```
DOCKED: ATOM     47  H   LIG    1      -25.370   6.782   5.989 +0.03
+0.06    +0.210 HD
DOCKED: ENDBRANCH  38  43
DOCKED: BRANCH  39  40
DOCKED: ATOM     48  C   LIG    1      -26.548   8.482   4.844 -0.00
+0.07    +0.190 C
DOCKED: BRANCH  40  41
DOCKED: ATOM     49  O   LIG    1      -27.176   8.397   4.071 +0.00 -
0.14    -0.392 OA
DOCKED: ATOM     50  H   LIG    1      -27.326   8.897   3.736 +0.00
+0.08    +0.210 HD
DOCKED: ENDBRANCH  40  41
DOCKED: ENDBRANCH  39  40
DOCKED: BRANCH  37  45
DOCKED: ATOM     51  O   LIG    1      -23.481   6.889   5.074 -0.10 -
0.07    -0.341 OA
DOCKED: BRANCH  45  46
DOCKED: ATOM     52  C   LIG    1      -23.388   6.110   4.454 -0.15
+0.07    +0.283 C
DOCKED: ATOM     53  C   LIG    1      -23.628   5.191   4.766 -0.21
+0.03    +0.201 C
DOCKED: ATOM     54  C   LIG    1      -23.536   4.412   4.146 -0.28
+0.04    +0.179 C
DOCKED: ATOM     55  C   LIG    1      -23.203   4.552   3.213 -0.21
+0.07    +0.185 C
DOCKED: ATOM     56  C   LIG    1      -22.963   5.471   2.901 -0.21
+0.10    +0.260 C
DOCKED: ATOM     57  O   LIG    1      -23.055   6.250   3.521 -0.17 -
0.12    -0.332 OA
DOCKED: BRANCH  50  51
DOCKED: ATOM     58  C   LIG    1      -22.630   5.611   1.969 -0.14
+0.15    +0.337 C
DOCKED: ATOM     59  O   LIG    1      -23.263   5.902   1.250 -0.09 -
0.11    -0.248 OA
DOCKED: BRANCH  51  53
DOCKED: ATOM     60  O   LIG    1      -21.665   5.461   1.754 -0.13 -
0.22    -0.479 OA
DOCKED: ATOM     61  H   LIG    1      -21.489   4.944   1.461 +0.10
+0.13    +0.295 HD
DOCKED: ENDBRANCH  51  53
DOCKED: ENDBRANCH  50  51
DOCKED: BRANCH  49  55
DOCKED: ATOM     62  O   LIG    1      -23.110   3.773   2.593 -0.04 -
0.16    -0.386 OA
DOCKED: ATOM     63  H   LIG    1      -23.517   3.695   2.131 +0.07
+0.09    +0.210 HD
DOCKED: ENDBRANCH  49  55
DOCKED: BRANCH  48  57
DOCKED: ATOM     64  O   LIG    1      -23.776   3.493   4.458 -0.23 -
0.07    -0.386 OA
DOCKED: ATOM     65  H   LIG    1      -23.342   3.126   4.706 +0.00
+0.02    +0.210 HD
DOCKED: ENDBRANCH  48  57
DOCKED: BRANCH  47  59
```

```
DOCKED: ATOM      66  O   LIG     1      -23.961   5.050   5.699 -0.13 -
0.01    -0.384 OA
DOCKED: ATOM      67  H   LIG     1      -24.570   5.045   5.813 +0.06
+0.02    +0.210 HD
DOCKED: ENDBRANCH  47  59
DOCKED: ENDBRANCH  45  46
DOCKED: ENDBRANCH  37  45
DOCKED: ENDBRANCH   1  35
DOCKED: TORSDOF 24
DOCKED: TER
DOCKED: ENDMDL
```

```
DPF> analysis                              # perform a ranked cluster
analysis
```

CLUSTER ANALYSIS OF CONFORMATIONS

Number of conformations = 50

RMSD cluster analysis will be performed using the ligand atoms only (67 / 67 total atoms).

