Quantum-mechanical simulation of protein crystals and water-protein interactions: the case of crambin

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SUPPORTING INFORMATION

COMPUTATIONAL DETAILS

The development version of the CRYSTAL14 code[1] was adopted for all the *ab initio* calculations in its massively parallel implementation.[2] CRYSTAL14 permits the study of systems of all dimensionalities, from molecules to crystals. It employs a Gaussian type basis, paired with both Density Functional Theory (DFT) and Hartree Fock (HF) Hamiltonians.

Hamiltonian

All calculations were performed within the Density Functional Theory, adopting the Becke, 3 parameters, Lee-Yang-Parr (B3LYP) hybrid functional.[3] Due to the use of a local basis set and suitable truncation of the exchange series, the present implementation of hybrid functionals in CRYSTAL14 is very efficient compared to other codes based on plane waves, being only about three times slower than pure GGAs.[2] The electron density and its gradient were integrated over a pruned grid consisting of 974 angular and 75 radial points per atom generated through the Gauss–Legendre quadrature and Lebedev schemes. The accuracy of this grid can be estimated from the integrated

number of electrons, that is 6760.0006 *e* for the largest studied system (6760 in the unit cell). Values of the tolerances that control the Coulomb and exchange series in periodical systems were kept at the default values (10^{-6} and 10^{-12} Ha).[4] For the periodic cases, the Hamiltonian matrix was diagonalized only at the Γ point, due to the large volume of the unit cells.[5] The eigenvalue level-shifting technique was used to initially lock the system in a non-conducting state, with the level shifter set to 0.6 Ha, which is then relaxed at the end of the self consistent field iterations.[6] To further help convergence of the Self Consistent Field (SCF), the Fock/KS matrix at a given cycle was mixed with 30% of the one of the previous cycle. The dispersion contribution was added to the DFT energies and gradients, by means of the empirical dispersion correction originally proposed by Grimme and known as D2 correction,[7] with the modified parameters proposed by Civalleri *et al*. for the treatment of molecular crystals using the B3LYP hybrid functional (hereafter referred as B3LYP-D*).[8]

Basis Set

A split valence double-ζ basis set (6-31G(d,p)) plus polarization functions was applied to C, N, S and O,[9] while an Ahlrichs's pVDZ basis was used for H.[10] For the sake of simplicity, the chosen combination of Hamiltonian and basis will be identified as B3LYP-D*/6-31G(d,p) in the following. As anticipated in the introduction, we modeled three crambin crystals differing for the amount of solvating water, namely with 0W, 84W and 172W water molecules investigated in the present work (*vide infra*) resulting in 12354, 14370 and 16482 Atomic Orbitals (AOs) in the unit cell, respectively. Both cell parameters and internal coordinates were optimized using the analytical gradient method.

Geometry optimizations

The Hessian is upgraded with the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm.[11] The initial Hessian for most calculations was generated by means of a classical model as proposed by Schlegel.[12] Due to memory constraints, for the largest studied system (172W, 1800 atoms/cell), the initial Hessian guess was changed to the identity matrix. Default convergence values were used for the maximum allowed gradient, the maximum atomic displacement and their maximum allowed root

mean square values for convergence (0.00045 Ha·bohr^{-1}, 0.00180 Bohr, 0.00030 Ha·bohr^{-1} and 0.00120 Bohr, respectively).

Computation of crystal formation energies

The energetics of the protein crystal and of the protein-protein and protein-water interactions was decomposed in various contributions as in Ref. [13] and detailed below.

For a general crystal CRY with n proteins P and m water molecules W in the unit cell, the formation energy ΔE can be defined as:

$$\Delta E = E(CRY/CRY) - n \cdot E(P/P) - m \cdot E(W/W) \quad (1)$$

where $E(CRY/CRY)$, $E(P/P)$ and $E(W/W)$ are the energies of the optimized crystal, free protein and free water, respectively (the symbol after the / refers to the geometry at which the energy was evaluated). ΔE is determined by the balance between the energy gain due to the new interactions present in the crystal with respect to the isolated compounds and the energy loss due to the structural deformations occurring for P and W from the gas to the condensed phase. For a crystal to be thermochemically stable $\Delta E < 0$. A deformation-free formation energy ΔE^* is defined as:

$$\Delta E^* = E(CRY/CRY) - \sum_{i=1}^{n} E(P_i/CRY) - \sum_{i=1}^{m} E(W_i/CRY) \quad (2)$$

where $E(P_i/CRY)$ is the energy of the i-th isolated protein taken at the geometry of the optimized crystal, and $E(W_i/CRY)$ is the energy of the i-th water molecule taken in the geometry of the optimized crystal. Eq. 2 can be easily reformulated to include the Basis Set Superposition Error (BSSE) correction, using the same counterpoise method adopted for intermolecular complexes:[14]

$$\Delta E^{*C} = E(CRY/CRY) - \sum_{i=1}^{n} E(P_i + gh/CRY) - \sum_{i=1}^{m} E(W_i + gh/CRY) \quad (3)$$

where "$+\ gh$" means that the energy is computed with the addition of the ghost functions of the surrounding molecules. In periodic systems, this is usually accomplished by including ghost functions within a chosen cutoff distance (here, 40 Å) around the molecule. The $BSSE$ can then be defined as:

$$BSSE = \Delta E^{*} - \Delta E^{*C} \tag{4}$$

and the final, BSSE corrected, formation energy ΔE^{C} is defined as:

$$\Delta E^{C} = \Delta E - BSSE \tag{5}$$

Eqs. 1-5 were then adapted to the different systems considered in the present work. For protein-protein and protein-water interactions of Table 4, the energetics was studied deformation-free, that is with the structure of the components frozen at the geometry of the interacting system. For some processes of Table 3, a water box representing liquid water was taken as a reference. To study such processes, Eqs. 1-3 must be reformulated as follows:

$$\Delta E = E(CRY/CRY) - n \cdot E(P/P) - E(W_m/W_m) \tag{6}$$

$$\Delta E^{*} = E(CRY/CRY) - \sum_{i=1}^{n} E(P_i/CRY) - E(W_m/CRY) \tag{7}$$

$$\Delta E^{*C} = E(CRY/CRY) - \sum_{i=1}^{n} E(P_i + gh/CRY) - E(W_m + gh/CRY) \tag{8}$$

where $E(W_m/W_m)$ is the energy of an optimized liquid water box containing m molecules, while $E(W_m + gh/CRY)$ and $E(W_m/CRY)$ are the energies of the 3D framework of m water molecules as found in the crystal with and without the protein ghost functions, respectively. Eqs. 4-5 remain valid. To evaluate $E(W_m/W_m)$, a water box of 84 molecules (side: 13.4 Å) was generated through the PACKMOL utility,[15] thermalized through a 10 ps by PBE-D2/TZVP *ab initio* molecular dynamics simulation at 300 K with the CP2K[16] software and then B3LYP-D*/6-31G(d,p) fully optimized with CRYSTAL14. For the 172W case $E(W_{84}/W_{84})$ was scaled by a factor 172/84.

Computation of BSSE-corrected charge transfers

Consider the interaction between two components, A and B, so that:

$$A + B \rightarrow AB \quad (1)$$

These two systems have, when isolated, total electronic charges Q_A and Q_B, corresponding to their total number of electrons. These electrons are distributed among the different atoms composing the systems:

$$Q_A = \sum_{i=1}^{N_A} Q_i \quad (2)$$

where N_A is the total number of atoms in A and Q_i is the electronic charge on the i^{th} atom, that may be estimated through a Mulliken population analysis.

The interaction complex AB has a total electronic charge Q_{AB}:

$$Q_{AB} = Q_{A*} + Q_{B*} \quad (3)$$

where Q_{A*} and Q_{B*} are the electronic charges on A and B when involved in the interaction. Of course, due to the charge transfer associated to this interaction, $Q_{A*} \neq Q_A$ and $Q_{B*} \neq Q_B$.

This charge transfer (QT) can then be defined as:

$$QT_{B \rightarrow A} = Q_{A*} - Q_A \quad (4)$$

If $QT_{B \rightarrow A} > 0$, a net flux of electronic charge from B to A has occurred, while B has obtained charge if $QT_{B \rightarrow A} < 0$. Of course, since the total electronic charge must be conserved:

$$QT_{B \rightarrow A} = -QT_{A \rightarrow B} \quad (5)$$

The Basis Set Superposition Error (BSSE) is known to affect any calculation based on atom-centered basis functions. This error is due to the superposition, in the AB complex, of the functions centered on both A and B atoms, so that AB is described by a richer basis set than the A and B components alone. This discrepancy causes inconsistencies when comparing total energies, such as when computing interaction energies. The same problem is present when dealing with equation (4), since

Q_{A*} and Q_A come from calculations with a different number of basis functions, *i.e.* Q_A misses functions centered on B. When these functions are present (when computing Q_{A*}), the effect of the BSSE is a net flux of electronic charge in order to partially occupy them.

This un-physical BSSE-caused charge transfer (QT^{BSSE}) can be evaluated by doing a calculation on A and B when the ghost functions of the other component are present:

$$\begin{aligned} QT^{BSSE}_{A} &= Q_{A[B]} - Q_A \\ QT^{BSSE}_{B} &= Q_{[A]B} - Q_B \end{aligned} \tag{6}$$

where the square brackets mean that only the ghost functions of the component are included. QT^{BSSE} is always a negative quantity.

The BSSE-corrected charge transfer due to the interaction (QT^{C}) is then computed by removing the spurious charge fluxes of equations (6) from the uncorrected charge transfer of equation (4):

$$QT_{B\to A}^{C} = QT_{B\to A} - QT^{BSSE}_{A} + QT^{BSSE}_{B} \tag{7}$$

where signs are conveniently put to account for charge fluxes directions.

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Supporting tables

Table S1. Energetics of the crambin crystal formation (HSE06-D*/6-31G(d,p)//B3LYP-D*/6-31G(d,p)).

Process	*n*	ΔE^{C} [a]	ΔE^{CD} [b]	disp [c]
2P + *n*W → CRY(*n*W)	0	+100 [+0.1]	-1350 [-1.1]	-1450 [-1.1]
	84	-4448 [-2.9]	-7380 [-4.8]	-2932 [-1.9]
CRY(0W) + *n*W → CRY(*n*W)	84	-4548 (-54)	-6029 (-72)	-1482 (-17)

[a] Reaction energies as in Table 3, without including dispersion, but at the HSE06/6-31G(d,p)//B3LYP-D*/6-31G(d,p) level of theory (in the *x//y* notation *x* is the level at which the energy is computed, *y* is the level at which the geometry has been optimized). [b] As [a], but obtained with dispersion (HSE06-D*/6-31G(d,p)//B3LYP-D*/6-31G(d,p)). In square brackets, the atom contribution to some formation energies. In parentheses, the contribution for each individual water molecule (when applicable) is reported. [c] Dispersion contribution evaluated as: $\Delta E^{CD} - \Delta E^{C}$. P: crambin molecule in gas phase. W: water molecule in gas phase. CRY: crambin crystal in the two 0W, 84W cases. All values are in kJ·mol^{-1}.

Table S2. Energetics of the crambin crystal formation (B3LYP-D*/6-31G//B3LYP-D*/6-31G(d,p)).

Process	*n*	ΔE^{C} [a]	ΔE^{CD} [b]	disp [c]
2P + *n*W → CRY(*n*W)	0	+353 [+0.3]	-1097 [-0.9]	-1450 [-1.1]
	84	-5416 [-3.5]	-8348 [-5.4]	-2932 [-1.9]
CRY(0W) + *n*W → CRY(*n*W)	84	-5769 (-69)	-7251 (-86)	-1482 (-17)

[a] Reaction energies as in Table 3, without including dispersion, but at the B3LYP/6-31G//B3LYP-D*/6-31G(d,p) level of theory (in the *x//y* notation *x* is the level at which the energy is computed, *y* is the level at which the geometry has been optimized). [b] As [a], but obtained with dispersion (B3LYP-D*/6-31G//B3LYP-D*/6-31G(d,p)). In square brackets, the atom contribution to some formation energies. In parentheses, the contribution for each individual water molecule (when applicable) is reported. [c] Dispersion contribution evaluated as: $\Delta E^{CD} - \Delta E^{C}$. P: crambin molecule in gas phase. W: water molecule in gas phase. CRY: crambin crystal in the two 0W, 84W cases. All values are in kJ·mol-1.

Table S3. Energetics of the crambin crystal formation (B3LYP-D3/6-31G(d,p)//B3LYP-D*/6-31G(d,p)).

Process	*n*	ΔE^{C} [a]	ΔE^{CD} [b]	disp [c]
2P + *n*W → CRY(*n*W)	0	+442 [+0.3]	-1031 [-0.8]	-1473 [-1.1]
	84	-3400 [-2.2]	-6593 [-4.3]	-3193 [-2.1]
CRY(0W) + *n*W → CRY(*n*W)	84	-3842 (-46)	-5562 (-66)	-1719 (-20)

[a] Reaction energies as in Table 3, without including dispersion, but at the B3LYP/6-31G//B3LYP-D*/6-31G(d,p) level of theory (in the *x//y* notation *x* is the level at which the energy is computed, *y* is the level at which the geometry has been optimized). [b] As [a], but obtained with dispersion (B3LYP-D3/6-31G//B3LYP-D*/6-31G(d,p)). In square brackets, the atom contribution to some formation energies. In parentheses, the

contribution for each individual water molecule (when applicable) is reported. [c] Dispersion contribution evaluated as: $\Delta E^{CD} - \Delta E^{C}$. P: crambin molecule in gas phase. W: water molecule in gas phase. CRY: crambin crystal in the two 0W, 84W cases. All values are in $kJ \cdot mol^{-1}$.

