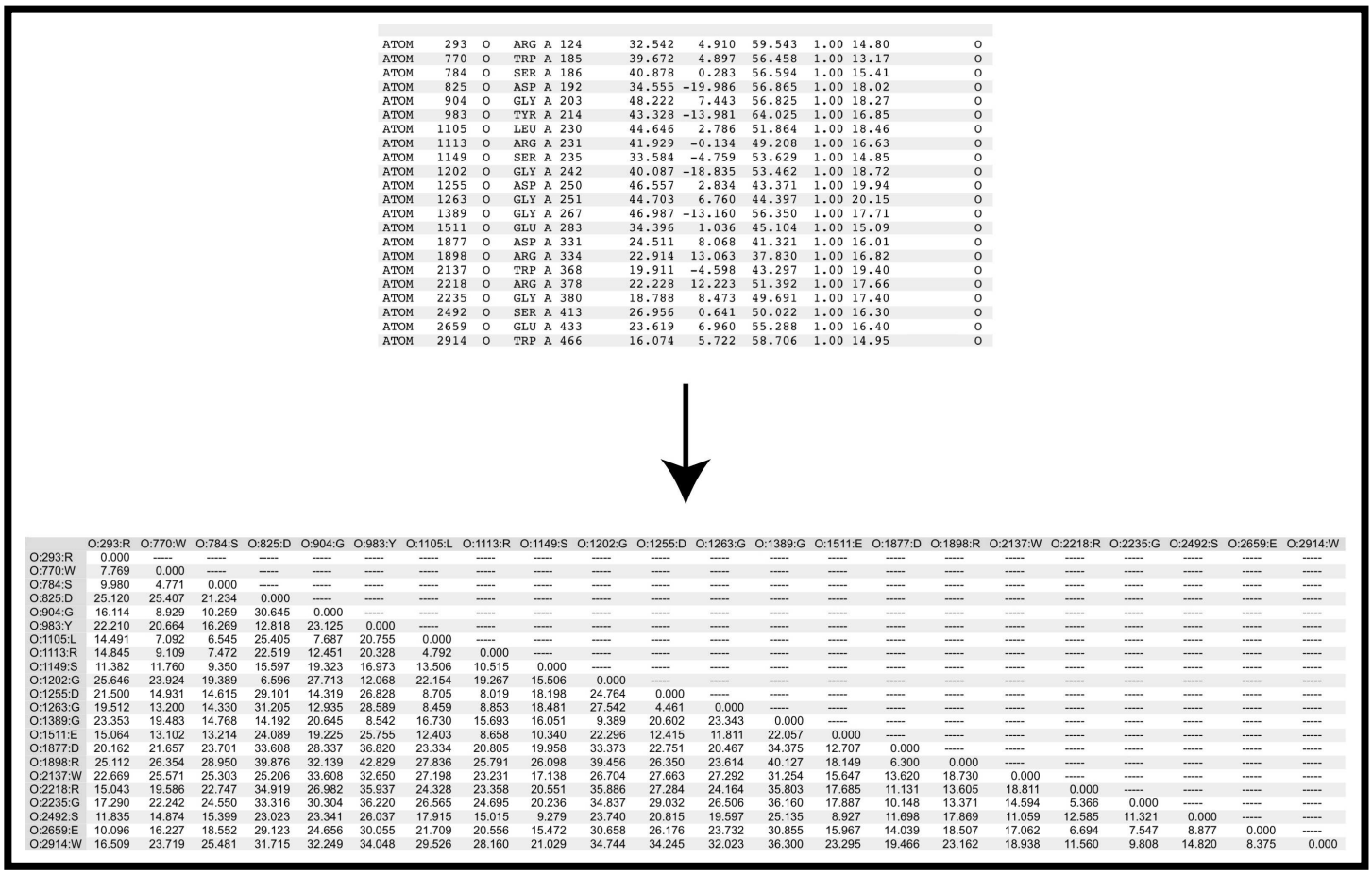

```
ATOM    293  O   ARG A 124      32.542   4.910  59.543  1.00 14.80           O
ATOM    770  O   TRP A 185      39.672   4.897  56.458  1.00 13.17           O
ATOM    784  O   SER A 186      40.878   0.283  56.594  1.00 15.41           O
ATOM    825  O   ASP A 192      34.555 -19.986  56.865  1.00 18.02           O
ATOM    904  O   GLY A 203      48.222   7.443  56.825  1.00 18.27           O
ATOM    983  O   TYR A 214      43.328 -13.981  64.025  1.00 16.85           O
ATOM   1105  O   LEU A 230      44.646   2.786  51.864  1.00 18.46           O
ATOM   1113  O   ARG A 231      41.929  -0.134  49.208  1.00 16.63           O
ATOM   1149  O   SER A 235      33.584  -4.759  53.629  1.00 14.85           O
ATOM   1202  O   GLY A 242      40.087 -18.835  53.462  1.00 18.72           O
ATOM   1255  O   ASP A 250      46.557   2.834  43.371  1.00 19.94           O
ATOM   1263  O   GLY A 251      44.703   6.760  44.397  1.00 20.15           O
ATOM   1389  O   GLY A 267      46.987 -13.160  56.350  1.00 17.71           O
ATOM   1511  O   GLU A 283      34.396   1.036  45.104  1.00 15.09           O
ATOM   1877  O   ASP A 331      24.511   8.068  41.321  1.00 16.01           O
ATOM   1898  O   ARG A 334      22.914  13.063  37.830  1.00 16.82           O
ATOM   2137  O   TRP A 368      19.911  -4.598  43.297  1.00 19.40           O
ATOM   2218  O   ARG A 378      22.228  12.223  51.392  1.00 17.66           O
ATOM   2235  O   GLY A 380      18.788   8.473  49.691  1.00 17.40           O
ATOM   2492  O   SER A 413      26.956   0.641  50.022  1.00 16.30           O
ATOM   2659  O   GLU A 433      23.619   6.960  55.288  1.00 16.40           O
ATOM   2914  O   TRP A 466      16.074   5.722  58.706  1.00 14.95           O
```