Outputting structurally similar clusters, ranked in order of increasing energy.

Number of distinct conformational clusters found = 49, out of 50 runs,
Using an rmsd-tolerance of 2.0 A

CLUSTERING HISTOGRAM

Clus-ter Rank	Lowest Binding Energy	Run	Mean Binding Energy	Num in Clus	Histogram 5 10 15 20 25 30 35
1	-4.71	44	-4.71	1	#
2	-4.68	30	-4.68	1	#
3	-4.25	40	-4.25	1	#
4	-3.75	3	-3.75	1	#
5	-3.35	12	-3.35	1	#

```
   6 |      -3.24 |  20 |      -3.24 |    1 |#
   7 |      -3.03 |  29 |      -3.03 |    1 |#
   8 |      -2.72 |  26 |      -2.72 |    1 |#
   9 |      -2.69 |   9 |      -2.69 |    1 |#
  10 |      -2.39 |  23 |      -2.04 |    2 |##
  11 |      -2.31 |  41 |      -2.31 |    1 |#
  12 |      -2.17 |  49 |      -2.17 |    1 |#
  13 |      -2.06 |   6 |      -2.06 |    1 |#
  14 |      -1.86 |  13 |      -1.86 |    1 |#
  15 |      -1.84 |  17 |      -1.84 |    1 |#
  16 |      -1.71 |  25 |      -1.71 |    1 |#
  17 |      -1.53 |  19 |      -1.53 |    1 |#
  18 |      -1.39 |  21 |      -1.39 |    1 |#
  19 |      -1.27 |   4 |      -1.27 |    1 |#
  20 |      -1.24 |  37 |      -1.24 |    1 |#
  21 |      -1.15 |  45 |      -1.15 |    1 |#
  22 |      -1.12 |  38 |      -1.12 |    1 |#
  23 |      -1.10 |  42 |      -1.10 |    1 |#
  24 |      -1.04 |  31 |      -1.04 |    1 |#
  25 |      -0.93 |  16 |      -0.93 |    1 |#
  26 |      -0.85 |  39 |      -0.85 |    1 |#
  27 |      -0.70 |  11 |      -0.70 |    1 |#
  28 |      -0.69 |   2 |      -0.69 |    1 |#
  29 |      -0.51 |   1 |      -0.51 |    1 |#
  30 |      -0.47 |  18 |      -0.47 |    1 |#
  31 |      -0.46 |  15 |      -0.46 |    1 |#
  32 |      -0.37 |  35 |      -0.37 |    1 |#
  33 |      -0.31 |  28 |      -0.31 |    1 |#
  34 |      -0.30 |  27 |      -0.30 |    1 |#
  35 |      +0.23 |  43 |      +0.23 |    1 |#
  36 |      +0.32 |  24 |      +0.32 |    1 |#
  37 |      +0.54 |  46 |      +0.54 |    1 |#
  38 |      +0.57 |  33 |      +0.57 |    1 |#
  39 |      +0.73 |  50 |      +0.73 |    1 |#
  40 |      +0.79 |  34 |      +0.79 |    1 |#
  41 |      +0.81 |  10 |      +0.81 |    1 |#
  42 |      +0.94 |  36 |      +0.94 |    1 |#
  43 |      +0.96 |   8 |      +0.96 |    1 |#
  44 |      +1.25 |   7 |      +1.25 |    1 |#
  45 |      +1.38 |  48 |      +1.38 |    1 |#
  46 |      +1.53 |  47 |      +1.53 |    1 |#
  47 |      +1.55 |  22 |      +1.55 |    1 |#
  48 |      +1.63 |  32 |      +1.63 |    1 |#
  49 |      +1.81 |  14 |      +1.81 |    1 |#
_____|____________|_____|____________|_____|_____________________________________
_______
```

Number of multi-member conformational clusters found = 1, out of 50 runs.

