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SIMULAID: simulation setup and analysis utilities, written by Mihaly Mezei
Version 02/25/2022; Memory use=1287 Mb; Maximum number of input records=250000
M. Mezei, J. Comp. Chem., Vol 31, 2658-2668 (2010). DOI:10.1002/jcc.21551
NOTE: input prompts showing ? will yield an explanation by typing just a ?
NOTE: input prompts showing + will yield a tip by typing just a +
Conversion files found in directory /simulaid
WARNING: could not determine if this is a cluster headnode
         Functions requiring sizable CPU time should be run on a compute node

SELECT run type:
Print all menu and submenu <F>unctions - - - - - - - - - -  : f
Geometry <O>ptimization (orientation, smallest sphere) [3]  : o
<C>leanup (sort, renumber, regroup, round charges) - - - -  : c
<S>tructure file and type conversions [15] - - - - - - - -  : s
<T>rajectory file and type conversions [4] - - - - - - - -  : t
Atom <N>ame and residue name conversions [4] - - - - - - -  : n
Trajectory - str<U>cture file conversions (pack/unpack) [4] : u
Conformation <E>dit (trans/rot/cent/algn/add/del, etc.) [15]: e
<M>iscellaneous (seq, RTF, UHBD, tors., Amber sum, etc.)[7] : m
<A>nalyze (TRAJELIX, RMSD, H-bonds, CV, etc.) [17] - - - -  : a
Cluste<R> atoms or data defined by a distance matrix [2] -  : r
Make the input <P>redictable - - - - - - - - - - - - - - -  : p
Open <L>ogfile logging the keyboard inputs - - - - - - - -  : l
<Q>uit Simulaid  - - - - - - - - - - - - - - - - - - - - -  : q  l
"Open logfile logging the keyboard inputs" selected
Name of the log file=oop.inp
File oop.inp (formatted) opened on unit  45
Keyboard inputs will be logged in the file oop.inp
Do you want to make the quizzes predictable (y/n/?) [y]
Interactive quizzes will not depend on the data.
Default options will be used and a message will be printed

SELECT run type:
Print all menu and submenu <F>unctions - - - - - - - - - -  : f
Geometry <O>ptimization (orientation, smallest sphere) [3]  : o
<C>leanup (sort, renumber, regroup, round charges) - - - -  : c
<S>tructure file and type conversions [15] - - - - - - - -  : s
<T>rajectory file and type conversions [4] - - - - - - - -  : t
Atom <N>ame and residue name conversions [4] - - - - - - -  : n
Trajectory - str<U>cture file conversions (pack/unpack) [4] : u
Conformation <E>dit (trans/rot/cent/algn/add/del, etc.) [15]: e
<M>iscellaneous (seq, RTF, UHBD, tors., Amber sum, etc.)[7] : m
<A>nalyze (TRAJELIX, RMSD, H-bonds, CV, etc.) [17] - - - -  : a
Cluste<R> atoms or data defined by a distance matrix [2] -  : r
Make the input <P>redictable - - - - - - - - - - - - - - -  : p
Open <L>ogfile logging the keyboard inputs - - - - - - - -  : l
<Q>uit Simulaid  - - - - - - - - - - - - - - - - - - - - -  : q  o
"Geometry optimization (orientation, smallest sphere) [3]" selected

SELECT optimization type:
<S>mallest sphere calculation  - - - - - - - - - : s
O<P>timize orientation in bounding cube/rectangle: p
<O>ptimize orientation in a periodic cell  - - - : o
<Q>uit optimization  - - - - - - - - - - - - - - : q  p
"Optimize orientation in bounding cube/rectangle" selected
Name of the input STRUCTURE file=mcd.pdb
File mcd.pdb (formatted) opened on unit  10
The input format is established as PDB
The PDB format is found to be Brookhaven
Is that OK (y/n) [y]
The input format is established as Brookh. PDB
Do you have charges in the temperature factor column (y/n) [n]
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Name of the output file=mcd_oop.pdb
Opening file mcd_opt.pdb
If the file exists, do you want to overwrite it (y/n) [n] y
File mcd_opt.pdb (formatted) opened on unit  20
The output format is established as PDB
New file - Brookhaven PDB selected
The output format is established as Brookh. PDB
Do you want to change atomnames to Brookhaven form (y/n/?) [n]
Note: all heteroatoms will be kept and
      only the first of alternate records will be used
Do you want to read chemical symbols from col 77-78 (y/n) [y] n
TITLE MCD - Mast Cell Degranulating Peptide

SELECT MODEL record treatment:
<K>eep MODEL/ENDMDL records  - - - - - - - - - - - - - - -  : k (default)
<D>elete MODEL/ENDMDL records  - - - - - - - - - - - - - - -  : d
Change ENDMDL to <E>ND and delete MODEL records  - - - - -  : e
Change ENDMDL to <T>ER and delete MODEL records  - - - - -  : t
"Keep MODEL/ENDMDL records" selected
REMARK A. Buku, I. Keselman, D. Lupyan, M. Mezei and J.A. Price,
REMARK Chem. Biol. Drug Des, 72, 13-139 (2008).