OPTIMIZED GEOMETRIES (PDB files)

1) CRAMBIN – optimized gas phase molecule

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COMPND    CRAMBIN OPTIMIZED GAS PHASE GEOMETRY
AUTHOR    DELLE PIANE, CORNO, ORLANDO, DOVESI, UGLIENGO
ATOM      1  N   THR A   1      -2.493  -4.567   8.109  1.00  0.00           N
ATOM      2  CA  THR A   1      -2.060  -3.222   7.634  1.00  0.00           C
ATOM      3  C   THR A   1      -1.713  -3.328   6.152  1.00  0.00           C
ATOM      4  O   THR A   1      -1.368  -4.430   5.706  1.00  0.00           O
ATOM      5  CB  THR A   1      -0.845  -2.831   8.536  1.00  0.00           C
ATOM      6  OG1 THR A   1      -1.235  -3.236   9.845  1.00  0.00           O
ATOM      7  CG2 THR A   1      -0.504  -1.352   8.479  1.00  0.00           C
ATOM      8  H1  THR A   1      -1.902  -5.349   7.727  1.00  0.00           H
ATOM      9  H2  THR A   1      -3.471  -4.785   7.905  1.00  0.00           H
ATOM     10  H3  THR A   1      -2.314  -4.520   9.139  1.00  0.00           H
ATOM     11  HA  THR A   1      -2.888  -2.520   7.818  1.00  0.00           H
ATOM     12  HB  THR A   1       0.022  -3.430   8.203  1.00  0.00           H
ATOM     13  HG1 THR A   1      -0.454  -3.685  10.265  1.00  0.00           H
ATOM     14 HG21 THR A   1       0.313  -1.153   9.186  1.00  0.00           H
ATOM     15 HG22 THR A   1      -1.369  -0.741   8.785  1.00  0.00           H
ATOM     16 HG23 THR A   1      -0.170  -1.043   7.478  1.00  0.00           H
ATOM     17  N   THR A   2      -1.793  -2.206   5.427  1.00  0.00           N
ATOM     18  CA  THR A   2      -1.137  -2.097   4.124  1.00  0.00           C
ATOM     19  C   THR A   2       0.122  -1.250   4.368  1.00  0.00           C
ATOM     20  O   THR A   2       0.075  -0.294   5.161  1.00  0.00           O
ATOM     21  CB  THR A   2      -2.063  -1.552   3.023  1.00  0.00           C
ATOM     22  OG1 THR A   2      -2.368  -0.190   3.328  1.00  0.00           O
ATOM     23  CG2 THR A   2      -3.331  -2.392   2.887  1.00  0.00           C
ATOM     24  H   THR A   2      -1.960  -1.315   5.892  1.00  0.00           H
ATOM     25  HA  THR A   2      -0.839  -3.106   3.821  1.00  0.00           H
ATOM     26  HB  THR A   2      -1.482  -1.607   2.083  1.00  0.00           H
ATOM     27  HG1 THR A   2      -2.944   0.139   2.612  1.00  0.00           H
ATOM     28 HG21 THR A   2      -3.077  -3.443   2.686  1.00  0.00           H
ATOM     29 HG22 THR A   2      -3.976  -2.032   2.073  1.00  0.00           H
ATOM     30 HG23 THR A   2      -3.919  -2.349   3.817  1.00  0.00           H
ATOM     31  N   CYS A   3       1.213  -1.660   3.715  1.00  0.00           N
ATOM     32  CA  CYS A   3       2.550  -1.144   3.967  1.00  0.00           C
ATOM     33  C   CYS A   3       3.195  -0.865   2.610  1.00  0.00           C
ATOM     34  O   CYS A   3       3.005  -1.676   1.688  1.00  0.00           O
ATOM     35  CB  CYS A   3       3.420  -2.169   4.709  1.00  0.00           C
ATOM     36  SG  CYS A   3       2.800  -2.673   6.361  1.00  0.00           S
ATOM     37  H   CYS A   3       1.135  -2.464   3.081  1.00  0.00           H
ATOM     38  HA  CYS A   3       2.476  -0.232   4.567  1.00  0.00           H
ATOM     39  HB1 CYS A   3       3.478  -3.108   4.140  1.00  0.00           H
ATOM     40  HB2 CYS A   3       4.429  -1.750   4.826  1.00  0.00           H
ATOM     41  N   CYS A   4       3.971   0.214   2.486  1.00  0.00           N
ATOM     42  CA  CYS A   4       4.538   0.541   1.190  1.00  0.00           C
ATOM     43  C   CYS A   4       6.042   0.804   1.323  1.00  0.00           C
ATOM     44  O   CYS A   4       6.498   1.386   2.314  1.00  0.00           O
ATOM     45  CB  CYS A   4       3.831   1.760   0.576  1.00  0.00           C
ATOM     46  SG  CYS A   4       2.031   1.514   0.294  1.00  0.00           S
ATOM     47  H   CYS A   4       4.102   0.892   3.252  1.00  0.00           H
ATOM     48  HA  CYS A   4       4.366  -0.328   0.549  1.00  0.00           H
ATOM     49  HB1 CYS A   4       3.888   2.622   1.256  1.00  0.00           H
ATOM     50  HB2 CYS A   4       4.289   2.055  -0.378  1.00  0.00           H
ATOM     51  N   PRO A   5       6.817   0.438   0.277  1.00  0.00           N
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ATOM     52  CA  PRO A   5       8.281   0.590   0.341  1.00  0.00           C
ATOM     53  C   PRO A   5       8.756   1.967  -0.134  1.00  0.00           C
ATOM     54  O   PRO A   5       9.945   2.246  -0.209  1.00  0.00           O
ATOM     55  CB  PRO A   5       8.778  -0.561  -0.543  1.00  0.00           C
ATOM     56  CG  PRO A   5       7.709  -0.659  -1.641  1.00  0.00           C
ATOM     57  CD  PRO A   5       6.392  -0.309  -0.930  1.00  0.00           C
ATOM     58  HA  PRO A   5       8.647   0.480   1.372  1.00  0.00           H
ATOM     59  HB1 PRO A   5       9.789  -0.365  -0.920  1.00  0.00           H
ATOM     60  HB2 PRO A   5       8.812  -1.476   0.066  1.00  0.00           H
ATOM     61  HG1 PRO A   5       7.912   0.067  -2.447  1.00  0.00           H
ATOM     62  HG2 PRO A   5       7.653  -1.657  -2.096  1.00  0.00           H
ATOM     63  HD1 PRO A   5       5.719   0.296  -1.556  1.00  0.00           H
ATOM     64  HD2 PRO A   5       5.863  -1.220  -0.635  1.00  0.00           H
ATOM     65  N   SER A   6       7.776   2.869  -0.478  1.00  0.00           N
ATOM     66  CA  SER A   6       8.091   4.274  -0.631  1.00  0.00           C
ATOM     67  C   SER A   6       6.809   5.094  -0.551  1.00  0.00           C
ATOM     68  O   SER A   6       5.714   4.615  -0.869  1.00  0.00           O
ATOM     69  CB  SER A   6       8.765   4.550  -1.995  1.00  0.00           C
ATOM     70  OG  SER A   6       7.904   4.281  -3.102  1.00  0.00           O
ATOM     71  H   SER A   6       6.806   2.633  -0.305  1.00  0.00           H
ATOM     72  HA  SER A   6       8.790   4.596   0.158  1.00  0.00           H
ATOM     73  HB1 SER A   6       9.045   5.611  -2.064  1.00  0.00           H
ATOM     74  HB2 SER A   6       9.682   3.945  -2.047  1.00  0.00           H
ATOM     75  H   SER A   6       7.762   3.319  -3.126  1.00  0.00           H
ATOM     76  N   ILE A   7       7.009   6.405  -0.250  1.00  0.00           N
ATOM     77  CA  ILE A   7       5.904   7.360  -0.292  1.00  0.00           C
ATOM     78  C   ILE A   7       5.288   7.414  -1.690  1.00  0.00           C
ATOM     79  O   ILE A   7       4.077   7.654  -1.816  1.00  0.00           O
ATOM     80  CB  ILE A   7       6.385   8.770   0.169  1.00  0.00           C
ATOM     81  CG1 ILE A   7       6.611   8.774   1.697  1.00  0.00           C
ATOM     82  CG2 ILE A   7       5.429   9.888  -0.269  1.00  0.00           C
ATOM     83  CD1 ILE A   7       7.327  10.014   2.236  1.00  0.00           C
ATOM     84  H   ILE A   7       7.737   6.533   0.474  1.00  0.00           H
ATOM     85  HA  ILE A   7       5.077   7.032   0.359  1.00  0.00           H
ATOM     86  HB  ILE A   7       7.359   8.939  -0.327  1.00  0.00           H
ATOM     87 HG11 ILE A   7       5.630   8.660   2.195  1.00  0.00           H
ATOM     88 HG12 ILE A   7       7.204   7.895   1.981  1.00  0.00           H
ATOM     89 HG21 ILE A   7       5.365   9.985  -1.362  1.00  0.00           H
ATOM     90 HG22 ILE A   7       5.776  10.857   0.116  1.00  0.00           H
ATOM     91 HG23 ILE A   7       4.409   9.719   0.110  1.00  0.00           H
ATOM     92 HD11 ILE A   7       8.303  10.157   1.743  1.00  0.00           H
ATOM     93 HD12 ILE A   7       7.518   9.906   3.315  1.00  0.00           H
ATOM     94 HD13 ILE A   7       6.744  10.938   2.099  1.00  0.00           H
ATOM     95  N   VAL A   8       6.093   7.247  -2.756  1.00  0.00           N
ATOM     96  CA  VAL A   8       5.562   7.224  -4.121  1.00  0.00           C
ATOM     97  C   VAL A   8       4.579   6.052  -4.308  1.00  0.00           C
ATOM     98  O   VAL A   8       3.460   6.240  -4.797  1.00  0.00           O
ATOM     99  CB  VAL A   8       6.704   7.195  -5.164  1.00  0.00           C
ATOM    100  CG1 VAL A   8       6.142   6.973  -6.576  1.00  0.00           C
ATOM    101  CG2 VAL A   8       7.545   8.477  -5.095  1.00  0.00           C
ATOM    102  H   VAL A   8       7.058   6.982  -2.586  1.00  0.00           H
ATOM    103  HA  VAL A   8       4.950   8.127  -4.266  1.00  0.00           H
ATOM    104  HB  VAL A   8       7.352   6.334  -4.914  1.00  0.00           H
ATOM    105 HG11 VAL A   8       5.634   6.003  -6.674  1.00  0.00           H
ATOM    106 HG12 VAL A   8       6.955   7.002  -7.316  1.00  0.00           H
ATOM    107 HG13 VAL A   8       5.410   7.753  -6.843  1.00  0.00           H
ATOM    108 HG21 VAL A   8       8.394   8.421  -5.794  1.00  0.00           H
ATOM    109 HG22 VAL A   8       7.958   8.659  -4.091  1.00  0.00           H
ATOM    110 HG23 VAL A   8       6.942   9.359  -5.370  1.00  0.00           H
ATOM    111  N   ALA A   9       5.025   4.839  -3.922  1.00  0.00           N
ATOM    112  CA  ALA A   9       4.155   3.667  -3.958  1.00  0.00           C
ATOM    113  C   ALA A   9       2.876   3.909  -3.135  1.00  0.00           C
ATOM    114  O   ALA A   9       1.777   3.569  -3.590  1.00  0.00           O
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ATOM    115  CB  ALA A   9       4.915   2.420  -3.502  1.00  0.00           C
ATOM    116  H   ALA A   9       5.948   4.753  -3.492  1.00  0.00           H
ATOM    117  HA  ALA A   9       3.792   3.526  -4.986  1.00  0.00           H
ATOM    118  HB1 ALA A   9       5.702   2.166  -4.228  1.00  0.00           H
ATOM    119  HB2 ALA A   9       4.247   1.551  -3.454  1.00  0.00           H
ATOM    120  HB3 ALA A   9       5.367   2.584  -2.513  1.00  0.00           H
ATOM    121  N   ARG A  10       3.026   4.500  -1.933  1.00  0.00           N
ATOM    122  CA  ARG A  10       1.881   4.824  -1.093  1.00  0.00           C
ATOM    123  C   ARG A  10       0.913   5.790  -1.775  1.00  0.00           C
ATOM    124  O   ARG A  10      -0.312   5.636  -1.644  1.00  0.00           O
ATOM    125  CB  ARG A  10       2.345   5.423   0.244  1.00  0.00           C
ATOM    126  CG  ARG A  10       1.194   5.798   1.187  1.00  0.00           C
