

=== GASBOR Version 2.2i build 21.06.06 started on 25-Jan-10 21:26:32

Computation mode ..... : User  
Project identifier ..... : GlkJrk  
Project description: gnom\_f.out 145 /sy P6 /lo GlkJrk  
Random sequence initialized from ..... : 212632  
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

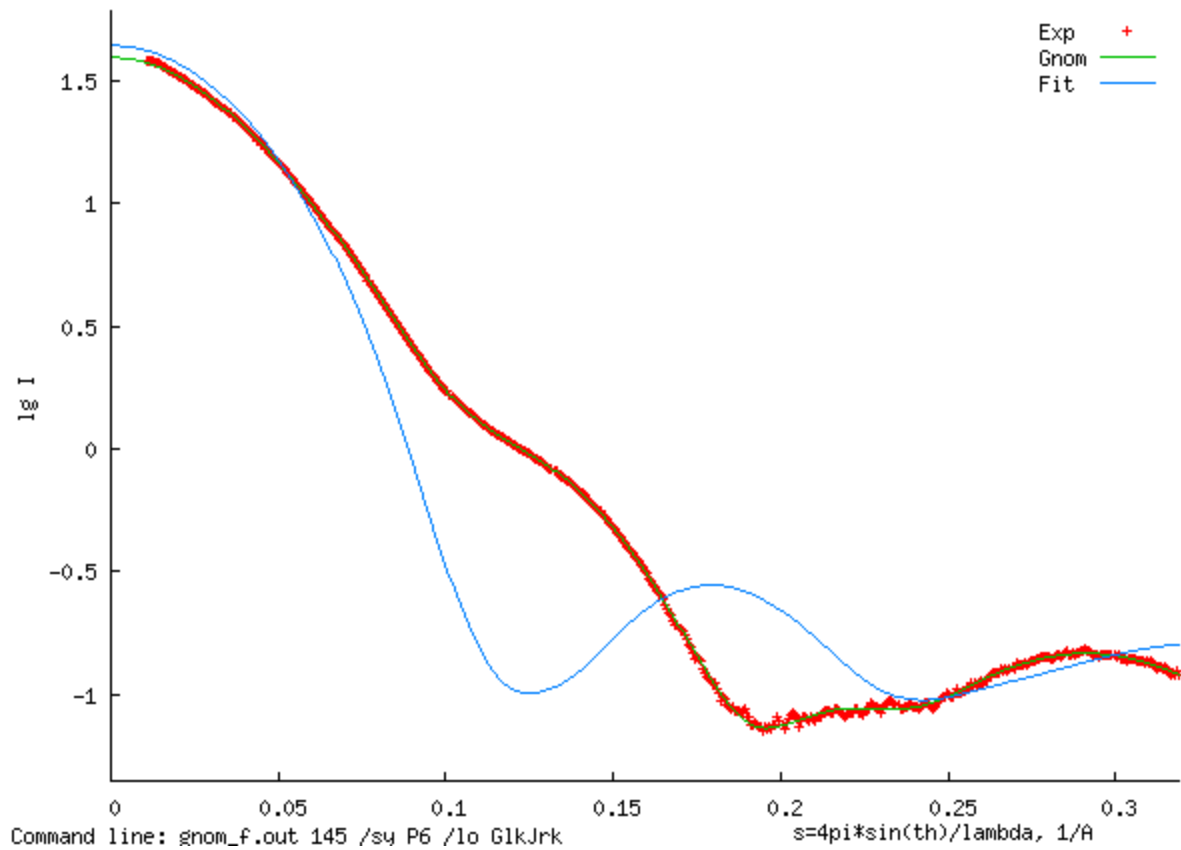
Maximum diameter of the particle ..... : 130.0  
Solution at Alpha = 0.499E+01 Rg : 0.363E+02 I(0) : 0.396E+02  
Radius of gyration ..... : 36.30  
Number of GNOM data points ..... : 525  
Maximum s value [1/angstrom] ..... : 0.3189  
Number of Shannon channels ..... : 13.20  
Number of knots in the curve to fit ..... : 26  
Point symmetry of the particle ..... : P6  
Number of equivalent positions ..... : 6  
Total number of residues ..... : 870  
Packing radius of dummy atoms ..... : 1.900  
Number of dummy waters ..... : 611  
Excluded volume per residue ..... : 28.73  
Radius of the search volume ..... : 65.00  
Histogram penalty weight ..... : 1.000e-3  
Bond length penalty weight ..... : 1.000e-2  
Discontiguity penalty weight ..... : 1.000e-2  
Peripheral penalty weight ..... : 1.000  
Expected particle anisotropy ..... : Unknown  
Contrast of the hydration layer ..... : 3.000e-2  
Histogram penalty value ..... : 39.42  
Bond length penalty value ..... : 1.529  
Initial DRM # of graphs ..... : 603  
Discontiguity value ..... : 2.674  
Peripheral penalty value ..... : 0.2496  
Weight: 0-2 = s<sup>2</sup>, 3-5 = s, 6 = log ..... : 2

\*\*\* Accounting for constant background \*\*\*

Initial scale factor ..... : 2.498e-7  
Constant background subtracted ..... : 5.613e-2  
Initial R<sup>2</sup> factor ..... : 0.1634  
Initial R factor ..... : 0.4042  
Initial penalty ..... : 0.3310  
Initial fVal ..... : 0.4944  
R-factor fixing threshold ..... : 0.0  
Fixing threshold for PenCha ..... : 0.0  
Fixing threshold for PenLen ..... : 0.0  
Initial annealing temperature ..... : 1.000e-3  
Annealing schedule factor ..... : 0.9000  
# of independent atoms to modify ..... : 1  
Max # of iterations at each T ..... : 60000  
Max # of successes at each T ..... : 6000  
Min # of successes to continue ..... : 60  
Max # of annealing steps ..... : 100

==== Simulated annealing procedure started ====

T: 0.100E-02 Rf:0.40417 Los: 39.42 Bnd: 1.529 Dis:2.6741 Per: 0.250



---