REMARK DOI:10.1111/j.1747-0285.2008.00684.x
Atom name starting with two upper-case charcters(HG) found
Are both characters part of the chemical symbol (y/n) [n]
Number of atoms found in the input file=    378
Title read:
MCD - Mast Cell Degranulating Peptide
Do you want to replace the title (y/n/+) [n]
Solvent residue name in the input file [HOH]=
Number of solute atoms found=         378
NOTE: no solvent residue HOH was found
Number of residues=          22  solute residues=          22
NOTE: residue numbers are not consecutive
Number of hydrogens in the solute=         200
There are   108 backbone atoms and     270 putative side chain solute atoms
 1    A      1-   378 Resid    1-   22 Resix    1-   22 MW=   2595 <B>=    0.0
The solute contains   22 amino acid residues   0 nucleic acid residues
and     0 unclassified residues
The volume of the solute is estimated to be    3281.29 A^3
Volume of the protein (part) is estimated to be     3281.29 A^3
Dimensions of the solute:
Smallest, middle and largest X coordinate values= -10.8400  -0.2500  10.3400
Smallest, middle and largest Y coordinate values= -12.8900  -1.6750   9.5400
Smallest, middle and largest Z coordinate values= -10.7070   0.8710  12.4490
Volume of enclosing rectangle=    11000.66 A^3

SELECT Bond information source:
<C>oordinates of the input structure - - - - - - - - - - -  : c (default)
User-supplied Charmm <P>SF file (Xplor format) - - - - - -  : p
User-supplied Amber <T>op file - - - - - - - - - - - - - -  : t  c
"Coordinates of the input structure" selected
Do you want to change bond thresholds (y/n/+) [n]
   21 chiral CAs were found,    21 in L and     0 in D conformation
    1 achiral CAs were found (glycine)
Do you want to include hydrogens (y/n/?) [y]
Hydrogens will be included in the optimization

Do you want to fix one axis of the solute (y/n/?) [n]
Optimizing orientation to minimize the bounding cube/rectange
Number of optimization attempts requested [ 100,?]=?
    Optimization is repeated from different (randomy selected)
    starting configurations and the best result will be used
Number of optimization attempts requested [ 100,?]=50
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Tolerance for minimization [ 0.00001]=
Smallest, middle and largest X coordinate values= -10.8400  -0.2500  10.3400
Smallest, middle and largest Y coordinate values= -12.8900  -1.6750   9.5400
Smallest, middle and largest Z coordinate values= -10.7070   0.8710  12.4490
Volume of enclosing rectangle=    11000.66 A^3

SELECT box or rectangle:
Bounding <C>ube  - - - - - - - - - - - - - - - - - - - - - - - -  : c
Bounding <R>ectangle - - - - - - - - - - - - - - - - - - - - - -  : r (default)   r
"Bounding rectangle" selected
Do you want to select the longest axis (y/n) [n]
 === Initial box size=  21.18000  22.43000  23.15600 A volume= 0.11001E+05 A^3
--- Iteration  10 Objective function=-0.95546592E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.90571143E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.73814912E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.72902261E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.72397104E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.72381948E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.72366797E+04 A (tolerance=0.0000100)
--- Number of iterations=          71
Smallest, middle and largest X coordinate values= -10.2255  -0.9231   8.3793
Smallest, middle and largest Y coordinate values= -10.7250  -1.5460   7.6330
Smallest, middle and largest Z coordinate values=  -9.7673   0.8266  11.4206
Volume of enclosing rectangle=     7236.68 A^3
=== Trial   1: edge=  18.6048  18.3581  21.1879 A vol= 0.72366797E+04 A^3
--- Iteration  10 Objective function=-0.92878223E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.92282529E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.92204268E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.91918555E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.89097656E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.87558496E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.86866875E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.81441650E+04 A (tolerance=0.0000100)
--- Iteration  90 Objective function=-0.77502905E+04 A (tolerance=0.0000100)
--- Iteration 100 Objective function=-0.76893867E+04 A (tolerance=0.0000100)
--- Iteration 110 Objective function=-0.76658042E+04 A (tolerance=0.0000100)
--- Iteration 120 Objective function=-0.76656606E+04 A (tolerance=0.0000100)
--- Iteration 130 Objective function=-0.76590869E+04 A (tolerance=0.0000100)
--- Iteration 140 Objective function=-0.76587051E+04 A (tolerance=0.0000100)
--- Number of iterations=         144
Smallest, middle and largest X coordinate values= -11.3291  -0.8730   9.5831
Smallest, middle and largest Y coordinate values=  -7.9778   0.9073   9.7924
Smallest, middle and largest Z coordinate values=  -8.7800   1.5246  11.8292
Volume of enclosing rectangle=     7658.70 A^3
=== Trial   2: edge=  20.9122  17.7702  20.6092 A vol= 0.76587012E+04 A^3
--- Iteration  10 Objective function=-0.97817812E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.94873936E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.93527861E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.91811602E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.87327871E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.84203291E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.80730308E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.77760835E+04 A (tolerance=0.0000100)
--- Iteration  90 Objective function=-0.72781465E+04 A (tolerance=0.0000100)
--- Iteration 100 Objective function=-0.72681494E+04 A (tolerance=0.0000100)
--- Iteration 110 Objective function=-0.72644082E+04 A (tolerance=0.0000100)
--- Iteration 120 Objective function=-0.72443027E+04 A (tolerance=0.0000100)
--- Iteration 130 Objective function=-0.72389448E+04 A (tolerance=0.0000100)
--- Iteration 140 Objective function=-0.72368784E+04 A (tolerance=0.0000100)
--- Number of iterations=         145
Smallest, middle and largest X coordinate values= -10.7262  -1.5465   7.6333
Smallest, middle and largest Y coordinate values= -11.4217  -0.8277   9.7663
Smallest, middle and largest Z coordinate values=  -8.3788   0.9229  10.2247
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Volume of enclosing rectangle=     7236.83 A^3
=== Trial   3: edge=  18.3595  21.1880  18.6036 A vol= 0.72368296E+04 A^3
--- Iteration  10 Objective function=-0.81445664E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.77196875E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.74023364E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.73666616E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.72840947E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.72526567E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.72388828E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.72368130E+04 A (tolerance=0.0000100)
--- Iteration  90 Objective function=-0.72365703E+04 A (tolerance=0.0000100)