ATOM    127  CD  ARG A  10       0.304   4.642   1.649  1.00  0.00           C
ATOM    128  NE  ARG A  10       1.041   3.785   2.569  1.00  0.00           N
ATOM    129  CZ  ARG A  10       0.518   2.740   3.216  1.00  0.00           C
ATOM    130  NH1 ARG A  10      -0.754   2.348   2.975  1.00  0.00           N
ATOM    131  NH2 ARG A  10       1.246   2.115   4.138  1.00  0.00           N
ATOM    132  H   ARG A  10       3.966   4.703  -1.584  1.00  0.00           H
ATOM    133  HA  ARG A  10       1.310   3.905  -0.915  1.00  0.00           H
ATOM    134  HB1 ARG A  10       3.028   4.721   0.740  1.00  0.00           H
ATOM    135  HB2 ARG A  10       2.929   6.331   0.034  1.00  0.00           H
ATOM    136  HG1 ARG A  10       1.628   6.287   2.074  1.00  0.00           H
ATOM    137  HG2 ARG A  10       0.545   6.542   0.703  1.00  0.00           H
ATOM    138  HD1 ARG A  10      -0.598   5.044   2.139  1.00  0.00           H
ATOM    139  HD2 ARG A  10      -0.057   4.066   0.780  1.00  0.00           H
ATOM    140  HE  ARG A  10       2.032   4.043   2.787  1.00  0.00           H
ATOM    141 HH11 ARG A  10      -1.209   2.661   2.125  1.00  0.00           H
ATOM    142 HH12 ARG A  10      -1.076   1.446   3.329  1.00  0.00           H
ATOM    143 HH21 ARG A  10       2.255   2.356   4.230  1.00  0.00           H
ATOM    144 HH22 ARG A  10       0.858   1.303   4.624  1.00  0.00           H
ATOM    145  N   SER A  11       1.453   6.823  -2.436  1.00  0.00           N
ATOM    146  CA  SER A  11       0.641   7.816  -3.122  1.00  0.00           C
ATOM    147  C   SER A  11      -0.217   7.140  -4.201  1.00  0.00           C
ATOM    148  O   SER A  11      -1.428   7.376  -4.300  1.00  0.00           O
ATOM    149  CB  SER A  11       1.539   8.925  -3.706  1.00  0.00           C
ATOM    150  OG  SER A  11       2.213   9.657  -2.706  1.00  0.00           O
ATOM    151  H   SER A  11       2.469   6.912  -2.455  1.00  0.00           H
ATOM    152  HA  SER A  11      -0.066   8.268  -2.411  1.00  0.00           H
ATOM    153  HB1 SER A  11       2.235   8.480  -4.439  1.00  0.00           H
ATOM    154  HB2 SER A  11       0.890   9.630  -4.247  1.00  0.00           H
ATOM    155  H   SER A  11       2.930   9.096  -2.353  1.00  0.00           H
ATOM    156  N   ASN A  12       0.445   6.281  -4.997  1.00  0.00           N
ATOM    157  CA  ASN A  12      -0.229   5.506  -6.028  1.00  0.00           C
ATOM    158  C   ASN A  12      -1.317   4.603  -5.412  1.00  0.00           C
ATOM    159  O   ASN A  12      -2.441   4.518  -5.926  1.00  0.00           O
ATOM    160  CB  ASN A  12       0.792   4.666  -6.797  1.00  0.00           C
ATOM    161  CG  ASN A  12       1.784   5.505  -7.600  1.00  0.00           C
ATOM    162  OD1 ASN A  12       1.639   6.698  -7.818  1.00  0.00           O
ATOM    163  ND2 ASN A  12       2.870   4.800  -8.049  1.00  0.00           N
ATOM    164  H   ASN A  12       1.454   6.166  -4.878  1.00  0.00           H
ATOM    165  HA  ASN A  12      -0.750   6.182  -6.719  1.00  0.00           H
ATOM    166  HB1 ASN A  12       1.339   4.010  -6.103  1.00  0.00           H
ATOM    167  HB2 ASN A  12       0.253   4.016  -7.503  1.00  0.00           H
ATOM    168 HD21 ASN A  12       2.881   3.786  -8.037  1.00  0.00           H
ATOM    169 HD22 ASN A  12       3.479   5.267  -8.713  1.00  0.00           H
ATOM    170  N   PHE A  13      -0.957   3.920  -4.310  1.00  0.00           N
ATOM    171  CA  PHE A  13      -1.876   3.059  -3.577  1.00  0.00           C
ATOM    172  C   PHE A  13      -3.116   3.848  -3.135  1.00  0.00           C
ATOM    173  O   PHE A  13      -4.253   3.380  -3.296  1.00  0.00           O
ATOM    174  CB  PHE A  13      -1.113   2.426  -2.384  1.00  0.00           C
ATOM    175  CG  PHE A  13      -2.004   1.778  -1.352  1.00  0.00           C
ATOM    176  CD2 PHE A  13      -2.581   2.556  -0.333  1.00  0.00           C
ATOM    177  CD1 PHE A  13      -2.306   0.410  -1.406  1.00  0.00           C
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ATOM    178  CE2 PHE A  13      -3.475   1.985   0.574  1.00  0.00           C
ATOM    179  CE1 PHE A  13      -3.205  -0.160  -0.501  1.00  0.00           C
ATOM    180  CZ  PHE A  13      -3.809   0.629   0.485  1.00  0.00           C
ATOM    181  H   PHE A  13       0.005   3.990  -3.962  1.00  0.00           H
ATOM    182  HA  PHE A  13      -2.254   2.266  -4.240  1.00  0.00           H
ATOM    183  HB1 PHE A  13      -0.396   1.699  -2.787  1.00  0.00           H
ATOM    184  HB2 PHE A  13      -0.532   3.223  -1.906  1.00  0.00           H
ATOM    185  HD2 PHE A  13      -2.368   3.623  -0.263  1.00  0.00           H
ATOM    186  HD1 PHE A  13      -1.842  -0.203  -2.181  1.00  0.00           H
ATOM    187  HE2 PHE A  13      -3.938   2.619   1.335  1.00  0.00           H
ATOM    188  HE1 PHE A  13      -3.467  -1.218  -0.577  1.00  0.00           H
ATOM    189  HZ  PHE A  13      -4.582   0.184   1.117  1.00  0.00           H
ATOM    190  N   ASN A  14      -2.871   5.037  -2.564  1.00  0.00           N
ATOM    191  CA  ASN A  14      -3.932   5.874  -2.037  1.00  0.00           C
ATOM    192  C   ASN A  14      -4.902   6.327  -3.141  1.00  0.00           C
ATOM    193  O   ASN A  14      -6.121   6.295  -2.947  1.00  0.00           O
ATOM    194  CB  ASN A  14      -3.347   7.099  -1.332  1.00  0.00           C
ATOM    195  CG  ASN A  14      -2.639   6.785  -0.015  1.00  0.00           C
ATOM    196  OD1 ASN A  14      -2.770   5.726   0.590  1.00  0.00           O
ATOM    197  ND2 ASN A  14      -1.902   7.818   0.481  1.00  0.00           N
ATOM    198  H   ASN A  14      -1.899   5.323  -2.406  1.00  0.00           H
ATOM    199  HA  ASN A  14      -4.539   5.296  -1.326  1.00  0.00           H
ATOM    200  HB1 ASN A  14      -2.668   7.636  -2.014  1.00  0.00           H
ATOM    201  HB2 ASN A  14      -4.177   7.786  -1.098  1.00  0.00           H
ATOM    202 HD21 ASN A  14      -1.680   8.633  -0.078  1.00  0.00           H
ATOM    203 HD22 ASN A  14      -1.384   7.670   1.339  1.00  0.00           H
ATOM    204  N   VAL A  15      -4.338   6.764  -4.288  1.00  0.00           N
ATOM    205  CA  VAL A  15      -5.155   7.132  -5.440  1.00  0.00           C
ATOM    206  C   VAL A  15      -6.014   5.939  -5.895  1.00  0.00           C
ATOM    207  O   VAL A  15      -7.222   6.056  -6.117  1.00  0.00           O
ATOM    208  CB  VAL A  15      -4.269   7.692  -6.581  1.00  0.00           C
ATOM    209  CG1 VAL A  15      -5.059   7.815  -7.889  1.00  0.00           C
ATOM    210  CG2 VAL A  15      -3.650   9.038  -6.179  1.00  0.00           C
ATOM    211  H   VAL A  15      -3.319   6.760  -4.383  1.00  0.00           H
ATOM    212  HA  VAL A  15      -5.886   7.896  -5.139  1.00  0.00           H
ATOM    213  HB  VAL A  15      -3.453   6.964  -6.740  1.00  0.00           H
ATOM    214 HG11 VAL A  15      -4.427   8.257  -8.674  1.00  0.00           H
ATOM    215 HG12 VAL A  15      -5.945   8.460  -7.766  1.00  0.00           H
ATOM    216 HG13 VAL A  15      -5.410   6.840  -8.258  1.00  0.00           H
ATOM    217 HG21 VAL A  15      -2.978   9.402  -6.972  1.00  0.00           H
ATOM    218 HG22 VAL A  15      -3.056   8.963  -5.259  1.00  0.00           H
ATOM    219 HG23 VAL A  15      -4.434   9.799  -6.028  1.00  0.00           H
ATOM    220  N   CYS A  16      -5.354   4.765  -6.027  1.00  0.00           N
ATOM    221  CA  CYS A  16      -6.041   3.529  -6.365  1.00  0.00           C
ATOM    222  C   CYS A  16      -7.206   3.233  -5.407  1.00  0.00           C
ATOM    223  O   CYS A  16      -8.273   2.763  -5.830  1.00  0.00           O
ATOM    224  CB  CYS A  16      -4.980   2.415  -6.377  1.00  0.00           C
ATOM    225  SG  CYS A  16      -5.593   0.707  -6.616  1.00  0.00           S
ATOM    226  H   CYS A  16      -4.350   4.723  -5.832  1.00  0.00           H
ATOM    227  HA  CYS A  16      -6.517   3.609  -7.354  1.00  0.00           H
ATOM    228  HB1 CYS A  16      -4.296   2.582  -7.220  1.00  0.00           H
ATOM    229  HB2 CYS A  16      -4.393   2.453  -5.451  1.00  0.00           H
ATOM    230  N   ARG A  17      -7.018   3.513  -4.108  1.00  0.00           N
ATOM    231  CA  ARG A  17      -8.056   3.221  -3.141  1.00  0.00           C
ATOM    232  C   ARG A  17      -9.307   4.092  -3.278  1.00  0.00           C
ATOM    233  O   ARG A  17     -10.370   3.648  -2.798  1.00  0.00           O
ATOM    234  CB  ARG A  17      -7.530   3.340  -1.699  1.00  0.00           C
ATOM    235  CG  ARG A  17      -6.622   2.187  -1.269  1.00  0.00           C
ATOM    236  CD  ARG A  17      -7.306   0.824  -1.245  1.00  0.00           C
ATOM    237  NE  ARG A  17      -8.323   0.670  -0.186  1.00  0.00           N
ATOM    238  CZ  ARG A  17      -9.608   0.349  -0.396  1.00  0.00           C
ATOM    239  NH1 ARG A  17     -10.359   0.895  -1.357  1.00  0.00           N
ATOM    240  NH2 ARG A  17     -10.170  -0.566   0.423  1.00  0.00           N
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ATOM    241  H   ARG A  17      -6.087   3.784  -3.780  1.00  0.00           H
ATOM    242  HA  ARG A  17      -8.429   2.204  -3.339  1.00  0.00           H
ATOM    243  HB1 ARG A  17      -7.010   4.306  -1.603  1.00  0.00           H
ATOM    244  HB2 ARG A  17      -8.402   3.387  -1.028  1.00  0.00           H
ATOM    245  HG1 ARG A  17      -5.746   2.119  -1.932  1.00  0.00           H
ATOM    246  HG2 ARG A  17      -6.220   2.404  -0.267  1.00  0.00           H
ATOM    247  HD1 ARG A  17      -7.774   0.577  -2.207  1.00  0.00           H
ATOM    248  HD2 ARG A  17      -6.548   0.051  -1.044  1.00  0.00           H
ATOM    249  HE  ARG A  17      -7.967   0.284   0.705  1.00  0.00           H
ATOM    250 HH11 ARG A  17     -10.081   1.728  -1.878  1.00  0.00           H
ATOM    251 HH12 ARG A  17     -11.110   0.331  -1.759  1.00  0.00           H
ATOM    252 HH21 ARG A  17      -9.554  -0.949   1.166  1.00  0.00           H
ATOM    253 HH22 ARG A  17     -11.172  -0.517   0.572  1.00  0.00           H
ATOM    254  N   LEU A  18      -9.185   5.300  -3.842  1.00  0.00           N
ATOM    255  CA  LEU A  18     -10.252   6.301  -3.843  1.00  0.00           C
ATOM    256  C   LEU A  18     -11.582   5.834  -4.466  1.00  0.00           C
