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=== DAMMIN53 started at          25-Jan-10    21:30:02
Computation mode ..... : Fast
Project identifier ..... : r3Yju9
  Project description: gnom_f.out /sy P6 /mo F /an Oblate /lo r3Yju9
Random sequence initialized from ..... : 213002
GNOM file name ..... : gnom_f.out
** Information read from the GNOM file **
Data set title:   Data divided by constant (Conc)

Raw data file name: trap_f.dat
Maximum diameter of the particle ..... : 130.0
  Solution at Alpha = 0.499E+01  Rg : 0.363E+02  I(0) : 0.396E+02
Radius of gyration read ..... : 36.30
Number of GNOM data points ..... : 525
Maximum s value [1/angstrom] ..... : 0.3189
Number of Shannon channels ..... : 13.20
Number of knots in the curve to fit ..... : 26
*** Warning: constant reduced to avoid oversubtraction
A constant was subtracted ..... : 5.826e-2
Maximum order of harmonics ..... : 10
Point symmetry of the particle ..... : P6
Sphere diameter [Angstrom] ..... : 130.0
Packing radius of dummy atoms ..... : 3.200
Radius of the sphere generated ..... : 65.00
Number of dummy atoms ..... : 5611
Number of equivalent positions ..... : 6
Expected particle anisotropy ..... : Oblate
Excluded volume per atom ..... : 185.5
Radius of 1st coordination sphere ..... : 9.024
Minimum number of contacts ..... : 8
Maximum number of contacts ..... : 18
Looseness penalty weight ..... : 3.000e-3
No of non-solvent atoms ..... : 5611
Initial DAM looseness ..... : 3.714e-4
Disconnectivity penalty weight ..... : 3.000e-3
Initial DAM # of graphs ..... : 1
Discontiguity value ..... : 0.0
Center of the initial DAM: 0.0000 0.0000 0.0000
Peripheral penalty weight ..... : 0.3000
Peripheral penalty value ..... : 0.6074
Looseness fixing threshold ..... : 5.000e-2
R-factor fixing threshold ..... : 1.500e-2
*** The structure was randomized ***
No of non-solvent atoms ..... : 2905
Randomized DAM looseness ..... : 5.211e-2
Randomized DAM # of graphs ..... : 1
Discontiguity value ..... : 0.0
Randomized peripheral penalty value ..... : 0.6174
Anisotropy penalty weight ..... : 0.1000
Weight: 0=s^2, 1=Emphas.s->0, 2=Log ..... : 1
*** Porod weight with emphasis at low s ***
Initial scale factor ..... : 2.124e-10
Scale factor fixed (Y=Yes, N=No) ..... : N
Initial R^2 factor ..... : 0.5428

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Initial R factor ..... : 0.7368
Initial penalty ..... : 0.1854
Initial fVal ..... : 0.7282
Variation of the target function ..... : 3.916e-4
CPU per function call, seconds ..... : 1.520e-3
Initial annealing temperature ..... : 1.175e-3
Annealing schedule factor ..... : 0.9000
# of independent atoms to modify ..... : 1
Max # of iterations at each T ..... : 98192
Max # of successes at each T ..... : 9819
Min # of successes to continue ..... : 32
Max # of annealing steps ..... : 100
==== Simulated annealing procedure started ====
j: 1 T: 0.117E-02 Suc: 9819 Eva: 15997 CPU: 0.197E+02 SqF: 0.6846
Rf: 0.58158 Los:0.1276 Dis:0.0771 Per: 0.4327 Sca: 0.502E-09
j: 2 T: 0.106E-02 Suc: 9819 Eva: 71674 CPU: 0.475E+02 SqF: 0.3018
Rf: 0.10579 Los:0.2147 Dis:0.2497 Per: 0.2908 Sca: 0.317E-08
j: 3 T: 0.952E-03 Suc: 9819 Eva: 135320 CPU: 0.764E+02 SqF: 0.2891
Rf: 0.09125 Los:0.2565 Dis:0.2716 Per: 0.3031 Sca: 0.321E-08
j: 4 T: 0.857E-03 Suc: 9819 Eva: 198377 CPU: 0.105E+03 SqF: 0.2710
Rf: 0.09812 Los:0.2686 Dis:0.3365 Per: 0.2835 Sca: 0.383E-08
j: 5 T: 0.771E-03 Suc: 9819 Eva: 266685 CPU: 0.135E+03 SqF: 0.2515
Rf: 0.06810 Los:0.2193 Dis:0.2168 Per: 0.2908 Sca: 0.338E-08
j: 6 T: 0.694E-03 Suc: 9819 Eva: 335189 CPU: 0.165E+03 SqF: 0.2410
Rf: 0.05915 Los:0.3115 Dis:0.3493 Per: 0.2968 Sca: 0.436E-08
j: 7 T: 0.624E-03 Suc: 9819 Eva: 405483 CPU: 0.195E+03 SqF: 0.2228
Rf: 0.05175 Los:0.2268 Dis:0.2668 Per: 0.2851 Sca: 0.362E-08
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