--- Number of iterations=          93
Smallest, middle and largest X coordinate values=  -8.3791   0.9240  10.2271
Smallest, middle and largest Y coordinate values= -10.7236  -1.5455   7.6326
Smallest, middle and largest Z coordinate values= -11.4208  -0.8268   9.7672
Volume of enclosing rectangle=     7236.48 A^3
=== Trial   4: edge=  18.6062  18.3561  21.1880 A vol= 0.72364766E+04 A^3
--- Iteration  10 Objective function=-0.82052031E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.76490151E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.76241333E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.76198120E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.76190049E+04 A (tolerance=0.0000100)
--- Number of iterations=          54
Smallest, middle and largest X coordinate values=  -9.4935  -0.6485   8.1964
Smallest, middle and largest Y coordinate values=  -9.3976   0.6059  10.6094
Smallest, middle and largest Z coordinate values= -11.4162  -0.6527  10.1109
Volume of enclosing rectangle=     7618.95 A^3
=== Trial   5: edge=  17.6899  20.0071  21.5271 A vol= 0.76189453E+04 A^3
--- Iteration  10 Objective function=-0.85737227E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.76093979E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.73965210E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.72701069E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.72545396E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.72407700E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.72376030E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.72374219E+04 A (tolerance=0.0000100)
--- Number of iterations=          81
Smallest, middle and largest X coordinate values=  -7.6327   1.5463  10.7252
Smallest, middle and largest Y coordinate values=  -9.7660   0.8268  11.4196
Smallest, middle and largest Z coordinate values=  -8.3839   0.9205  10.2250
Volume of enclosing rectangle=     7237.41 A^3
=== Trial   6: edge=  18.3579  21.1856  18.6088 A vol= 0.72374111E+04 A^3
--- Iteration  10 Objective function=-0.77477153E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.72927212E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.72787207E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.72397568E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.72381221E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.72367100E+04 A (tolerance=0.0000100)
--- Number of iterations=          69
Smallest, middle and largest X coordinate values= -10.7253  -1.5463   7.6327
Smallest, middle and largest Y coordinate values= -11.4210  -0.8270   9.7670
Smallest, middle and largest Z coordinate values=  -8.3790   0.9232  10.2254
Volume of enclosing rectangle=     7236.54 A^3
=== Trial   7: edge=  18.3581  21.1880  18.6044 A vol= 0.72365420E+04 A^3
--- Iteration  10 Objective function=-0.91707402E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.88348965E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.88171904E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.88099863E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.87576670E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.86977607E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.86913398E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.86852197E+04 A (tolerance=0.0000100)
--- Iteration  90 Objective function=-0.86823340E+04 A (tolerance=0.0000100)
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--- Iteration 100 Objective function=-0.86816328E+04 A (tolerance=0.0000100)
--- Number of iterations=         102
Smallest, middle and largest X coordinate values=  -8.9945   0.2227   9.4399
Smallest, middle and largest Y coordinate values=  -9.2994   1.1001  11.4997
Smallest, middle and largest Z coordinate values= -12.1629  -0.8416  10.4797
Volume of enclosing rectangle=     8681.63 A^3
=== Trial   8: edge=  18.4344  20.7991  22.6427 A vol= 0.86816328E+04 A^3
--- Iteration  10 Objective function=-0.82393916E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.74415278E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.73613262E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.72446396E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.72406533E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.72390659E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.72386035E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.72383687E+04 A (tolerance=0.0000100)
--- Number of iterations=          82
Smallest, middle and largest X coordinate values=  -7.6369   1.5562  10.7493
Smallest, middle and largest Y coordinate values= -10.2028  -0.9129   8.3770
Smallest, middle and largest Z coordinate values=  -9.7613   0.8331  11.4274
Volume of enclosing rectangle=     7238.32 A^3
=== Trial   9: edge=  18.3862  18.5798  21.1887 A vol= 0.72383242E+04 A^3
--- Iteration  10 Objective function=-0.87665049E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.87456670E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.87456670E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.87449658E+04 A (tolerance=0.0000100)
--- Number of iterations=          44
Smallest, middle and largest X coordinate values= -11.6680  -0.3351  10.9979
Smallest, middle and largest Y coordinate values=  -8.9986   0.2275   9.4536
Smallest, middle and largest Z coordinate values=  -9.5985   0.8561  11.3108
Volume of enclosing rectangle=     8744.97 A^3
=== Trial  10: edge=  22.6658  18.4521  20.9093 A vol= 0.87449658E+04 A^3
--- Iteration  10 Objective function=-0.76607314E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.76305972E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.76266597E+04 A (tolerance=0.0000100)
--- Number of iterations=          37
Smallest, middle and largest X coordinate values=  -9.6828  -0.7621   8.1587
Smallest, middle and largest Y coordinate values= -10.6041  -0.6022   9.3997
Smallest, middle and largest Z coordinate values= -10.2068   0.4774  11.1615
Volume of enclosing rectangle=     7626.26 A^3
=== Trial  11: edge=  17.8415  20.0038  21.3682 A vol= 0.76262627E+04 A^3
--- Iteration  10 Objective function=-0.88646113E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.78885947E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.77530176E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.76628330E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.74594019E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.72770337E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.72434229E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.72381826E+04 A (tolerance=0.0000100)
--- Iteration  90 Objective function=-0.72370371E+04 A (tolerance=0.0000100)
--- Iteration 100 Objective function=-0.72365649E+04 A (tolerance=0.0000100)
--- Number of iterations=         103
Smallest, middle and largest X coordinate values=  -9.7674   0.8266  11.4207
Smallest, middle and largest Y coordinate values= -10.2268  -0.9238   8.3792
Smallest, middle and largest Z coordinate values= -10.7239  -1.5456   7.6326