ATOM    257  O   LEU A  18     -12.628   6.095  -3.875  1.00  0.00           O
ATOM    258  CB  LEU A  18      -9.782   7.614  -4.487  1.00  0.00           C
ATOM    259  CG  LEU A  18      -8.632   8.346  -3.768  1.00  0.00           C
ATOM    260  CD1 LEU A  18      -8.214   9.573  -4.588  1.00  0.00           C
ATOM    261  CD2 LEU A  18      -8.979   8.729  -2.325  1.00  0.00           C
ATOM    262  H   LEU A  18      -8.284   5.554  -4.246  1.00  0.00           H
ATOM    263  HA  LEU A  18     -10.547   6.486  -2.800  1.00  0.00           H
ATOM    264  HB1 LEU A  18      -9.470   7.416  -5.524  1.00  0.00           H
ATOM    265  HB2 LEU A  18     -10.665   8.274  -4.536  1.00  0.00           H
ATOM    266  HG  LEU A  18      -7.766   7.668  -3.724  1.00  0.00           H
ATOM    267 HD11 LEU A  18      -7.938   9.289  -5.617  1.00  0.00           H
ATOM    268 HD12 LEU A  18      -7.345  10.079  -4.136  1.00  0.00           H
ATOM    269 HD13 LEU A  18      -9.029  10.314  -4.656  1.00  0.00           H
ATOM    270 HD21 LEU A  18      -8.144   9.274  -1.854  1.00  0.00           H
ATOM    271 HD22 LEU A  18      -9.173   7.844  -1.699  1.00  0.00           H
ATOM    272 HD23 LEU A  18      -9.871   9.377  -2.277  1.00  0.00           H
ATOM    273  N   PRO A  19     -11.575   5.129  -5.638  1.00  0.00           N
ATOM    274  CA  PRO A  19     -12.855   4.637  -6.169  1.00  0.00           C
ATOM    275  C   PRO A  19     -13.315   3.312  -5.533  1.00  0.00           C
ATOM    276  O   PRO A  19     -14.281   2.706  -5.989  1.00  0.00           O
ATOM    277  CB  PRO A  19     -12.592   4.483  -7.675  1.00  0.00           C
ATOM    278  CG  PRO A  19     -11.099   4.142  -7.728  1.00  0.00           C
ATOM    279  CD  PRO A  19     -10.490   5.030  -6.640  1.00  0.00           C
ATOM    280  HA  PRO A  19     -13.654   5.359  -5.948  1.00  0.00           H
ATOM    281  HB1 PRO A  19     -13.246   3.722  -8.118  1.00  0.00           H
ATOM    282  HB2 PRO A  19     -12.789   5.442  -8.181  1.00  0.00           H
ATOM    283  HG1 PRO A  19     -10.941   3.078  -7.488  1.00  0.00           H
ATOM    284  HG2 PRO A  19     -10.641   4.325  -8.710  1.00  0.00           H
ATOM    285  HD1 PRO A  19      -9.576   4.610  -6.217  1.00  0.00           H
ATOM    286  HD2 PRO A  19     -10.254   6.031  -7.040  1.00  0.00           H
ATOM    287  N   GLY A  20     -12.593   2.869  -4.464  1.00  0.00           N
ATOM    288  CA  GLY A  20     -13.001   1.719  -3.703  1.00  0.00           C
ATOM    289  C   GLY A  20     -12.147   0.471  -3.904  1.00  0.00           C
ATOM    290  O   GLY A  20     -12.325  -0.534  -3.193  1.00  0.00           O
ATOM    291  H   GLY A  20     -11.856   3.444  -4.053  1.00  0.00           H
ATOM    292  HA1 GLY A  20     -13.007   1.947  -2.626  1.00  0.00           H
ATOM    293  HA2 GLY A  20     -14.025   1.445  -3.999  1.00  0.00           H
ATOM    294  N   THR A  21     -11.205   0.534  -4.861  1.00  0.00           N
ATOM    295  CA  THR A  21     -10.501  -0.628  -5.359  1.00  0.00           C
ATOM    296  C   THR A  21      -9.988  -1.505  -4.211  1.00  0.00           C
ATOM    297  O   THR A  21      -9.243  -1.066  -3.334  1.00  0.00           O
ATOM    298  CB  THR A  21      -9.294  -0.175  -6.218  1.00  0.00           C
ATOM    299  OG1 THR A  21      -9.714   0.851  -7.101  1.00  0.00           O
ATOM    300  CG2 THR A  21      -8.705  -1.351  -6.987  1.00  0.00           C
ATOM    301  H   THR A  21     -11.133   1.370  -5.437  1.00  0.00           H
ATOM    302  HA  THR A  21     -11.184  -1.200  -6.006  1.00  0.00           H
ATOM    303  HB  THR A  21      -8.550   0.228  -5.518  1.00  0.00           H
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ATOM    304  HG1 THR A  21      -9.134   1.620  -6.909  1.00  0.00           H
ATOM    305 HG21 THR A  21      -8.398  -2.157  -6.304  1.00  0.00           H
ATOM    306 HG22 THR A  21      -7.823  -1.024  -7.554  1.00  0.00           H
ATOM    307 HG23 THR A  21      -9.439  -1.749  -7.707  1.00  0.00           H
ATOM    308  N   PRO A  22     -10.290  -2.834  -4.267  1.00  0.00           N
ATOM    309  CA  PRO A  22      -9.824  -3.699  -3.195  1.00  0.00           C
ATOM    310  C   PRO A  22      -8.313  -3.624  -2.964  1.00  0.00           C
ATOM    311  O   PRO A  22      -7.493  -3.619  -3.888  1.00  0.00           O
ATOM    312  CB  PRO A  22     -10.258  -5.098  -3.664  1.00  0.00           C
ATOM    313  CG  PRO A  22     -11.583  -4.814  -4.379  1.00  0.00           C
ATOM    314  CD  PRO A  22     -11.335  -3.475  -5.087  1.00  0.00           C
ATOM    315  HA  PRO A  22     -10.336  -3.427  -2.252  1.00  0.00           H
ATOM    316  HB1 PRO A  22      -9.509  -5.486  -4.375  1.00  0.00           H
ATOM    317  HB2 PRO A  22     -10.347  -5.808  -2.830  1.00  0.00           H
ATOM    318  HG1 PRO A  22     -11.875  -5.609  -5.079  1.00  0.00           H
ATOM    319  HG2 PRO A  22     -12.393  -4.704  -3.640  1.00  0.00           H
ATOM    320  HD1 PRO A  22     -10.977  -3.622  -6.118  1.00  0.00           H
ATOM    321  HD2 PRO A  22     -12.240  -2.853  -5.112  1.00  0.00           H
ATOM    322  N   GLU A  23      -7.972  -3.743  -1.655  1.00  0.00           N
ATOM    323  CA  GLU A  23      -6.615  -3.615  -1.127  1.00  0.00           C
ATOM    324  C   GLU A  23      -5.588  -4.395  -1.941  1.00  0.00           C
ATOM    325  O   GLU A  23      -4.486  -3.904  -2.195  1.00  0.00           O
ATOM    326  CB  GLU A  23      -6.558  -4.113   0.335  1.00  0.00           C
ATOM    327  CG  GLU A  23      -7.444  -3.346   1.316  1.00  0.00           C
ATOM    328  CD  GLU A  23      -7.094  -1.847   1.443  1.00  0.00           C
ATOM    329  OE1 GLU A  23      -5.968  -1.484   1.029  1.00  0.00           O
ATOM    330  OE2 GLU A  23      -7.991  -1.104   1.948  1.00  0.00           O
ATOM    331  H   GLU A  23      -8.713  -3.546  -0.988  1.00  0.00           H
ATOM    332  HA  GLU A  23      -6.286  -2.567  -1.155  1.00  0.00           H
ATOM    333  HB1 GLU A  23      -6.812  -5.186   0.357  1.00  0.00           H
ATOM    334  HB2 GLU A  23      -5.513  -4.013   0.655  1.00  0.00           H
ATOM    335  HG1 GLU A  23      -8.519  -3.441   1.082  1.00  0.00           H
ATOM    336  HG2 GLU A  23      -7.341  -3.798   2.317  1.00  0.00           H
ATOM    337  N   ALA A  24      -5.903  -5.672  -2.278  1.00  0.00           N
ATOM    338  CA  ALA A  24      -4.950  -6.544  -2.951  1.00  0.00           C
ATOM    339  C   ALA A  24      -4.503  -5.993  -4.315  1.00  0.00           C
ATOM    340  O   ALA A  24      -3.342  -6.176  -4.692  1.00  0.00           O
ATOM    341  CB  ALA A  24      -5.529  -7.950  -3.107  1.00  0.00           C
ATOM    342  H   ALA A  24      -6.833  -6.014  -2.060  1.00  0.00           H
ATOM    343  HA  ALA A  24      -4.029  -6.590  -2.355  1.00  0.00           H
ATOM    344  HB1 ALA A  24      -5.756  -8.390  -2.124  1.00  0.00           H
ATOM    345  HB2 ALA A  24      -4.797  -8.596  -3.612  1.00  0.00           H
ATOM    346  HB3 ALA A  24      -6.449  -7.938  -3.713  1.00  0.00           H
ATOM    347  N   LEU A  25      -5.451  -5.391  -5.066  1.00  0.00           N
ATOM    348  CA  LEU A  25      -5.115  -4.798  -6.357  1.00  0.00           C
ATOM    349  C   LEU A  25      -4.272  -3.526  -6.201  1.00  0.00           C
ATOM    350  O   LEU A  25      -3.357  -3.274  -6.984  1.00  0.00           O
ATOM    351  CB  LEU A  25      -6.381  -4.497  -7.173  1.00  0.00           C
ATOM    352  CG  LEU A  25      -7.313  -5.696  -7.430  1.00  0.00           C
ATOM    353  CD1 LEU A  25      -8.547  -5.234  -8.216  1.00  0.00           C
ATOM    354  CD2 LEU A  25      -6.600  -6.860  -8.128  1.00  0.00           C
ATOM    355  H   LEU A  25      -6.307  -5.075  -4.606  1.00  0.00           H
ATOM    356  HA  LEU A  25      -4.452  -5.494  -6.886  1.00  0.00           H
ATOM    357  HB1 LEU A  25      -6.949  -3.703  -6.664  1.00  0.00           H
ATOM    358  HB2 LEU A  25      -6.048  -4.069  -8.135  1.00  0.00           H
ATOM    359  HG  LEU A  25      -7.668  -6.063  -6.448  1.00  0.00           H
ATOM    360 HD11 LEU A  25      -9.067  -4.412  -7.699  1.00  0.00           H
ATOM    361 HD12 LEU A  25      -9.267  -6.057  -8.353  1.00  0.00           H
ATOM    362 HD13 LEU A  25      -8.269  -4.867  -9.218  1.00  0.00           H
ATOM    363 HD21 LEU A  25      -7.299  -7.687  -8.333  1.00  0.00           H
ATOM    364 HD22 LEU A  25      -5.782  -7.270  -7.516  1.00  0.00           H
ATOM    365 HD23 LEU A  25      -6.170  -6.542  -9.093  1.00  0.00           H
ATOM    366  N   CYS A  26      -4.586  -2.706  -5.167  1.00  0.00           N
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ATOM    367  CA  CYS A  26      -3.778  -1.525  -4.934  1.00  0.00           C
ATOM    368  C   CYS A  26      -2.362  -1.879  -4.448  1.00  0.00           C
ATOM    369  O   CYS A  26      -1.430  -1.101  -4.705  1.00  0.00           O
ATOM    370  CB  CYS A  26      -4.476  -0.525  -4.018  1.00  0.00           C
ATOM    371  SG  CYS A  26      -6.085   0.064  -4.693  1.00  0.00           S
ATOM    372  H   CYS A  26      -5.403  -2.889  -4.588  1.00  0.00           H
ATOM    373  HA  CYS A  26      -3.600  -1.034  -5.903  1.00  0.00           H
ATOM    374  HB1 CYS A  26      -4.736  -0.972  -3.044  1.00  0.00           H
ATOM    375  HB2 CYS A  26      -3.822   0.334  -3.824  1.00  0.00           H
ATOM    376  N   ALA A  27      -2.219  -3.038  -3.789  1.00  0.00           N
ATOM    377  CA  ALA A  27      -0.925  -3.611  -3.434  1.00  0.00           C
ATOM    378  C   ALA A  27      -0.139  -4.032  -4.694  1.00  0.00           C
ATOM    379  O   ALA A  27       0.999  -3.594  -4.890  1.00  0.00           O
ATOM    380  CB  ALA A  27      -1.113  -4.769  -2.453  1.00  0.00           C
ATOM    381  H   ALA A  27      -3.059  -3.550  -3.521  1.00  0.00           H
ATOM    382  HA  ALA A  27      -0.298  -2.835  -2.978  1.00  0.00           H
ATOM    383  HB1 ALA A  27      -1.612  -4.409  -1.541  1.00  0.00           H
ATOM    384  HB2 ALA A  27      -0.127  -5.168  -2.185  1.00  0.00           H
ATOM    385  HB3 ALA A  27      -1.726  -5.566  -2.898  1.00  0.00           H