	O:293:R	O:770:W	O:784:S	O:825:D	O:904:G	O:983:Y	O:1105:L	O:1113:R	O:1149:S	O:1202:G	O:1255:D	O:1263:G	O:1389:G	O:1511:E	O:1877:D	O:1898:R	O:2137:W	O:2218:R	O:2235:G	O:2492:S	O:2659:E	O:2914:W
O:293:R	0.000	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
O:770:W	7.769	0.000	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
O:784:S	9.980	4.771	0.000	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
O:825:D	25.120	25.407	21.234	0.000	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
O:904:G	16.114	8.929	10.259	30.645	0.000	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
O:983:Y	22.210	20.664	16.269	12.818	23.125	0.000	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
O:1105:L	14.491	7.092	6.545	25.405	7.687	20.755	0.000	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
O:1113:R	14.845	9.109	7.472	22.519	12.451	20.328	4.792	0.000	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
O:1149:S	11.382	11.760	9.350	15.597	19.323	16.973	13.506	10.515	0.000	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
O:1202:G	25.646	23.924	19.389	6.596	27.713	12.068	22.154	19.267	15.506	0.000	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
O:1255:D	21.500	14.931	14.615	29.101	14.319	26.828	8.705	8.019	18.198	24.764	0.000	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
O:1263:G	19.512	13.200	14.330	31.205	12.935	28.589	8.459	8.853	18.481	27.542	4.461	0.000	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
O:1389:G	23.353	19.483	14.768	14.192	20.645	8.542	16.730	15.693	16.051	9.389	20.602	23.343	0.000	-----	-----	-----	-----	-----	-----	-----	-----	-----
O:1511:E	15.064	13.102	13.214	24.089	19.225	25.755	12.403	8.658	10.340	22.296	12.415	11.811	22.057	0.000	-----	-----	-----	-----	-----	-----	-----	-----
O:1877:D	20.162	21.657	23.701	33.608	28.337	36.820	23.334	20.805	19.958	33.373	22.751	20.467	34.375	12.707	0.000	-----	-----	-----	-----	-----	-----	-----
O:1898:R	25.112	26.354	28.950	39.876	32.139	42.829	27.836	25.791	26.098	39.456	26.350	23.614	40.127	18.149	6.300	0.000	-----	-----	-----	-----	-----	-----
O:2137:W	22.669	25.571	25.303	25.206	33.608	32.650	27.198	23.231	17.138	26.704	27.663	27.292	31.254	15.647	13.620	18.730	0.000	-----	-----	-----	-----	-----
O:2218:R	15.043	19.586	22.747	34.919	26.982	35.937	24.328	23.358	20.551	35.886	27.284	24.164	35.803	17.685	11.131	13.605	18.811	0.000	-----	-----	-----	-----
O:2235:G	17.290	22.242	24.550	33.316	30.304	36.220	26.565	24.695	20.236	34.837	29.032	26.506	36.160	17.887	10.148	13.371	14.594	5.366	0.000	-----	-----	-----
O:2492:S	11.835	14.874	15.399	23.023	23.341	26.037	17.915	15.015	9.279	23.740	20.815	19.597	25.135	8.927	11.698	17.869	11.059	12.585	11.321	0.000	-----	-----
O:2659:E	10.096	16.227	18.552	29.123	24.656	30.055	21.709	20.556	15.472	30.658	26.176	23.732	30.855	15.967	14.039	18.507	17.062	6.694	7.547	8.877	0.000	-----
O:2914:W	16.509	23.719	25.481	31.715	32.249	34.048	29.526	28.160	21.029	34.744	34.245	32.023	36.300	23.295	19.466	23.162	18.938	11.560	9.808	14.820	8.375	0.000