Volume of enclosing rectangle=     7236.56 A^3
=== Trial  12: edge=  21.1881  18.6059  18.3564 A vol= 0.72365645E+04 A^3
--- Iteration  10 Objective function=-0.90952627E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.87342998E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.86932510E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.86796455E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.86779570E+04 A (tolerance=0.0000100)
--- Number of iterations=          59
Smallest, middle and largest X coordinate values=  -9.2622   0.2623   9.7868
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Smallest, middle and largest Y coordinate values=  -8.7802   1.2681  11.3165
Smallest, middle and largest Z coordinate values= -12.1775  -0.8441  10.4892
Volume of enclosing rectangle=     8677.27 A^3
=== Trial  13: edge=  19.0489  20.0967  22.6666 A vol= 0.86772705E+04 A^3
--- Iteration  10 Objective function=-0.93536504E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.87159131E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.81119951E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.76525781E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.72985864E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.72709692E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.72476055E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.72395889E+04 A (tolerance=0.0000100)
--- Iteration  90 Objective function=-0.72370601E+04 A (tolerance=0.0000100)
--- Iteration 100 Objective function=-0.72365698E+04 A (tolerance=0.0000100)
--- Number of iterations=         101
Smallest, middle and largest X coordinate values= -10.7254  -1.5463   7.6328
Smallest, middle and largest Y coordinate values=  -9.7668   0.8272  11.4212
Smallest, middle and largest Z coordinate values= -10.2253  -0.9232   8.3789
Volume of enclosing rectangle=     7236.56 A^3
=== Trial  14: edge=  18.3582  21.1880  18.6043 A vol= 0.72365620E+04 A^3
--- Iteration  10 Objective function=-0.79244248E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.75282197E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.74670342E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.74448457E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.74378330E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.74346196E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.74344722E+04 A (tolerance=0.0000100)
--- Number of iterations=          71
Smallest, middle and largest X coordinate values=  -9.7270   0.3484  10.4238
Smallest, middle and largest Y coordinate values= -10.4715  -0.4217   9.6280
Smallest, middle and largest Z coordinate values= -10.7234  -1.5455   7.6324
Volume of enclosing rectangle=     7434.46 A^3
=== Trial  15: edge=  20.1507  20.0995  18.3558 A vol= 0.74344624E+04 A^3
--- Iteration  10 Objective function=-0.10051655E+05 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.96975107E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.96417715E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.96301758E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.96239355E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.95585518E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.95585518E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.95566006E+04 A (tolerance=0.0000100)
--- Number of iterations=          81
Smallest, middle and largest X coordinate values= -10.0217   0.5132  11.0481
Smallest, middle and largest Y coordinate values= -10.2207  -0.2522   9.7164
Smallest, middle and largest Z coordinate values=  -8.8139   2.5610  13.9360
Volume of enclosing rectangle=     9556.60 A^3
=== Trial  16: edge=  21.0699  19.9371  22.7499 A vol= 0.95566016E+04 A^3
--- Iteration  10 Objective function=-0.93868428E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.93238262E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.93157998E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.92901299E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.87455693E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.87116914E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.86926865E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.86881025E+04 A (tolerance=0.0000100)
--- Iteration  90 Objective function=-0.86843984E+04 A (tolerance=0.0000100)
--- Iteration 100 Objective function=-0.86818330E+04 A (tolerance=0.0000100)
--- Number of iterations=         107
Smallest, middle and largest X coordinate values= -10.4797   0.8416  12.1630
Smallest, middle and largest Y coordinate values= -11.4997  -1.1000   9.2996
Smallest, middle and largest Z coordinate values=  -9.4397  -0.2226   8.9945
Volume of enclosing rectangle=     8681.64 A^3
=== Trial  17: edge=  22.6427  20.7994  18.4342 A vol= 0.86816377E+04 A^3
```

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--- Iteration  10 Objective function=-0.78008506E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.75610918E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.75149502E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.74769419E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.74676416E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.74454634E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.74364033E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.74350444E+04 A (tolerance=0.0000100)
--- Number of iterations=          86
Smallest, middle and largest X coordinate values= -10.7236  -1.5456   7.6324
Smallest, middle and largest Y coordinate values=  -9.6288   0.4228  10.4744
Smallest, middle and largest Z coordinate values=  -9.7283   0.3456  10.4195
Volume of enclosing rectangle=     7434.78 A^3
=== Trial  18: edge=  18.3559  20.1032  20.1478 A vol= 0.74347842E+04 A^3
--- Iteration  10 Objective function=-0.90291836E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.76831729E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.76231274E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.76167144E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.75256484E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.74784819E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.74683091E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.74660815E+04 A (tolerance=0.0000100)
--- Iteration  90 Objective function=-0.74651753E+04 A (tolerance=0.0000100)
--- Iteration 100 Objective function=-0.74417705E+04 A (tolerance=0.0000100)
--- Iteration 110 Objective function=-0.74381528E+04 A (tolerance=0.0000100)
--- Iteration 120 Objective function=-0.74377197E+04 A (tolerance=0.0000100)
--- Number of iterations=         123
Smallest, middle and largest X coordinate values=  -9.7391   0.3260  10.3911
Smallest, middle and largest Y coordinate values=  -7.6326   1.5459  10.7243
Smallest, middle and largest Z coordinate values= -10.4938  -0.4301   9.6335
Volume of enclosing rectangle=     7437.60 A^3
=== Trial  19: edge=  20.1301  18.3569  20.1273 A vol= 0.74375977E+04 A^3