ATOM    386  N   THR A  28      -0.739  -4.891  -5.549  1.00  0.00           N
ATOM    387  CA  THR A  28      -0.010  -5.367  -6.720  1.00  0.00           C
ATOM    388  C   THR A  28       0.355  -4.256  -7.732  1.00  0.00           C
ATOM    389  O   THR A  28       1.386  -4.351  -8.390  1.00  0.00           O
ATOM    390  CB  THR A  28      -0.727  -6.523  -7.428  1.00  0.00           C
ATOM    391  OG1 THR A  28      -1.977  -6.014  -7.900  1.00  0.00           O
ATOM    392  CG2 THR A  28      -0.912  -7.765  -6.556  1.00  0.00           C
ATOM    393  H   THR A  28      -1.704  -5.193  -5.399  1.00  0.00           H
ATOM    394  HA  THR A  28       0.973  -5.738  -6.392  1.00  0.00           H
ATOM    395  HB  THR A  28      -0.077  -6.775  -8.286  1.00  0.00           H
ATOM    396  HG1 THR A  28      -2.363  -6.673  -8.498  1.00  0.00           H
ATOM    397 HG21 THR A  28       0.058  -8.135  -6.188  1.00  0.00           H
ATOM    398 HG22 THR A  28      -1.373  -8.574  -7.147  1.00  0.00           H
ATOM    399 HG23 THR A  28      -1.567  -7.559  -5.698  1.00  0.00           H
ATOM    400  N   TYR A  29      -0.495  -3.202  -7.803  1.00  0.00           N
ATOM    401  CA  TYR A  29      -0.228  -2.054  -8.659  1.00  0.00           C
ATOM    402  C   TYR A  29       1.059  -1.300  -8.268  1.00  0.00           C
ATOM    403  O   TYR A  29       1.664  -0.629  -9.097  1.00  0.00           O
ATOM    404  CB  TYR A  29      -1.479  -1.137  -8.574  1.00  0.00           C
ATOM    405  CG  TYR A  29      -1.366   0.294  -9.052  1.00  0.00           C
ATOM    406  CD1 TYR A  29      -0.742   0.664 -10.249  1.00  0.00           C
ATOM    407  CD2 TYR A  29      -1.907   1.318  -8.262  1.00  0.00           C
ATOM    408  CE1 TYR A  29      -0.629   2.003 -10.622  1.00  0.00           C
ATOM    409  CE2 TYR A  29      -1.811   2.661  -8.619  1.00  0.00           C
ATOM    410  CZ  TYR A  29      -1.148   3.008  -9.800  1.00  0.00           C
ATOM    411  OH  TYR A  29      -1.019   4.343 -10.076  1.00  0.00           O
ATOM    412  H   TYR A  29      -1.426  -3.295  -7.393  1.00  0.00           H
ATOM    413  HA  TYR A  29      -0.054  -2.381  -9.696  1.00  0.00           H
ATOM    414  HB1 TYR A  29      -2.293  -1.658  -9.106  1.00  0.00           H
ATOM    415  HB2 TYR A  29      -1.788  -1.116  -7.520  1.00  0.00           H
ATOM    416  HD1 TYR A  29      -0.295  -0.096 -10.889  1.00  0.00           H
ATOM    417  HD2 TYR A  29      -2.399   1.058  -7.322  1.00  0.00           H
ATOM    418  HE1 TYR A  29      -0.114   2.269 -11.551  1.00  0.00           H
ATOM    419  HE2 TYR A  29      -2.211   3.448  -7.980  1.00  0.00           H
ATOM    420  HH  TYR A  29      -0.521   4.451 -10.901  1.00  0.00           H
ATOM    421  N   THR A  30       1.415  -1.371  -6.954  1.00  0.00           N
ATOM    422  CA  THR A  30       2.351  -0.433  -6.371  1.00  0.00           C
ATOM    423  C   THR A  30       3.598  -1.036  -5.723  1.00  0.00           C
ATOM    424  O   THR A  30       4.501  -0.298  -5.324  1.00  0.00           O
ATOM    425  CB  THR A  30       1.632   0.432  -5.308  1.00  0.00           C
ATOM    426  OG1 THR A  30       1.204  -0.402  -4.224  1.00  0.00           O
ATOM    427  CG2 THR A  30       0.476   1.211  -5.909  1.00  0.00           C
ATOM    428  H   THR A  30       0.845  -1.936  -6.329  1.00  0.00           H
ATOM    429  HA  THR A  30       2.706   0.211  -7.187  1.00  0.00           H
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ATOM    430  HB  THR A  30       2.373   1.123  -4.883  1.00  0.00           H
ATOM    431  HG1 THR A  30       0.286  -0.712  -4.393  1.00  0.00           H
ATOM    432 HG21 THR A  30       0.780   1.713  -6.837  1.00  0.00           H
ATOM    433 HG22 THR A  30       0.119   1.966  -5.205  1.00  0.00           H
ATOM    434 HG23 THR A  30      -0.356   0.544  -6.156  1.00  0.00           H
ATOM    435  N   GLY A  31       3.605  -2.380  -5.539  1.00  0.00           N
ATOM    436  CA  GLY A  31       4.569  -2.985  -4.655  1.00  0.00           C
ATOM    437  C   GLY A  31       4.290  -2.809  -3.163  1.00  0.00           C
ATOM    438  O   GLY A  31       5.093  -3.257  -2.329  1.00  0.00           O
ATOM    439  H   GLY A  31       2.781  -2.919  -5.797  1.00  0.00           H
ATOM    440  HA1 GLY A  31       4.612  -4.067  -4.840  1.00  0.00           H
ATOM    441  HA2 GLY A  31       5.569  -2.569  -4.844  1.00  0.00           H
ATOM    442  N   CYS A  32       3.163  -2.171  -2.801  1.00  0.00           N
ATOM    443  CA  CYS A  32       2.723  -2.212  -1.424  1.00  0.00           C
ATOM    444  C   CYS A  32       2.300  -3.669  -1.071  1.00  0.00           C
ATOM    445  O   CYS A  32       1.984  -4.475  -1.943  1.00  0.00           O
ATOM    446  CB  CYS A  32       1.567  -1.240  -1.157  1.00  0.00           C
ATOM    447  SG  CYS A  32       1.910   0.538  -1.547  1.00  0.00           S
ATOM    448  H   CYS A  32       2.478  -1.916  -3.514  1.00  0.00           H
ATOM    449  HA  CYS A  32       3.562  -1.943  -0.773  1.00  0.00           H
ATOM    450  HB1 CYS A  32       0.693  -1.494  -1.773  1.00  0.00           H
ATOM    451  HB2 CYS A  32       1.274  -1.298  -0.102  1.00  0.00           H
ATOM    452  N   ILE A  33       2.313  -3.957   0.252  1.00  0.00           N
ATOM    453  CA  ILE A  33       1.980  -5.270   0.747  1.00  0.00           C
ATOM    454  C   ILE A  33       0.868  -5.165   1.796  1.00  0.00           C
ATOM    455  O   ILE A  33       0.483  -4.087   2.269  1.00  0.00           O
ATOM    456  CB  ILE A  33       3.224  -6.052   1.276  1.00  0.00           C
ATOM    457  CG1 ILE A  33       3.823  -5.350   2.510  1.00  0.00           C
ATOM    458  CG2 ILE A  33       4.214  -6.293   0.130  1.00  0.00           C
ATOM    459  CD1 ILE A  33       5.067  -6.007   3.106  1.00  0.00           C
ATOM    460  H   ILE A  33       2.566  -3.222   0.917  1.00  0.00           H
ATOM    461  HA  ILE A  33       1.574  -5.825  -0.112  1.00  0.00           H
ATOM    462  HB  ILE A  33       2.860  -7.045   1.605  1.00  0.00           H
ATOM    463 HG11 ILE A  33       4.072  -4.313   2.246  1.00  0.00           H
ATOM    464 HG12 ILE A  33       3.037  -5.291   3.285  1.00  0.00           H
ATOM    465 HG21 ILE A  33       5.068  -6.898   0.462  1.00  0.00           H
ATOM    466 HG22 ILE A  33       4.613  -5.356  -0.276  1.00  0.00           H
ATOM    467 HG23 ILE A  33       3.723  -6.827  -0.699  1.00  0.00           H
ATOM    468 HD11 ILE A  33       4.898  -7.075   3.328  1.00  0.00           H
ATOM    469 HD12 ILE A  33       5.353  -5.510   4.045  1.00  0.00           H
ATOM    470 HD13 ILE A  33       5.932  -5.926   2.433  1.00  0.00           H
ATOM    471  N   ILE A  34       0.326  -6.348   2.165  1.00  0.00           N
ATOM    472  CA  ILE A  34      -0.724  -6.479   3.161  1.00  0.00           C
ATOM    473  C   ILE A  34      -0.215  -7.497   4.185  1.00  0.00           C
ATOM    474  O   ILE A  34       0.159  -8.614   3.826  1.00  0.00           O
ATOM    475  CB  ILE A  34      -2.082  -6.919   2.553  1.00  0.00           C
ATOM    476  CG1 ILE A  34      -2.408  -6.085   1.300  1.00  0.00           C
ATOM    477  CG2 ILE A  34      -3.172  -6.838   3.632  1.00  0.00           C
ATOM    478  CD1 ILE A  34      -3.715  -6.446   0.597  1.00  0.00           C
ATOM    479  H   ILE A  34       0.702  -7.213   1.787  1.00  0.00           H
ATOM    480  HA  ILE A  34      -0.838  -5.494   3.625  1.00  0.00           H
ATOM    481  HB  ILE A  34      -1.973  -7.976   2.248  1.00  0.00           H
ATOM    482 HG11 ILE A  34      -2.414  -5.015   1.568  1.00  0.00           H
ATOM    483 HG12 ILE A  34      -1.584  -6.199   0.578  1.00  0.00           H
ATOM    484 HG21 ILE A  34      -2.889  -7.396   4.538  1.00  0.00           H
ATOM    485 HG22 ILE A  34      -4.125  -7.257   3.278  1.00  0.00           H
ATOM    486 HG23 ILE A  34      -3.350  -5.792   3.934  1.00  0.00           H
ATOM    487 HD11 ILE A  34      -3.725  -7.504   0.281  1.00  0.00           H
ATOM    488 HD12 ILE A  34      -3.838  -5.822  -0.298  1.00  0.00           H
ATOM    489 HD13 ILE A  34      -4.596  -6.283   1.235  1.00  0.00           H
ATOM    490  N   ILE A  35      -0.187  -7.066   5.472  1.00  0.00           N
ATOM    491  CA  ILE A  35       0.406  -7.876   6.511  1.00  0.00           C
ATOM    492  C   ILE A  35      -0.486  -7.896   7.748  1.00  0.00           C
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ATOM    493  O   ILE A  35      -1.280  -6.979   8.016  1.00  0.00           O
ATOM    494  CB  ILE A  35       1.849  -7.408   6.903  1.00  0.00           C
ATOM    495  CG1 ILE A  35       1.857  -6.057   7.644  1.00  0.00           C
ATOM    496  CG2 ILE A  35       2.769  -7.422   5.676  1.00  0.00           C
ATOM    497  CD1 ILE A  35       3.196  -5.713   8.298  1.00  0.00           C
ATOM    498  H   ILE A  35      -0.505  -6.121   5.685  1.00  0.00           H
ATOM    499  HA  ILE A  35       0.482  -8.886   6.084  1.00  0.00           H
ATOM    500  HB  ILE A  35       2.233  -8.173   7.606  1.00  0.00           H
ATOM    501 HG11 ILE A  35       1.572  -5.254   6.943  1.00  0.00           H
ATOM    502 HG12 ILE A  35       1.085  -6.050   8.429  1.00  0.00           H
ATOM    503 HG21 ILE A  35       3.811  -7.220   5.962  1.00  0.00           H
ATOM    504 HG22 ILE A  35       2.474  -6.650   4.951  1.00  0.00           H
ATOM    505 HG23 ILE A  35       2.740  -8.390   5.155  1.00  0.00           H
ATOM    506 HD11 ILE A  35       3.575  -6.556   8.906  1.00  0.00           H
ATOM    507 HD12 ILE A  35       3.095  -4.854   8.972  1.00  0.00           H
ATOM    508 HD13 ILE A  35       3.973  -5.474   7.557  1.00  0.00           H
ATOM    509  N   PRO A  36      -0.298  -8.914   8.627  1.00  0.00           N
ATOM    510  CA  PRO A  36      -0.998  -8.907   9.922  1.00  0.00           C
ATOM    511  C   PRO A  36      -0.332  -8.000  10.966  1.00  0.00           C
ATOM    512  O   PRO A  36      -0.944  -7.655  11.972  1.00  0.00           O
ATOM    513  CB  PRO A  36      -0.967 -10.386  10.353  1.00  0.00           C
ATOM    514  CG  PRO A  36       0.326 -10.914   9.719  1.00  0.00           C