dist Overview

DIST

dist Overview

dist creates a distance matrix from a points list, generating a lower triangle matrix with distances between all the points, a zero-valued diagonal, and an upper triangle matrix with hyphens or zeroes (e.g. '---' or '0.00'). There are options for specifying upper triangle contents, handling input and output labels, and output format. dist can optionally parse a PDB file, and has options for specifying user defined output atom labels.

dist Help Output (“dist -h” output)

```
NAME

  dist (version 1.0.2) -- creates distance matrix from points list

SYNOPSIS

  dist [options]

  CHARACTER OPTION_____KEYWORD OPTION________DESCRIPTION_____________________________DEFAULT____

  Options for input:

  -i <filename> .... --input=<filename> .... input points list filename ........... stdin
  -n ............... --no_input_labels ..... input points list has no labels ...... has labels

  Options for output:

  -o <filename> .... --output=<filename> ... output distance matrix filename ...... stdout
  -f #.#  .......... --format=#.# .......... real number format (width.precision) . 5.3
  -s # ............. --spaces=# ............. separate fields with # spaces ........ 0 (tabs used)
  -t ............... --truncate_labels ..... action to fit col width to labels .... no truncation
  -x ............... --no_output_labels .... do not output labels .................. output labels
  -z ............... --upper_zeroes ........ fill upper matrix with zeroes ........ '---'

  Options for PDB input and atom label output:

  -a [<labelfmt>] .. --atom_labels ......... input points list is PDB file ........ not PDB file
                     --atom_labels=<labelfmt>
     <labelfmt> characters specify atom label content ............................. '@:#:*'
         @ _________________ atom name _____________________ <= 3 characters
         # _________________ atom serial number __________ <= 5 digits
         & _________________ residue name ________________    3 characters
         * _________________ residue name ________________    1 character
         ? _________________ residue sequence # __________ <= 4 digits
         % _________________ chain identifier _____________    1 character

  Other options:

  -d ............... --info ................. outputs processing info to stderr .... no info
  -h ............... --help ................. prints help (Enter 'dist -h' for help.)
                     --license ............. prints license terms for dist.

DESCRIPTION

  dist creates a distance matrix from a points list, generating a lower triangle matrix
  with distances between all the points, a zero-valued diagonal, and an upper triangle
  matrix with either hyphens or zeroes (e.g. '---' or '0.00').

  By default, input comes from stdin and output goes to stdout.
  Option '--input=' ('-i') allows command line specification of the input file.
  Option '--output=' ('-o') allows command line specification of the output file.
  Errors and warnings go to stderr.

  The points list should consist of points on separate lines as "[label] x y z", i.e.
  an optional label followed by 3 real numbers. Labels and real numbers must be separated
  by white space (i.e., spaces or tabs). Labels are assumed to be present in the input
  points list file by default. If there are no labels in the input points list file, then
  the option '--no_input_labels' ('-n') must be used and no input labels will be parsed.

  Labels are output as the topmost row and the leftmost column by default.
  The option '--no_output_labels' ('-x') can be used to suppress all labels from the output.
  In the case where option '--no_output_labels' ('-x') is not used (and labels are to be
  output by default) and option '--no_input_labels' ('-n') is used at the same time (and no
  labels are read in from input), then output labels will be generated as 'pt#'.

  Distance values are output as real numbers. The option '--format=' ('-f') must be followed
  by an option value specifying the output format as 'mmm.ddd', where 'mmm' is the minimum
  field width for the entire real number, and where 'ddd' is the precision. The default
  format is '5.3', where the minimum field width for the entire number is 5 characters,
  and there are 3 digits following the decimal point.

  By default, tabs delimit output columns and spaces are not output. The option '--spaces='
  ('-s') specifies that spaces will be output to delimit column values instead of tabs; the
  option '--spaces=' ('-s') must be followed by an integer option value specifying the number
  of spaces to be used.
```