--- Iteration  10 Objective function=-0.84735186E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.76295820E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.75964385E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.75718130E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.75671152E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.75656323E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.75649268E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.75628315E+04 A (tolerance=0.0000100)
--- Iteration  90 Objective function=-0.75625903E+04 A (tolerance=0.0000100)
--- Number of iterations=          90
Smallest, middle and largest X coordinate values= -11.8393  -0.9588   9.9218
Smallest, middle and largest Y coordinate values=  -9.3999   0.6048  10.6095
Smallest, middle and largest Z coordinate values=  -8.2418   0.4424   9.1265
Volume of enclosing rectangle=     7562.59 A^3
=== Trial  20: edge=  21.7610  20.0094  17.3683 A vol= 0.75625903E+04 A^3
--- Iteration  10 Objective function=-0.87006230E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.85999043E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.85793232E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.85774775E+04 A (tolerance=0.0000100)
--- Number of iterations=          47
Smallest, middle and largest X coordinate values= -12.6684  -1.8067   9.0551
Smallest, middle and largest Y coordinate values=  -9.7758  -0.7265   8.3228
Smallest, middle and largest Z coordinate values= -10.6579   0.2497  11.1573
Volume of enclosing rectangle=     8576.94 A^3
=== Trial  21: edge=  21.7235  18.0985  21.8152 A vol= 0.85769414E+04 A^3
--- Iteration  10 Objective function=-0.76341455E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.75728638E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.75654917E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.75626846E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.75621299E+04 A (tolerance=0.0000100)
--- Number of iterations=          55
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Smallest, middle and largest X coordinate values= -10.6084  -0.6000   9.4084
Smallest, middle and largest Y coordinate values=  -9.9206   0.9669  11.8545
Smallest, middle and largest Z coordinate values=  -9.0954  -0.4207   8.2539
Volume of enclosing rectangle=     7561.99 A^3
=== Trial  22: edge=  20.0168  21.7751  17.3493 A vol= 0.75619878E+04 A^3
--- Iteration  10 Objective function=-0.80455518E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.75531445E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.72682451E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.72404302E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.72380825E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.72370405E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.72364795E+04 A (tolerance=0.0000100)
--- Number of iterations=          72
Smallest, middle and largest X coordinate values= -11.4206  -0.8267   9.7672
Smallest, middle and largest Y coordinate values=  -8.3792   0.9239  10.2271
Smallest, middle and largest Z coordinate values= -10.7235  -1.5455   7.6325
Volume of enclosing rectangle=     7236.45 A^3
=== Trial  23: edge=  21.1878  18.6063  18.3560 A vol= 0.72364463E+04 A^3
--- Iteration  10 Objective function=-0.90827295E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.87942393E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.86733311E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.86534141E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.86506230E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.86501406E+04 A (tolerance=0.0000100)
--- Number of iterations=          62
Smallest, middle and largest X coordinate values= -10.9219   0.3996  11.7211
Smallest, middle and largest Y coordinate values= -10.9683  -1.1127   8.7428
Smallest, middle and largest Z coordinate values=  -9.9551  -0.2646   9.4259
Volume of enclosing rectangle=     8650.14 A^3
=== Trial  24: edge=  22.6430  19.7111  19.3811 A vol= 0.86501406E+04 A^3
--- Iteration  10 Objective function=-0.96541758E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.74490151E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.73555547E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.72654111E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.72421953E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.72381465E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.72364849E+04 A (tolerance=0.0000100)
--- Number of iterations=          79
Smallest, middle and largest X coordinate values= -10.2264  -0.9237   8.3790
Smallest, middle and largest Y coordinate values=  -7.6326   1.5459  10.7243
Smallest, middle and largest Z coordinate values= -11.4209  -0.8269   9.7671
Volume of enclosing rectangle=     7236.48 A^3
=== Trial  25: edge=  18.6054  18.3569  21.1880 A vol= 0.72364805E+04 A^3
--- Iteration  10 Objective function=-0.98505332E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.84080928E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.77686147E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.76107949E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.75848242E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.75756084E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.75713833E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.75704199E+04 A (tolerance=0.0000100)
--- Iteration  90 Objective function=-0.75638467E+04 A (tolerance=0.0000100)
--- Iteration 100 Objective function=-0.75621748E+04 A (tolerance=0.0000100)
--- Number of iterations=         105
Smallest, middle and largest X coordinate values=  -9.4069   0.6010  10.6089
Smallest, middle and largest Y coordinate values=  -9.1006  -0.4244   8.2517
Smallest, middle and largest Z coordinate values=  -9.9207   0.9656  11.8518
Volume of enclosing rectangle=     7562.04 A^3
=== Trial  26: edge=  20.0158  17.3523  21.7725 A vol= 0.75620366E+04 A^3
--- Iteration  10 Objective function=-0.85571455E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.84490684E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.80296216E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.73149917E+04 A (tolerance=0.0000100)
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--- Iteration  50 Objective function=-0.72418096E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.72393193E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.72373828E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.72367612E+04 A (tolerance=0.0000100)
--- Number of iterations=          84
Smallest, middle and largest X coordinate values= -11.4210  -0.8269   9.7671
Smallest, middle and largest Y coordinate values= -10.7234  -1.5453   7.6327
Smallest, middle and largest Z coordinate values= -10.2273  -0.9240   8.3793
Volume of enclosing rectangle=     7236.70 A^3
=== Trial  27: edge=  21.1881  18.3562  18.6066 A vol= 0.72366958E+04 A^3
--- Iteration  10 Objective function=-0.83484082E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.82609238E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.81517212E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.75660044E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.72974067E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.72732920E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.72413848E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.72387070E+04 A (tolerance=0.0000100)