ATOM    515  CD  PRO A  36       0.371 -10.209   8.359  1.00  0.00           C
ATOM    516  HA  PRO A  36      -2.018  -8.525   9.805  1.00  0.00           H
ATOM    517  HB1 PRO A  36      -1.005 -10.492  11.445  1.00  0.00           H
ATOM    518  HB2 PRO A  36      -1.845 -10.903   9.934  1.00  0.00           H
ATOM    519  HG1 PRO A  36       1.196 -10.619  10.326  1.00  0.00           H
ATOM    520  HG2 PRO A  36       0.346 -12.007   9.616  1.00  0.00           H
ATOM    521  HD1 PRO A  36       1.396 -10.067   7.993  1.00  0.00           H
ATOM    522  HD2 PRO A  36      -0.191 -10.767   7.592  1.00  0.00           H
ATOM    523  N   GLY A  37       0.973  -7.662  10.759  1.00  0.00           N
ATOM    524  CA  GLY A  37       1.624  -6.747  11.673  1.00  0.00           C
ATOM    525  C   GLY A  37       0.919  -5.393  11.714  1.00  0.00           C
ATOM    526  O   GLY A  37       0.728  -4.762  10.669  1.00  0.00           O
ATOM    527  H   GLY A  37       1.379  -7.807   9.844  1.00  0.00           H
ATOM    528  HA1 GLY A  37       1.678  -7.193  12.678  1.00  0.00           H
ATOM    529  HA2 GLY A  37       2.646  -6.552  11.321  1.00  0.00           H
ATOM    530  N   ALA A  38       0.586  -4.922  12.935  1.00  0.00           N
ATOM    531  CA  ALA A  38      -0.016  -3.601  13.129  1.00  0.00           C
ATOM    532  C   ALA A  38       0.972  -2.470  12.764  1.00  0.00           C
ATOM    533  O   ALA A  38       0.564  -1.415  12.305  1.00  0.00           O
ATOM    534  CB  ALA A  38      -0.498  -3.445  14.571  1.00  0.00           C
ATOM    535  H   ALA A  38       0.563  -5.587  13.702  1.00  0.00           H
ATOM    536  HA  ALA A  38      -0.866  -3.474  12.443  1.00  0.00           H
ATOM    537  HB1 ALA A  38      -1.276  -4.186  14.809  1.00  0.00           H
ATOM    538  HB2 ALA A  38      -0.926  -2.442  14.704  1.00  0.00           H
ATOM    539  HB3 ALA A  38       0.334  -3.560  15.284  1.00  0.00           H
ATOM    540  N   THR A  39       2.277  -2.730  13.098  1.00  0.00           N
ATOM    541  CA  THR A  39       3.371  -1.925  12.570  1.00  0.00           C
ATOM    542  C   THR A  39       3.934  -2.645  11.333  1.00  0.00           C
ATOM    543  O   THR A  39       3.895  -3.877  11.251  1.00  0.00           O
ATOM    544  CB  THR A  39       4.439  -1.731  13.681  1.00  0.00           C
ATOM    545  OG1 THR A  39       3.816  -1.197  14.836  1.00  0.00           O
ATOM    546  CG2 THR A  39       5.567  -0.789  13.295  1.00  0.00           C
ATOM    547  H   THR A  39       2.514  -3.718  13.162  1.00  0.00           H
ATOM    548  HA  THR A  39       2.951  -0.946  12.300  1.00  0.00           H
ATOM    549  HB  THR A  39       4.864  -2.736  13.899  1.00  0.00           H
ATOM    550  HG1 THR A  39       2.995  -1.701  14.967  1.00  0.00           H
ATOM    551 HG21 THR A  39       6.169  -1.167  12.456  1.00  0.00           H
ATOM    552 HG22 THR A  39       6.229  -0.651  14.162  1.00  0.00           H
ATOM    553 HG23 THR A  39       5.164   0.202  13.028  1.00  0.00           H
ATOM    554  N   CYS A  40       4.444  -1.827  10.390  1.00  0.00           N
ATOM    555  CA  CYS A  40       5.172  -2.275   9.216  1.00  0.00           C
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ATOM    556  C   CYS A  40       6.683  -2.321   9.538  1.00  0.00           C
ATOM    557  O   CYS A  40       7.162  -1.470  10.295  1.00  0.00           O
ATOM    558  CB  CYS A  40       4.959  -1.280   8.067  1.00  0.00           C
ATOM    559  SG  CYS A  40       3.207  -1.024   7.567  1.00  0.00           S
ATOM    560  H   CYS A  40       4.559  -0.849  10.636  1.00  0.00           H
ATOM    561  HA  CYS A  40       4.785  -3.264   8.948  1.00  0.00           H
ATOM    562  HB1 CYS A  40       5.303  -0.279   8.377  1.00  0.00           H
ATOM    563  HB2 CYS A  40       5.552  -1.535   7.181  1.00  0.00           H
ATOM    564  N   PRO A  41       7.432  -3.276   8.943  1.00  0.00           N
ATOM    565  CA  PRO A  41       8.892  -3.223   9.066  1.00  0.00           C
ATOM    566  C   PRO A  41       9.392  -1.983   8.298  1.00  0.00           C
ATOM    567  O   PRO A  41       8.691  -1.455   7.431  1.00  0.00           O
ATOM    568  CB  PRO A  41       9.351  -4.569   8.478  1.00  0.00           C
ATOM    569  CG  PRO A  41       8.296  -4.872   7.405  1.00  0.00           C
ATOM    570  CD  PRO A  41       6.989  -4.262   7.937  1.00  0.00           C
ATOM    571  HA  PRO A  41       9.165  -3.107  10.125  1.00  0.00           H
ATOM    572  HB1 PRO A  41      10.351  -4.511   8.023  1.00  0.00           H
ATOM    573  HB2 PRO A  41       9.340  -5.323   9.283  1.00  0.00           H
ATOM    574  HG1 PRO A  41       8.613  -4.422   6.454  1.00  0.00           H
ATOM    575  HG2 PRO A  41       8.194  -5.950   7.215  1.00  0.00           H
ATOM    576  HD1 PRO A  41       6.409  -3.777   7.137  1.00  0.00           H
ATOM    577  HD2 PRO A  41       6.345  -5.013   8.423  1.00  0.00           H
ATOM    578  N   GLY A  42      10.598  -1.484   8.650  1.00  0.00           N
ATOM    579  CA  GLY A  42      11.088  -0.201   8.155  1.00  0.00           C
ATOM    580  C   GLY A  42      11.163  -0.050   6.621  1.00  0.00           C
ATOM    581  O   GLY A  42      10.791   1.002   6.088  1.00  0.00           O
ATOM    582  H   GLY A  42      11.166  -2.005   9.306  1.00  0.00           H
ATOM    583  HA1 GLY A  42      10.447   0.615   8.512  1.00  0.00           H
ATOM    584  HA2 GLY A  42      12.094  -0.052   8.573  1.00  0.00           H
ATOM    585  N   ASP A  43      11.659  -1.118   5.977  1.00  0.00           N
ATOM    586  CA  ASP A  43      11.635  -1.319   4.528  1.00  0.00           C
ATOM    587  C   ASP A  43      10.282  -0.999   3.862  1.00  0.00           C
ATOM    588  O   ASP A  43      10.216  -0.620   2.695  1.00  0.00           O
ATOM    589  CB  ASP A  43      11.973  -2.815   4.262  1.00  0.00           C
ATOM    590  CG  ASP A  43      11.174  -3.755   5.211  1.00  0.00           C
ATOM    591  OD2 ASP A  43      11.526  -3.683   6.440  1.00  0.00           O
ATOM    592  OD1 ASP A  43      10.247  -4.446   4.743  1.00  0.00           O
ATOM    593  H   ASP A  43      11.768  -2.030   6.485  1.00  0.00           H
ATOM    594  HA  ASP A  43      12.365  -0.666   4.028  1.00  0.00           H
ATOM    595  HB1 ASP A  43      11.760  -3.038   3.209  1.00  0.00           H
ATOM    596  HB2 ASP A  43      13.049  -2.965   4.444  1.00  0.00           H
ATOM    597  N   TYR A  44       9.214  -1.245   4.652  1.00  0.00           N
ATOM    598  CA  TYR A  44       7.839  -1.181   4.240  1.00  0.00           C
ATOM    599  C   TYR A  44       7.037  -0.202   5.110  1.00  0.00           C
ATOM    600  O   TYR A  44       5.804  -0.302   5.224  1.00  0.00           O
ATOM    601  CB  TYR A  44       7.226  -2.603   4.173  1.00  0.00           C
ATOM    602  CG  TYR A  44       7.249  -3.155   2.771  1.00  0.00           C
ATOM    603  CD2 TYR A  44       8.321  -3.910   2.271  1.00  0.00           C
ATOM    604  CD1 TYR A  44       6.196  -2.853   1.904  1.00  0.00           C
ATOM    605  CE2 TYR A  44       8.330  -4.337   0.942  1.00  0.00           C
ATOM    606  CE1 TYR A  44       6.181  -3.298   0.587  1.00  0.00           C
ATOM    607  CZ  TYR A  44       7.266  -4.029   0.082  1.00  0.00           C
ATOM    608  OH  TYR A  44       7.320  -4.456  -1.208  1.00  0.00           O
ATOM    609  H   TYR A  44       9.368  -1.572   5.603  1.00  0.00           H
ATOM    610  HA  TYR A  44       7.823  -0.734   3.236  1.00  0.00           H
ATOM    611  HB1 TYR A  44       7.798  -3.250   4.851  1.00  0.00           H
ATOM    612  HB2 TYR A  44       6.194  -2.564   4.538  1.00  0.00           H
ATOM    613  HD2 TYR A  44       9.149  -4.167   2.939  1.00  0.00           H
ATOM    614  HD1 TYR A  44       5.352  -2.270   2.267  1.00  0.00           H
ATOM    615  HE2 TYR A  44       9.168  -4.918   0.550  1.00  0.00           H
ATOM    616  HE1 TYR A  44       5.330  -3.100  -0.058  1.00  0.00           H
ATOM    617  HH  TYR A  44       6.545  -4.108  -1.702  1.00  0.00           H
ATOM    618  N   ALA A  45       7.738   0.805   5.668  1.00  0.00           N
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ATOM    619  CA  ALA A  45       7.139   1.767   6.580  1.00  0.00           C
ATOM    620  C   ALA A  45       6.936   3.131   5.902  1.00  0.00           C
ATOM    621  O   ALA A  45       7.095   4.202   6.511  1.00  0.00           O
ATOM    622  CB  ALA A  45       7.905   1.873   7.893  1.00  0.00           C
ATOM    623  H   ALA A  45       8.759   0.799   5.597  1.00  0.00           H
ATOM    624  HA  ALA A  45       6.113   1.403   6.759  1.00  0.00           H
ATOM    625  HB1 ALA A  45       7.906   0.901   8.405  1.00  0.00           H
ATOM    626  HB2 ALA A  45       7.438   2.630   8.537  1.00  0.00           H
ATOM    627  HB3 ALA A  45       8.945   2.179   7.705  1.00  0.00           H
ATOM    628  N   ASN A  46       6.518   3.078   4.623  1.00  0.00           N
ATOM    629  CA  ASN A  46       5.803   4.167   3.994  1.00  0.00           C
ATOM    630  C   ASN A  46       4.359   3.720   3.637  1.00  0.00           C
ATOM    631  OXT ASN A  46       3.955   2.618   4.107  1.00  0.00           O
ATOM    632  CB  ASN A  46       6.552   4.761   2.795  1.00  0.00           C
ATOM    633  CG  ASN A  46       7.847   5.520   3.063  1.00  0.00           C
ATOM    634  OD1 ASN A  46       8.496   6.006   2.111  1.00  0.00           O
ATOM    635  ND2 ASN A  46       8.252   5.688   4.330  1.00  0.00           N
ATOM    636  O   ASN A  46       3.682   4.523   2.939  1.00  0.00           O
ATOM    637  H   ASN A  46       6.406   2.173   4.170  1.00  0.00           H
ATOM    638  HA  ASN A  46       5.671   4.949   4.759  1.00  0.00           H
ATOM    639  HB1 ASN A  46       6.799   3.954   2.089  1.00  0.00           H
ATOM    640  HB2 ASN A  46       5.875   5.451   2.271  1.00  0.00           H
ATOM    641 HD21 ASN A  46       7.812   5.253   5.154  1.00  0.00           H
ATOM    642 HD22 ASN A  46       9.139   6.166   4.455  1.00  0.00           H
END
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2) CRAMBIN – molecule as in the optimized 0W crystal