RMSD TABLE

_____

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	44	-4.71	0.00	21.54	RANKING
2	1	30	-4.68	0.00	53.66	RANKING
3	1	40	-4.25	0.00	35.75	RANKING
4	1	3	-3.75	0.00	33.53	RANKING
5	1	12	-3.35	0.00	41.14	RANKING
6	1	20	-3.24	0.00	42.06	RANKING
7	1	29	-3.03	0.00	31.46	RANKING
8	1	26	-2.72	0.00	32.54	RANKING
9	1	9	-2.69	0.00	13.19	RANKING
10	1	23	-2.39	0.00	35.22	RANKING
10	2	5	-1.69	1.80	35.16	RANKING
11	1	41	-2.31	0.00	11.37	RANKING
12	1	49	-2.17	0.00	15.87	RANKING
13	1	6	-2.06	0.00	41.69	RANKING
14	1	13	-1.86	0.00	15.39	RANKING
15	1	17	-1.84	0.00	33.37	RANKING
16	1	25	-1.71	0.00	27.20	RANKING
17	1	19	-1.53	0.00	24.71	RANKING
18	1	21	-1.39	0.00	53.44	RANKING
19	1	4	-1.27	0.00	35.23	RANKING
20	1	37	-1.24	0.00	13.71	RANKING
21	1	45	-1.15	0.00	32.24	RANKING
22	1	38	-1.12	0.00	33.73	RANKING
23	1	42	-1.10	0.00	57.49	RANKING
24	1	31	-1.04	0.00	28.64	RANKING
25	1	16	-0.93	0.00	11.09	RANKING
26	1	39	-0.85	0.00	18.63	RANKING
27	1	11	-0.70	0.00	34.03	RANKING
28	1	2	-0.69	0.00	52.15	RANKING
29	1	1	-0.51	0.00	30.64	RANKING
30	1	18	-0.47	0.00	46.03	RANKING
31	1	15	-0.46	0.00	18.53	RANKING
32	1	35	-0.37	0.00	29.24	RANKING
33	1	28	-0.31	0.00	38.64	RANKING
34	1	27	-0.30	0.00	40.33	RANKING
35	1	43	+0.23	0.00	41.83	RANKING
36	1	24	+0.32	0.00	29.38	RANKING
37	1	46	+0.54	0.00	37.79	RANKING
38	1	33	+0.57	0.00	41.34	RANKING
39	1	50	+0.73	0.00	29.52	RANKING
40	1	34	+0.79	0.00	24.68	RANKING
41	1	10	+0.81	0.00	48.14	RANKING
42	1	36	+0.94	0.00	55.52	RANKING
43	1	8	+0.96	0.00	34.67	RANKING
44	1	7	+1.25	0.00	44.27	RANKING
45	1	48	+1.38	0.00	27.08	RANKING
46	1	47	+1.53	0.00	36.70	RANKING
47	1	22	+1.55	0.00	55.80	RANKING
48	1	32	+1.63	0.00	36.28	RANKING
49	1	14	+1.81	0.00	12.27	RANKING

_____

INFORMATION ENTROPY ANALYSIS FOR THIS CLUSTERING

Information entropy for this clustering = 0.99 (rmstol = 2.00 Angstrom)

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STATISTICAL MECHANICAL ANALYSIS

```
Partition function, Q =    50.08            at Temperature, T = 298.15 K
Free energy,        A ~ -2318.78 kcal/mol   at Temperature, T = 298.15 K
Internal energy,    U =    -0.98 kcal/mol   at Temperature, T = 298.15 K
Entropy,            S =     7.77 kcal/mol/K at Temperature, T = 298.15 K
```