--- Iteration  90 Objective function=-0.72373662E+04 A (tolerance=0.0000100)
--- Number of iterations=          98
Smallest, middle and largest X coordinate values= -10.2259  -0.9223   8.3813
Smallest, middle and largest Y coordinate values=  -7.6330   1.5457  10.7244
Smallest, middle and largest Z coordinate values= -11.4198  -0.8263   9.7672
Volume of enclosing rectangle=     7237.02 A^3
=== Trial  28: edge=  18.6071  18.3574  21.1869 A vol= 0.72370156E+04 A^3
--- Iteration  10 Objective function=-0.93329805E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.83101074E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.80939019E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.77052695E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.75803774E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.75803774E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.75699062E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.75633506E+04 A (tolerance=0.0000100)
--- Iteration  90 Objective function=-0.75626929E+04 A (tolerance=0.0000100)
--- Iteration 100 Objective function=-0.75619312E+04 A (tolerance=0.0000100)
--- Number of iterations=         106
Smallest, middle and largest X coordinate values=  -8.2541   0.4202   9.0945
Smallest, middle and largest Y coordinate values=  -9.4083   0.6003  10.6090
Smallest, middle and largest Z coordinate values=  -9.9201   0.9675  11.8550
Volume of enclosing rectangle=     7561.86 A^3
=== Trial  29: edge=  17.3486  20.0173  21.7750 A vol= 0.75618574E+04 A^3
--- Iteration  10 Objective function=-0.83170225E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.76873716E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.76416592E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.76286670E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.76262783E+04 A (tolerance=0.0000100)
--- Number of iterations=          54
Smallest, middle and largest X coordinate values=  -9.6470  -0.7476   8.1517
Smallest, middle and largest Y coordinate values= -10.5500  -0.5652   9.4196
Smallest, middle and largest Z coordinate values= -10.2279   0.5000  11.2279
Volume of enclosing rectangle=     7626.08 A^3
=== Trial  30: edge=  17.7987  19.9696  21.4558 A vol= 0.76260835E+04 A^3
--- Iteration  10 Objective function=-0.88546543E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.87485537E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.87238623E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.86656162E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.86531738E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.86508174E+04 A (tolerance=0.0000100)
--- Number of iterations=          67
Smallest, middle and largest X coordinate values= -11.7216  -0.4000  10.9215
Smallest, middle and largest Y coordinate values=  -9.4259   0.2646   9.9551
Smallest, middle and largest Z coordinate values=  -8.7430   1.1127  10.9684
Volume of enclosing rectangle=     8650.22 A^3
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=== Trial  31: edge=  22.6430  19.3809  19.7114 A vol= 0.86502158E+04 A^3
--- Iteration  10 Objective function=-0.86954150E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.86954150E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.86694121E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.83340498E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.78017485E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.76912915E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.76839707E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.76826509E+04 A (tolerance=0.0000100)
--- Iteration  90 Objective function=-0.76701313E+04 A (tolerance=0.0000100)
--- Iteration 100 Objective function=-0.74328906E+04 A (tolerance=0.0000100)
--- Iteration 110 Objective function=-0.74073984E+04 A (tolerance=0.0000100)
--- Iteration 120 Objective function=-0.74032847E+04 A (tolerance=0.0000100)
--- Iteration 130 Objective function=-0.73874722E+04 A (tolerance=0.0000100)
--- Iteration 140 Objective function=-0.72742651E+04 A (tolerance=0.0000100)
--- Iteration 150 Objective function=-0.72574653E+04 A (tolerance=0.0000100)
--- Iteration 160 Objective function=-0.72531108E+04 A (tolerance=0.0000100)
--- Number of iterations=         169
Smallest, middle and largest X coordinate values=  -9.7526   0.8466  11.4459
Smallest, middle and largest Y coordinate values=  -7.6814   1.6015  10.8844
Smallest, middle and largest Z coordinate values= -10.0670  -0.8529   8.3611
Volume of enclosing rectangle=     7252.65 A^3
=== Trial  32: edge=  21.1985  18.5658  18.4280 A vol= 0.72526528E+04 A^3
--- Iteration  10 Objective function=-0.79327388E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.76653457E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.75819272E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.75737495E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.75733472E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.75715342E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.75628945E+04 A (tolerance=0.0000100)
--- Number of iterations=          78
Smallest, middle and largest X coordinate values=  -9.9227   0.9647  11.8521
Smallest, middle and largest Y coordinate values= -10.6076  -0.5993   9.4090
Smallest, middle and largest Z coordinate values=  -8.2535   0.4218   9.0971
Volume of enclosing rectangle=     7562.38 A^3
=== Trial  33: edge=  21.7748  20.0166  17.3506 A vol= 0.75623794E+04 A^3
--- Iteration  10 Objective function=-0.85459980E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.77876758E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.74010234E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.72839238E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.72518911E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.72397979E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.72369307E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.72365786E+04 A (tolerance=0.0000100)
--- Number of iterations=          84
Smallest, middle and largest X coordinate values= -10.2272  -0.9238   8.3795
Smallest, middle and largest Y coordinate values=  -9.7672   0.8266  11.4205
Smallest, middle and largest Z coordinate values=  -7.6324   1.5455  10.7235
Volume of enclosing rectangle=     7236.51 A^3
=== Trial  34: edge=  18.6067  21.1877  18.3559 A vol= 0.72365117E+04 A^3
--- Iteration  10 Objective function=-0.99883779E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.75843838E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.74630972E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.74418691E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.74378281E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.74349331E+04 A (tolerance=0.0000100)
--- Number of iterations=          65