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COMPND    CRAMBIN OPTIMIZED CRYSTAL 0W GEOMETRY
AUTHOR    DELLE PIANE, CORNO, ORLANDO, DOVESI, UGLIENGO
ATOM      1  N   THR N   1      -7.130  -5.367  -3.415  1.00  0.00           N
ATOM      2  H1  THR N   1      -7.808  -5.844  -4.016  1.00  0.00           H
ATOM      3  H2  THR N   1      -7.455  -5.409  -2.434  1.00  0.00           H
ATOM      4  H3  THR N   1      -6.249  -5.927  -3.476  1.00  0.00           H
ATOM      5  CA  THR N   1      -6.943  -3.934  -3.779  1.00  0.00           C
ATOM      6  HA  THR N   1      -7.907  -3.544  -4.134  1.00  0.00           H
ATOM      7  C   THR N   1      -5.859  -3.842  -4.847  1.00  0.00           C
ATOM      8  CB  THR N   1      -6.480  -3.169  -2.492  1.00  0.00           C
ATOM      9  O   THR N   1      -4.905  -4.641  -4.820  1.00  0.00           O
ATOM     10  N   THR N   2      -5.980  -2.809  -5.680  1.00  0.00           N
ATOM     11  HB  THR N   1      -5.416  -3.420  -2.342  1.00  0.00           H
ATOM     12  OG1 THR N   1      -7.240  -3.648  -1.392  1.00  0.00           O
ATOM     13  CG2 THR N   1      -6.639  -1.665  -2.642  1.00  0.00           C
ATOM     14  H   THR N   2      -6.887  -2.331  -5.781  1.00  0.00           H
ATOM     15  CA  THR N   2      -4.922  -2.459  -6.603  1.00  0.00           C
ATOM     16  HG1 THR N   1      -6.662  -4.306  -0.939  1.00  0.00           H
ATOM     17 HG21 THR N   1      -6.323  -1.179  -1.708  1.00  0.00           H
ATOM     18 HG22 THR N   1      -6.018  -1.275  -3.461  1.00  0.00           H
ATOM     19 HG23 THR N   1      -7.693  -1.400  -2.825  1.00  0.00           H
ATOM     20  HA  THR N   2      -4.511  -3.379  -7.022  1.00  0.00           H
ATOM     21  C   THR N   2      -3.775  -1.719  -5.910  1.00  0.00           C
ATOM     22  CB  THR N   2      -5.496  -1.627  -7.782  1.00  0.00           C
ATOM     23  O   THR N   2      -3.948  -0.892  -5.009  1.00  0.00           O
ATOM     24  N   CYS N   3      -2.574  -2.037  -6.444  1.00  0.00           N
ATOM     25  HB  THR N   2      -4.637  -1.175  -8.308  1.00  0.00           H
ATOM     26  OG1 THR N   2      -6.278  -0.558  -7.265  1.00  0.00           O
ATOM     27  CG2 THR N   2      -6.217  -2.562  -8.755  1.00  0.00           C
ATOM     28  H   CYS N   3      -2.562  -2.704  -7.215  1.00  0.00           H
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ATOM     29  CA  CYS N   3      -1.309  -1.392  -6.145  1.00  0.00           C
ATOM     30  HG1 THR N   2      -7.238  -0.655  -7.511  1.00  0.00           H
ATOM     31 HG21 THR N   2      -6.835  -2.012  -9.466  1.00  0.00           H
ATOM     32 HG22 THR N   2      -5.471  -3.141  -9.310  1.00  0.00           H
ATOM     33 HG23 THR N   2      -6.866  -3.258  -8.211  1.00  0.00           H
ATOM     34  HA  CYS N   3      -1.504  -0.436  -5.645  1.00  0.00           H
ATOM     35  C   CYS N   3      -0.600  -1.155  -7.488  1.00  0.00           C
ATOM     36  CB  CYS N   3      -0.392  -2.240  -5.247  1.00  0.00           C
ATOM     37  O   CYS N   3      -0.759  -1.963  -8.421  1.00  0.00           O
ATOM     38  N   CYS N   4       0.201  -0.082  -7.559  1.00  0.00           N
ATOM     39  HB1 CYS N   3      -0.198  -3.216  -5.713  1.00  0.00           H
ATOM     40  HB2 CYS N   3       0.582  -1.746  -5.106  1.00  0.00           H
ATOM     41  SG  CYS N   3      -1.101  -2.668  -3.608  1.00  0.00           S
ATOM     42  H   CYS N   4       0.186   0.617  -6.791  1.00  0.00           H
ATOM     43  CA  CYS N   4       0.708   0.360  -8.843  1.00  0.00           C
ATOM     44  SG  CYS N  40      -0.971  -0.887  -2.536  1.00  0.00           S
ATOM     45  HA  CYS N   4       0.448  -0.422  -9.561  1.00  0.00           H
ATOM     46  C   CYS N   4       2.226   0.537  -8.829  1.00  0.00           C
ATOM     47  CB  CYS N   4       0.031   1.676  -9.259  1.00  0.00           C
ATOM     48  CB  CYS N  40       0.807  -0.801  -2.025  1.00  0.00           C
ATOM     49  O   CYS N   4       2.817   1.042  -7.866  1.00  0.00           O
ATOM     50  N   PRO N   5       2.882   0.167  -9.952  1.00  0.00           N
ATOM     51  HB1 CYS N   4      -0.017   2.359  -8.399  1.00  0.00           H
ATOM     52  HB2 CYS N   4       0.574   2.187 -10.065  1.00  0.00           H
ATOM     53  SG  CYS N   4      -1.708   1.443  -9.792  1.00  0.00           S
ATOM     54  HB1 CYS N  40       1.412  -0.460  -2.877  1.00  0.00           H
ATOM     55  HB2 CYS N  40       0.827  -0.014  -1.256  1.00  0.00           H
ATOM     56  CA  CYS N  40       1.374  -2.122  -1.511  1.00  0.00           C
ATOM     57  CA  PRO N   5       4.354   0.202 -10.031  1.00  0.00           C
ATOM     58  CD  PRO N   5       2.271  -0.355 -11.196  1.00  0.00           C
ATOM     59  SG  CYS N  32      -1.453   0.620 -11.699  1.00  0.00           S
ATOM     60  HA  CYS N  40       1.253  -2.866  -2.301  1.00  0.00           H
ATOM     61  N   CYS N  40       0.669  -2.650  -0.346  1.00  0.00           N
ATOM     62  C   CYS N  40       2.857  -1.973  -1.129  1.00  0.00           C
ATOM     63  HA  PRO N   5       4.815  -0.332  -9.190  1.00  0.00           H
ATOM     64  C   PRO N   5       4.950   1.602  -9.973  1.00  0.00           C
ATOM     65  CB  PRO N   5       4.653  -0.496 -11.378  1.00  0.00           C
ATOM     66  HD1 PRO N   5       1.381   0.216 -11.481  1.00  0.00           H
ATOM     67  HD2 PRO N   5       1.990  -1.408 -11.067  1.00  0.00           H
ATOM     68  CG  PRO N   5       3.395  -0.230 -12.208  1.00  0.00           C
ATOM     69  CB  CYS N  32      -1.841  -1.187 -11.524  1.00  0.00           C
ATOM     70  H   CYS N  40       0.318  -2.006   0.355  1.00  0.00           H
ATOM     71  C   THR N  39       0.652  -3.985  -0.104  1.00  0.00           C
ATOM     72  O   CYS N  40       3.151  -1.162  -0.228  1.00  0.00           O
ATOM     73  N   PRO N  41       3.753  -2.778  -1.730  1.00  0.00           N
ATOM     74  O   PRO N   5       6.163   1.751  -9.762  1.00  0.00           O
ATOM     75  N   SER N   6       4.143   2.647 -10.207  1.00  0.00           N
ATOM     76  HB1 PRO N   5       5.567  -0.120 -11.851  1.00  0.00           H
ATOM     77  HB2 PRO N   5       4.783  -1.573 -11.197  1.00  0.00           H
ATOM     78  HG1 PRO N   5       3.281  -0.902 -13.061  1.00  0.00           H
ATOM     79  HG2 PRO N   5       3.417   0.789 -12.609  1.00  0.00           H
ATOM     80  HB1 CYS N  32      -2.260  -1.321 -10.520  1.00  0.00           H
ATOM     81  HB2 CYS N  32      -2.649  -1.360 -12.245  1.00  0.00           H
ATOM     82  CA  CYS N  32      -0.689  -2.187 -11.755  1.00  0.00           C
ATOM     83  O   THR N  39       1.141  -4.805  -0.882  1.00  0.00           O
ATOM     84  CA  THR N  39      -0.068  -4.441   1.179  1.00  0.00           C
ATOM     85  CA  PRO N  41       5.178  -2.750  -1.405  1.00  0.00           C
ATOM     86  CD  PRO N  41       3.530  -3.848  -2.724  1.00  0.00           C
ATOM     87  H   SER N   6       3.138   2.529 -10.271  1.00  0.00           H
ATOM     88  CA  SER N   6       4.631   4.003 -10.107  1.00  0.00           C
ATOM     89  HA  CYS N  32       0.069  -2.035 -10.976  1.00  0.00           H
ATOM     90  N   CYS N  32      -0.075  -2.031 -13.053  1.00  0.00           N
ATOM     91  C   CYS N  32      -1.152  -3.666 -11.558  1.00  0.00           C
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ATOM     92  HA  THR N  39      -0.037  -3.660   1.951  1.00  0.00           H
ATOM     93  N   THR N  39      -1.480  -4.619   0.851  1.00  0.00           N
ATOM     94  CB  THR N  39       0.581  -5.736   1.730  1.00  0.00           C
ATOM     95  HA  PRO N  41       5.298  -2.363  -0.391  1.00  0.00           H
ATOM     96  C   PRO N  41       5.918  -1.796  -2.355  1.00  0.00           C
ATOM     97  CB  PRO N  41       5.638  -4.227  -1.546  1.00  0.00           C
ATOM     98  HD1 PRO N  41       2.489  -4.173  -2.725  1.00  0.00           H
ATOM     99  HD2 PRO N  41       3.809  -3.460  -3.712  1.00  0.00           H
ATOM    100  CG  PRO N  41       4.472  -4.957  -2.251  1.00  0.00           C
ATOM    101  HA  SER N   6       5.304   4.071  -9.239  1.00  0.00           H
ATOM    102  C   SER N   6       3.436   4.920  -9.895  1.00  0.00           C
ATOM    103  CB  SER N   6       5.383   4.440 -11.368  1.00  0.00           C
ATOM    104  H   CYS N  32      -0.671  -1.687 -13.806  1.00  0.00           H
ATOM    105  C   GLY N  31       1.054  -2.707 -13.384  1.00  0.00           C
ATOM    106  O   CYS N  32      -0.995  -4.508 -12.449  1.00  0.00           O
ATOM    107  N   ILE N  33      -1.688  -3.928 -10.350  1.00  0.00           N
ATOM    108  H   THR N  39      -1.712  -5.288   0.122  1.00  0.00           H
ATOM    109  C   ALA N  38      -2.480  -3.890   1.404  1.00  0.00           C
ATOM    110  HB  THR N  39       0.612  -6.460   0.892  1.00  0.00           H
ATOM    111  OG1 THR N  39      -0.133  -6.261   2.823  1.00  0.00           O
ATOM    112  CG2 THR N  39       2.004  -5.482   2.217  1.00  0.00           C
ATOM    113  O   PRO N  41       5.354  -1.256  -3.298  1.00  0.00           O
ATOM    114  N   GLY N  42       7.249  -1.605  -2.120  1.00  0.00           N
ATOM    115  HB1 PRO N  41       6.552  -4.297  -2.147  1.00  0.00           H
ATOM    116  HB2 PRO N  41       5.842  -4.656  -0.554  1.00  0.00           H
ATOM    117  HG1 PRO N  41       4.840  -5.545  -3.100  1.00  0.00           H
ATOM    118  HG2 PRO N  41       3.935  -5.607  -1.544  1.00  0.00           H
ATOM    119  O   SER N   6       2.271   4.543 -10.077  1.00  0.00           O
ATOM    120  N   ILE N   7       3.757   6.199  -9.604  1.00  0.00           N
ATOM    121  HB1 SER N   6       6.149   3.691 -11.614  1.00  0.00           H
ATOM    122  HB2 SER N   6       5.907   5.392 -11.172  1.00  0.00           H
ATOM    123  OG  SER N   6       4.451   4.590 -12.428  1.00  0.00           O
ATOM    124  O   GLY N  31       1.793  -3.244 -12.553  1.00  0.00           O
ATOM    125  CA  GLY N  31       1.418  -2.786 -14.874  1.00  0.00           C
ATOM    126  H   ILE N  33      -1.631  -3.194  -9.641  1.00  0.00           H
ATOM    127  CA  ILE N  33      -1.881  -5.273  -9.835  1.00  0.00           C
ATOM    128  O   ALA N  38      -2.290  -3.044   2.280  1.00  0.00           O
ATOM    129  CA  ALA N  38      -3.888  -4.156   0.811  1.00  0.00           C
ATOM    130  HG1 THR N  39      -1.105  -6.218   2.685  1.00  0.00           H
ATOM    131 HG21 THR N  39       2.653  -5.123   1.405  1.00  0.00           H
ATOM    132 HG22 THR N  39       2.424  -6.419   2.611  1.00  0.00           H
ATOM    133 HG23 THR N  39       1.995  -4.755   3.046  1.00  0.00           H
ATOM    134  H   GLY N  42       7.625  -1.833  -1.205  1.00  0.00           H
ATOM    135  CA  GLY N  42       7.982  -0.608  -2.887  1.00  0.00           C
ATOM    136  H   ILE N   7       4.673   6.357  -9.198  1.00  0.00           H
ATOM    137  CA  ILE N   7       2.731   7.196  -9.351  1.00  0.00           C
ATOM    138  H   SER N   6       4.889   5.157 -13.109  1.00  0.00           H
ATOM    139  HA1 GLY N  31       1.443  -3.857 -15.121  1.00  0.00           H
ATOM    140  HA2 GLY N  31       2.435  -2.384 -14.982  1.00  0.00           H
ATOM    141  N   GLY N  31       0.529  -2.105 -15.786  1.00  0.00           N
ATOM    142  HA  ILE N  33      -1.930  -5.968 -10.679  1.00  0.00           H
ATOM    143  C   ILE N  33      -3.183  -5.283  -9.061  1.00  0.00           C
ATOM    144  CB  ILE N  33      -0.685  -5.738  -8.913  1.00  0.00           C