If spaces are specified to be used instead of tabs, column width can either be expanded to the size of each label associated with that individual column or labels can be truncated to a common column size. The default behaviour is to expand any specific column width to fit its label. The option '--truncate_labels' ('-t') truncates, if necessary, the labels' to fit a common column size.

By default, hypens (i.e., '---') are output for the values of the upper triangle matrix. Option '--upper_zeroes' ('-z') changes these output values to zeroes (e.g., '0.00').

Option '--atom_labels=' ('-a') allows parsing of an atom list provided in 'PDB' file format. An optional accompanying option value specifies the label format, i.e., the content of the labels. Six reserved characters are used to specify substitution with specific fields from 'ATOM' or 'HETATM' pdb lines:

Char	Substitution	Size
@	... atom name	<= 3 char output
#	... atom serial number	<= 5 digits output
%	... chain identifier	1 char output
&	... residue name	3 char output
*	... residue name	1 char output
?	... residue sequence number ...	<= 4 digits output

All other characters specified in the option value will be directly used in each label. Labels will be written out in the order of the position of all characters in the option value. When option '--atom_labels=' ('-a') is used without an option value, the default label format specification is '@:#:*', and would produce labels that look similar to 'NH1:1171:R'. Note: If you use option '--atom_labels=' ('-a') without an accompanying option value, make sure to put '--atom_labels=' ('-a') at the end of the command. Reserved characters can be directly used without being substituted by: (1) adding single quotes to front and back of the label format option value, and also (2) using a backslash in front of the reserved characters that are intended to be directly used without substitution; e.g., "-a 'ATOM\##'" will produce labels that look similar to 'ATOM#1171'. Note: Always use single quotes on front and back of the label format option value; this will keep the reserved characters from being used as unix shell directives.

Option '--info' ('-d') is used to output, to stderr, processing information: number of points read, the list of points, and completion statement. No processing information is output by default.

Option '--help' ('-h') prints this help.

EXAMPLES

The following command line would read input, including labels, from the file 'points_list' and write a new file, named 'distance_matrix', with the contents of a labelled, tab-delimited distance matrix.

With keyword options:

```
dist --input=points_list --output=distance_matrix
```

With character options:

```
dist -i points_list -o distance_matrix
```

The following command line would read input, including labels, from the file 'points_list' and write a new file, named 'distance_matrix', with the contents of a labelled, space-delimited distance matrix.

With keyword options:

```
dist --input=points_list --output=distance_matrix --spaces=2
```

With character options:

```
dist -i points_list -o distance_matrix -s 2
```

The following command line would read input from the file 'points_list' (a file not containing labels) and write a new file, named 'distance_matrix', with the contents of a space-delimited distance matrix with no labels, and zero values for the upper triangle matrix.

With keyword options:

```
dist --input=points_list --output=distance_matrix --spaces=2            \
     --no_input_labels   --no_output_labels       --upper_zeroes
```

With character options:

```
dist -i points_list -o distance_matrix -s 2  -n -x -z
```

```
  The following command line would read input from the file 'atoms.pdb' and write a new file,
  named 'distance_matrix', with the contents of a tab-delimited distance matrix with labels
  that look similar to 'NH1:1171:R' (by default).

     With keyword options:

        dist --input=atoms.pdb --output=distance_matrix --atom_labels

     With character options:

        dist -i atoms.pdb -o distance_matrix -a

LICENSE INFORMATION

  dist is a software program from Arthur Weininger (www.weiningerworks.com).
  dist is subject to a license; use the keyword option '--license' in order to view
  the license terms. Your use of this software contitutes an agreement to the
  license terms. Do not use this software if you do not agree to the license terms.
```

---

dist Tutorial

The **dist and deviation Tutorial Page** gives examples of using **deviation.**