Smallest, middle and largest X coordinate values=  -7.6328   1.5452  10.7232
Smallest, middle and largest Y coordinate values= -10.4716  -0.4221   9.6275
Smallest, middle and largest Z coordinate values=  -9.7270   0.3485  10.4241
Volume of enclosing rectangle=     7434.58 A^3
=== Trial  35: edge=  18.3561  20.0992  20.1511 A vol= 0.74345791E+04 A^3
--- Iteration  10 Objective function=-0.81929873E+04 A (tolerance=0.0000100)
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--- Iteration  20 Objective function=-0.80167192E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.79726919E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.79162651E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.75996611E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.75827666E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.75804351E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.75786401E+04 A (tolerance=0.0000100)
--- Iteration  90 Objective function=-0.75777515E+04 A (tolerance=0.0000100)
--- Number of iterations=          93
Smallest, middle and largest X coordinate values= -11.6963  -0.7980  10.1004
Smallest, middle and largest Y coordinate values= -10.4653  -0.5079   9.4495
Smallest, middle and largest Z coordinate values=  -9.2730  -0.5444   8.1842
Volume of enclosing rectangle=     7577.75 A^3
=== Trial  36: edge=  21.7966  19.9147  17.4573 A vol= 0.75777520E+04 A^3
--- Iteration  10 Objective function=-0.99886240E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.95362559E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.95270859E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.95250498E+04 A (tolerance=0.0000100)
--- Number of iterations=          46
Smallest, middle and largest X coordinate values= -10.5064  -0.9082   8.6900
Smallest, middle and largest Y coordinate values= -10.2865   0.6626  11.6118
Smallest, middle and largest Z coordinate values= -12.4861  -1.1571  10.1719
Volume of enclosing rectangle=     9524.74 A^3
=== Trial  37: edge=  19.1964  21.8983  22.6581 A vol= 0.95247363E+04 A^3
--- Iteration  10 Objective function=-0.91266230E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.85191426E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.73661157E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.72689072E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.72614600E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.72421851E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.72375186E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.72367261E+04 A (tolerance=0.0000100)
--- Number of iterations=          84
Smallest, middle and largest X coordinate values= -10.2243  -0.9227   8.3788
Smallest, middle and largest Y coordinate values=  -7.6330   1.5468  10.7266
Smallest, middle and largest Z coordinate values= -11.4216  -0.8275   9.7666
Volume of enclosing rectangle=     7236.72 A^3
=== Trial  38: edge=  18.6031  18.3596  21.1881 A vol= 0.72367148E+04 A^3
--- Iteration  10 Objective function=-0.10293053E+05 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.85529590E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.75877173E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.75644570E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.75644570E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.75626797E+04 A (tolerance=0.0000100)
--- Number of iterations=          68
Smallest, middle and largest X coordinate values=  -9.9213   0.9627  11.8466
Smallest, middle and largest Y coordinate values=  -9.4041   0.6025  10.6091
Smallest, middle and largest Z coordinate values=  -9.1112  -0.4317   8.2477
Volume of enclosing rectangle=     7562.31 A^3
=== Trial  39: edge=  21.7679  20.0132  17.3589 A vol= 0.75623115E+04 A^3
--- Iteration  10 Objective function=-0.80029009E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.73881685E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.73394717E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.73208115E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.72484844E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.72428945E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.72399214E+04 A (tolerance=0.0000100)
--- Number of iterations=          75
Smallest, middle and largest X coordinate values= -11.4335  -0.8386   9.7563
Smallest, middle and largest Y coordinate values= -10.1812  -0.9034   8.3744
Smallest, middle and largest Z coordinate values=  -7.6410   1.5656  10.7722
Volume of enclosing rectangle=     7239.86 A^3
=== Trial  40: edge=  21.1898  18.5556  18.4132 A vol= 0.72398643E+04 A^3
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--- Iteration  10 Objective function=-0.83917803E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.76398486E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.76011582E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.75828711E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.75661343E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.75625547E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.75624907E+04 A (tolerance=0.0000100)
--- Number of iterations=          72
Smallest, middle and largest X coordinate values=  -9.0998  -0.4232   8.2533
Smallest, middle and largest Y coordinate values=  -9.4062   0.6016  10.6095
Smallest, middle and largest Z coordinate values= -11.8543  -0.9680   9.9184
Volume of enclosing rectangle=     7562.45 A^3
=== Trial  41: edge=  17.3532  20.0158  21.7726 A vol= 0.75624482E+04 A^3
--- Iteration  10 Objective function=-0.10369898E+05 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.93989414E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.93929072E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.93925811E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.93914375E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.92011670E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.91759688E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.91748672E+04 A (tolerance=0.0000100)
--- Number of iterations=          85
Smallest, middle and largest X coordinate values= -10.7985   0.5898  11.9781
Smallest, middle and largest Y coordinate values= -11.5815  -1.0543   9.4729
Smallest, middle and largest Z coordinate values=  -9.4107   0.1555   9.7216
Volume of enclosing rectangle=     9174.87 A^3
=== Trial  42: edge=  22.7766  21.0545  19.1323 A vol= 0.91748662E+04 A^3
--- Iteration  10 Objective function=-0.92187139E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.92021816E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.91959004E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.91951875E+04 A (tolerance=0.0000100)
--- Number of iterations=          40
Smallest, middle and largest X coordinate values= -11.5574  -0.5018  10.5538
Smallest, middle and largest Y coordinate values= -12.9934  -2.3723   8.2488
Smallest, middle and largest Z coordinate values= -11.5421  -1.7536   8.0350
Volume of enclosing rectangle=     9195.16 A^3
=== Trial  43: edge=  22.1111  21.2423  19.5771 A vol= 0.91951621E+04 A^3