_____

LOWEST ENERGY DOCKED CONFORMATION from EACH CLUSTER

Keeping original residue number (specified in the input PDBQ file) for outputting.

```
MODEL       44
USER    Run = 44
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 1
USER
USER    RMSD from reference structure       = 21.544 A
USER
USER    Estimated Free Energy of Binding    =   -4.71 kcal/mol
[=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  350.71 uM (micromolar)
[Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =   -8.29 kcal/mol
USER        vdW + Hbond + desolv Energy     =   -8.02 kcal/mol
USER        Electrostatic Energy            =   -0.27 kcal/mol
USER    (2) Final Total Internal Energy     =  +61.27 kcal/mol
USER    (3) Torsional Free Energy           =   +3.58 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =  +61.27 kcal/mol
USER
USER
USER
```

```
USER    DPF = ./try2.dpf
USER    NEWDPF move    CID_3084050LIGNAD.pdbqt
USER    NEWDPF about   6.867000 -0.098800 0.000000
USER    NEWDPF tran0   -6.016331 -23.019099 6.014919
USER    NEWDPF axisangle0    -0.062840 -0.786580 -0.614283 -63.523743
USER    NEWDPF quaternion0   -0.033078 -0.414048 -0.323353 -0.850243
USER    NEWDPF dihe0   73.72 89.70 91.33 5.25 139.27 -138.51 93.63 105.49
-58.86 -94.48 100.29 150.59 -34.42 -126.40 -88.56 86.89 -88.91 90.43 -
59.93 -86.70 -89.51 49.87 76.86 53.37
USER
USER                                x       y       z    vdW   Elec
q     RMS
ATOM      1  O   LIG    1       -6.059 -22.094   5.513 -0.08 -0.08    -
0.340    21.544
ATOM      2  C   LIG    1       -5.382 -22.152   6.247 -0.12 +0.04
+0.192    21.544
ATOM      3  C   LIG    1       -5.565 -21.722   7.131 -0.16 +0.05
+0.260    21.544
ATOM      4  O   LIG    1       -4.889 -21.780   7.865 -0.09 -0.07    -
0.331    21.544
ATOM      5  C   LIG    1       -4.029 -22.269   7.715 -0.06 +0.05
+0.283    21.544
ATOM      6  C   LIG    1       -3.846 -22.699   6.831 -0.05 +0.04
+0.201    21.544
ATOM      7  C   LIG    1       -4.522 -22.641   6.097 -0.07 +0.03
+0.180    21.544
ATOM      8  C   LIG    1       -6.425 -21.234   7.281 -0.19 +0.08
+0.337    21.544
ATOM      9  O   LIG    1       -6.494 -20.262   7.056 -0.10 -0.08    -
0.248    21.544
ATOM     10  O   LIG    1       -7.215 -21.718   7.657 -0.13 -0.05    -
0.479    21.544
ATOM     11  H   LIG    1       -7.694 -21.862   7.290 +0.07 +0.04
+0.295    21.544
ATOM     12  O   LIG    1       -2.986 -23.187   6.681 +0.00 -0.07    -
0.384    21.544
ATOM     13  H   LIG    1       -2.946 -23.792   6.811 +0.03 +0.03
+0.210    21.544
ATOM     14  O   LIG    1       -4.339 -23.071   5.213 -0.00 -0.08    -
0.386    21.544
ATOM     15  H   LIG    1       -4.521 -23.654   5.109 +0.05 +0.04
+0.210    21.544
ATOM     16  O   LIG    1       -3.352 -22.327   8.449 -0.03 -0.07    -
0.341    21.544
ATOM     17  C   LIG    1       -3.631 -22.620   9.364 -0.14 +0.03
+0.177    21.544
ATOM     18  C   LIG    1       -3.939 -21.944  10.033 -0.20 +0.04
+0.176    21.544
ATOM     19  C   LIG    1       -4.217 -22.237  10.948 -0.29 +0.03
+0.178    21.544
ATOM     20  O   LIG    1       -4.188 -23.206  11.193 -0.20 -0.00    -
0.341    21.544
ATOM     21  C   LIG    1       -3.879 -23.882  10.524 -0.20 -0.00
+0.270    21.544
```