--- Iteration  10 Objective function=-0.81760303E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.74126426E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.72627041E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.72455991E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.72387520E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.72367441E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.72365498E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.72363877E+04 A (tolerance=0.0000100)
--- Number of iterations=          80
Smallest, middle and largest X coordinate values=  -7.6324   1.5456  10.7236
Smallest, middle and largest Y coordinate values=  -8.3790   0.9240  10.2270
Smallest, middle and largest Z coordinate values= -11.4206  -0.8267   9.7673
Volume of enclosing rectangle=     7236.39 A^3
=== Trial  44: edge=  18.3560  18.6061  21.1879 A vol= 0.72363877E+04 A^3
--- Iteration  10 Objective function=-0.76675400E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.74757061E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.74696792E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.74684868E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.74681255E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.74666201E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.74491606E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.74484224E+04 A (tolerance=0.0000100)
--- Iteration  90 Objective function=-0.74472295E+04 A (tolerance=0.0000100)
--- Number of iterations=          99
Smallest, middle and largest X coordinate values= -10.4412  -0.4110   9.6193
Smallest, middle and largest Y coordinate values=  -7.6327   1.5452  10.7232
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Smallest, middle and largest Z coordinate values= -10.4687  -0.3565   9.7557
Volume of enclosing rectangle=     7447.23 A^3
=== Trial  45: edge=  20.0605  18.3560  20.2244 A vol= 0.74472305E+04 A^3
--- Iteration  10 Objective function=-0.10419869E+05 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.94482334E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.93732471E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.92300918E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.87622900E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.87286709E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.86793418E+04 A (tolerance=0.0000100)
--- Iteration  80 Objective function=-0.86573770E+04 A (tolerance=0.0000100)
--- Iteration  90 Objective function=-0.86527256E+04 A (tolerance=0.0000100)
--- Iteration 100 Objective function=-0.86515742E+04 A (tolerance=0.0000100)
--- Number of iterations=         103
Smallest, middle and largest X coordinate values=  -8.7438   1.1148  10.9735
Smallest, middle and largest Y coordinate values= -11.7273  -0.4051  10.9170
Smallest, middle and largest Z coordinate values=  -9.4240   0.2646   9.9532
Volume of enclosing rectangle=     8651.57 A^3
=== Trial  46: edge=  19.7172  22.6442  19.3772 A vol= 0.86515674E+04 A^3
--- Iteration  10 Objective function=-0.90722598E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.76560806E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.74600386E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.74512627E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.74458120E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.74455161E+04 A (tolerance=0.0000100)
--- Number of iterations=          63
Smallest, middle and largest X coordinate values= -10.8999  -0.5905   9.7190
Smallest, middle and largest Y coordinate values= -10.7239  -1.5457   7.6325
Smallest, middle and largest Z coordinate values=  -9.9767  -0.1408   9.6950
Volume of enclosing rectangle=     7445.50 A^3
=== Trial  47: edge=  20.6189  18.3563  19.6718 A vol= 0.74455054E+04 A^3
--- Iteration  10 Objective function=-0.82162969E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.79089336E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.74920146E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.74527422E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.74360117E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.74344351E+04 A (tolerance=0.0000100)
--- Number of iterations=          69
Smallest, middle and largest X coordinate values= -10.4237  -0.3485   9.7267
Smallest, middle and largest Y coordinate values=  -9.6279   0.4218  10.4716
Smallest, middle and largest Z coordinate values= -10.7234  -1.5455   7.6324
Volume of enclosing rectangle=     7434.39 A^3
=== Trial  48: edge=  20.1505  20.0995  18.3559 A vol= 0.74343921E+04 A^3
--- Iteration  10 Objective function=-0.93722705E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.83330508E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.76421406E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.75816582E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.75649351E+04 A (tolerance=0.0000100)
--- Iteration  60 Objective function=-0.75622783E+04 A (tolerance=0.0000100)
--- Iteration  70 Objective function=-0.75620420E+04 A (tolerance=0.0000100)
--- Number of iterations=          78
Smallest, middle and largest X coordinate values=  -9.9202   0.9660  11.8522
Smallest, middle and largest Y coordinate values= -10.6092  -0.6012   9.4067
Smallest, middle and largest Z coordinate values=  -8.2518   0.4243   9.1003
Volume of enclosing rectangle=     7562.00 A^3
=== Trial  49: edge=  21.7724  20.0160  17.3522 A vol= 0.75620044E+04 A^3
--- Iteration  10 Objective function=-0.88581650E+04 A (tolerance=0.0000100)
--- Iteration  20 Objective function=-0.87397773E+04 A (tolerance=0.0000100)
--- Iteration  30 Objective function=-0.86909912E+04 A (tolerance=0.0000100)
--- Iteration  40 Objective function=-0.86854512E+04 A (tolerance=0.0000100)
--- Iteration  50 Objective function=-0.86819209E+04 A (tolerance=0.0000100)
--- Number of iterations=          59
Smallest, middle and largest X coordinate values=  -9.3025   1.0990  11.5004
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Smallest, middle and largest Y coordinate values= -12.1636  -0.8422  10.4791
Smallest, middle and largest Z coordinate values=  -8.9937   0.2218   9.4373
Volume of enclosing rectangle=     8681.62 A^3
=== Trial  50: edge=  20.8029  22.6427  18.4310 A vol= 0.86816162E+04 A^3
=== Edges of the smallest box still enclosing the solute:
=== Optimum:   18.35602  18.60607  21.18795 A vol= 0.72363877E+04 A^3 Nslt=   378
Optimal orientation is from the   44th try
The number of times the optimal cell volume was reached=  5
Input configuration is multiplied by the matrix
          -0.0378212 -0.9283683  0.3697322
          -0.8227965 -0.1810353 -0.5387321
           0.5670763 -0.3245898 -0.7570111
Do you want to center the system to (0,0,0) (y/n) [y]
Optimized configuration was shifed to (0,0,0) from
               1.545600       0.923986      -0.826651
Do you want the atoms sorted (y/n) [n]
Conf    1 Number of atoms deleted=        0 (out of      378)
Do you want to adjust atom and residue numbers (y/n) [n]
Do you want a sequence list (y/n) [n]
```