ATOM    145  HA  ALA N  38      -3.829  -3.921  -0.265  1.00  0.00           H
ATOM    146  N   ALA N  38      -4.211  -5.581   0.930  1.00  0.00           N
ATOM    147  CB  ALA N  38      -4.948  -3.268   1.461  1.00  0.00           C
ATOM    148  HA1 GLY N  42       8.991  -0.532  -2.460  1.00  0.00           H
ATOM    149  HA2 GLY N  42       7.517   0.387  -2.803  1.00  0.00           H
ATOM    150  C   GLY N  42       8.113  -0.876  -4.392  1.00  0.00           C
ATOM    151  HA  ILE N   7       1.958   6.765  -8.697  1.00  0.00           H
ATOM    152  C   ILE N   7       1.972   7.532 -10.645  1.00  0.00           C
ATOM    153  CB  ILE N   7       3.348   8.430  -8.646  1.00  0.00           C
ATOM    154  H   GLY N  31      -0.318  -2.594 -16.068  1.00  0.00           H
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ATOM    155  C   THR N  30       0.613  -0.760 -15.949  1.00  0.00           C
ATOM    156  O   ILE N  33      -3.627  -4.232  -8.594  1.00  0.00           O
ATOM    157  N   ILE N  34      -3.785  -6.485  -8.831  1.00  0.00           N
ATOM    158  HB  ILE N  33      -0.644  -6.837  -9.014  1.00  0.00           H
ATOM    159  CG2 ILE N  33       0.616  -5.147  -9.456  1.00  0.00           C
ATOM    160  CG1 ILE N  33      -0.889  -5.388  -7.422  1.00  0.00           C
ATOM    161  H   ALA N  38      -3.827  -6.047   1.775  1.00  0.00           H
ATOM    162  C   GLY N  37      -5.087  -6.214   0.137  1.00  0.00           C
ATOM    163  HB1 ALA N  38      -5.903  -3.360   0.929  1.00  0.00           H
ATOM    164  HB2 ALA N  38      -4.634  -2.216   1.435  1.00  0.00           H
ATOM    165  HB3 ALA N  38      -5.097  -3.557   2.510  1.00  0.00           H
ATOM    166  O   GLY N  42       8.383   0.061  -5.149  1.00  0.00           O
ATOM    167  N   ASP N  43       7.967  -2.155  -4.800  1.00  0.00           N
ATOM    168  O   ILE N   7       0.745   7.671 -10.617  1.00  0.00           O
ATOM    169  N   VAL N   8       2.697   7.684 -11.780  1.00  0.00           N
ATOM    170  HB  ILE N   7       4.268   8.706  -9.198  1.00  0.00           H
ATOM    171  CG2 ILE N   7       2.390   9.608  -8.723  1.00  0.00           C
ATOM    172  CG1 ILE N   7       3.724   8.058  -7.194  1.00  0.00           C
ATOM    173  O   THR N  30       1.553  -0.091 -15.517  1.00  0.00           O
ATOM    174  CA  THR N  30      -0.585  -0.046 -16.594  1.00  0.00           C
ATOM    175  H   ILE N  34      -3.277  -7.325  -9.101  1.00  0.00           H
ATOM    176  CA  ILE N  34      -4.654  -6.626  -7.659  1.00  0.00           C
ATOM    177 HG21 ILE N  33       1.478  -5.520  -8.906  1.00  0.00           H
ATOM    178 HG22 ILE N  33       0.624  -4.057  -9.342  1.00  0.00           H
ATOM    179 HG23 ILE N  33       0.775  -5.380 -10.517  1.00  0.00           H
ATOM    180 HG11 ILE N  33      -1.048  -4.304  -7.340  1.00  0.00           H
ATOM    181 HG12 ILE N  33      -1.810  -5.861  -7.047  1.00  0.00           H
ATOM    182  CD1 ILE N  33       0.257  -5.796  -6.492  1.00  0.00           C
ATOM    183  O   GLY N  37      -5.619  -5.695  -0.864  1.00  0.00           O
ATOM    184  CA  GLY N  37      -5.454  -7.640   0.563  1.00  0.00           C
ATOM    185  H   ASP N  43       7.497  -2.843  -4.202  1.00  0.00           H
ATOM    186  CA  ASP N  43       7.834  -2.479  -6.217  1.00  0.00           C
ATOM    187  H   VAL N   8       3.676   7.407 -11.772  1.00  0.00           H
ATOM    188  CA  VAL N   8       2.025   7.902 -13.061  1.00  0.00           C
ATOM    189 HG21 ILE N   7       2.784  10.462  -8.167  1.00  0.00           H
ATOM    190 HG22 ILE N   7       2.240   9.935  -9.760  1.00  0.00           H
ATOM    191 HG23 ILE N   7       1.405   9.344  -8.311  1.00  0.00           H
ATOM    192 HG11 ILE N   7       4.412   7.200  -7.209  1.00  0.00           H
ATOM    193 HG12 ILE N   7       2.810   7.688  -6.696  1.00  0.00           H
ATOM    194  CD1 ILE N   7       4.347   9.162  -6.341  1.00  0.00           C
ATOM    195  HA  THR N  30      -0.194   0.578 -17.409  1.00  0.00           H
ATOM    196  N   THR N  30      -1.623  -0.895 -17.154  1.00  0.00           N
ATOM    197  CB  THR N  30      -1.198   0.852 -15.491  1.00  0.00           C
ATOM    198  HA  ILE N  34      -4.611  -5.665  -7.134  1.00  0.00           H
ATOM    199  C   ILE N  34      -4.056  -7.736  -6.798  1.00  0.00           C
ATOM    200  CB  ILE N  34      -6.152  -6.983  -7.917  1.00  0.00           C
ATOM    201 HD11 ILE N  33       0.479  -6.871  -6.564  1.00  0.00           H
ATOM    202 HD12 ILE N  33       1.188  -5.254  -6.714  1.00  0.00           H
ATOM    203 HD13 ILE N  33      -0.004  -5.589  -5.442  1.00  0.00           H
ATOM    204  HA1 GLY N  37      -4.762  -8.010   1.329  1.00  0.00           H
ATOM    205  HA2 GLY N  37      -6.467  -7.590   0.988  1.00  0.00           H
ATOM    206  N   GLY N  37      -5.479  -8.554  -0.552  1.00  0.00           N
ATOM    207  HA  ASP N  43       8.654  -1.992  -6.752  1.00  0.00           H
ATOM    208  CB  ASP N  43       7.921  -4.003  -6.415  1.00  0.00           C
ATOM    209  C   ASP N  43       6.546  -1.863  -6.812  1.00  0.00           C
ATOM    210  HA  VAL N   8       1.228   8.637 -12.881  1.00  0.00           H
ATOM    211  C   VAL N   8       1.268   6.651 -13.520  1.00  0.00           C
ATOM    212  CB  VAL N   8       2.985   8.471 -14.134  1.00  0.00           C
ATOM    213 HD11 ILE N   7       5.286   9.557  -6.753  1.00  0.00           H
ATOM    214 HD12 ILE N   7       3.668  10.015  -6.194  1.00  0.00           H
ATOM    215 HD13 ILE N   7       4.586   8.770  -5.340  1.00  0.00           H
ATOM    216  H   THR N  30      -2.154  -1.487 -16.517  1.00  0.00           H
ATOM    217  C   TYR N  29      -2.127  -0.721 -18.403  1.00  0.00           C
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ATOM    218  HB  THR N  30      -0.368   1.395 -15.022  1.00  0.00           H
ATOM    219  OG1 THR N  30      -1.745   0.009 -14.470  1.00  0.00           O
ATOM    220  CG2 THR N  30      -2.224   1.840 -16.020  1.00  0.00           C
ATOM    221  O   ILE N  34      -3.739  -8.824  -7.301  1.00  0.00           O
ATOM    222  N   ILE N  35      -3.943  -7.452  -5.487  1.00  0.00           N
ATOM    223  HB  ILE N  34      -6.215  -8.078  -7.998  1.00  0.00           H
ATOM    224  CG1 ILE N  34      -6.710  -6.420  -9.230  1.00  0.00           C
ATOM    225  CG2 ILE N  34      -7.004  -6.561  -6.708  1.00  0.00           C
ATOM    226  H   GLY N  37      -4.581  -8.979  -0.785  1.00  0.00           H
ATOM    227  C   PRO N  36      -6.613  -9.091  -1.054  1.00  0.00           C
ATOM    228  HB1 ASP N  43       7.753  -4.246  -7.475  1.00  0.00           H
ATOM    229  HB2 ASP N  43       8.949  -4.324  -6.179  1.00  0.00           H
ATOM    230  CG  ASP N  43       6.973  -4.902  -5.565  1.00  0.00           C
ATOM    231  O   ASP N  43       6.593  -1.032  -7.742  1.00  0.00           O
ATOM    232  N   TYR N  44       5.403  -2.274  -6.247  1.00  0.00           N
ATOM    233  O   VAL N   8       0.183   6.784 -14.100  1.00  0.00           O
ATOM    234  N   ALA N   9       1.784   5.436 -13.248  1.00  0.00           N
ATOM    235  HB  VAL N   8       3.902   7.856 -14.120  1.00  0.00           H
ATOM    236  CG2 VAL N   8       3.359   9.912 -13.752  1.00  0.00           C
ATOM    237  CG1 VAL N   8       2.380   8.390 -15.544  1.00  0.00           C
ATOM    238  O   TYR N  29      -1.618   0.007 -19.257  1.00  0.00           O
ATOM    239  CA  TYR N  29      -3.448  -1.446 -18.711  1.00  0.00           C
ATOM    240  HG1 THR N  30      -2.654  -0.276 -14.706  1.00  0.00           H
ATOM    241 HG21 THR N  30      -2.437   2.594 -15.258  1.00  0.00           H
ATOM    242 HG22 THR N  30      -3.157   1.325 -16.284  1.00  0.00           H
ATOM    243 HG23 THR N  30      -1.855   2.352 -16.921  1.00  0.00           H
ATOM    244  H   ILE N  35      -4.268  -6.536  -5.166  1.00  0.00           H
ATOM    245  CA  ILE N  35      -3.725  -8.490  -4.497  1.00  0.00           C
ATOM    246 HG11 ILE N  34      -6.697  -5.319  -9.199  1.00  0.00           H
ATOM    247 HG12 ILE N  34      -6.041  -6.697 -10.062  1.00  0.00           H
ATOM    248  CD1 ILE N  34      -8.119  -6.939  -9.515  1.00  0.00           C
ATOM    249 HG21 ILE N  34      -6.560  -6.914  -5.769  1.00  0.00           H
ATOM    250 HG22 ILE N  34      -8.010  -7.001  -6.769  1.00  0.00           H
ATOM    251 HG23 ILE N  34      -7.123  -5.466  -6.665  1.00  0.00           H
ATOM    252  O   PRO N  36      -7.740  -8.902  -0.591  1.00  0.00           O
ATOM    253  CA  PRO N  36      -6.464  -9.999  -2.293  1.00  0.00           C
ATOM    254  OD1 ASP N  43       6.939  -6.102  -5.866  1.00  0.00           O
ATOM    255  OD2 ASP N  43       6.317  -4.313  -4.627  1.00  0.00           O
ATOM    256  H   TYR N  44       5.502  -2.973  -5.487  1.00  0.00           H
ATOM    257  CA  TYR N  44       4.091  -1.789  -6.645  1.00  0.00           C
ATOM    258  H   ALA N   9       2.687   5.311 -12.782  1.00  0.00           H
ATOM    259  CA  ALA N   9       0.967   4.261 -13.525  1.00  0.00           C
ATOM    260 HG21 VAL N   8       4.089  10.326 -14.463  1.00  0.00           H
ATOM    261 HG22 VAL N   8       3.799   9.953 -12.744  1.00  0.00           H
ATOM    262 HG23 VAL N   8       2.476  10.572 -13.762  1.00  0.00           H
ATOM    263 HG11 VAL N   8       3.027   8.896 -16.273  1.00  0.00           H
ATOM    264 HG12 VAL N   8       2.258   7.348 -15.878  1.00  0.00           H
ATOM    265 HG13 VAL N   8       1.384   8.855 -15.603  1.00  0.00           H
ATOM    266  HA  TYR N  29      -3.402  -1.658 -19.791  1.00  0.00           H
ATOM    267  N   TYR N  29      -3.604  -2.682 -17.958  1.00  0.00           N
ATOM    268  CB  TYR N  29      -4.659  -0.533 -18.387  1.00  0.00           C
ATOM    269  HA  ILE N  35      -3.566  -9.414  -5.069  1.00  0.00           H
ATOM    270  C   ILE N  35      -5.006  -8.636  -3.676  1.00  0.00           C
ATOM    271  CB  ILE N  35      -2.471  -8.233  -3.613  1.00  0.00           C
ATOM    272 HD11 ILE N  34      -8.501  -6.545 -10.460  1.00  0.00           H
ATOM    273 HD12 ILE N  34      -8.837  -6.643  -8.737  1.00  0.00           H
ATOM    274 HD13 ILE N  34      -8.131  -8.039  -9.569  1.00  0.00           H
ATOM    275  HA  PRO N  36      -7.313  -9.698  -2.922  1.00  0.00           H
ATOM    276  N   PRO N  36      -5.207  -9.807  -3.032  1.00  0.00           N
ATOM    277  CB  PRO N  36      -6.496 -11.520  -2.020  1.00  0.00           C
ATOM    278  HA  TYR N  44       4.240  -1.231  -7.576  1.00  0.00           H
ATOM    279  CB  TYR N  44       3.125  -2.947  -6.927  1.00  0.00           C
ATOM    280  C   TYR N  44       3.602  -0.781  -5.593  1.00  0.00           C
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ATOM    281  HA  ALA N   9       0.712   4.248 -14.594  1.00  0.00           H
ATOM    282  CB  ALA N   9       1.682   2.965 -13.164  1.00  0.00           C
ATOM    283  C   ALA N   9      -0.375   4.378 -12.794  1.00  0.00           C
ATOM    284  H   TYR N  29      -4.521  -2.885 -17.555  1.00  0.00           H
ATOM    285  C   THR N  28      -2.708  -3.696 -18.077  1.00  0.00           C
ATOM    286  HB1 TYR N  29      -4.605  -0.268 -17.322  1.00  0.00           H
ATOM    287  HB2 TYR N  29      -5.562  -1.151 -18.496  1.00  0.00           H
ATOM    288  CG  TYR N  29      -4.809   0.719 -19.218  1.00  0.00           C
ATOM    289  O   ILE N  35      -5.836  -7.718  -3.588  1.00  0.00           O
ATOM    290  HB  ILE N  35      -2.556  -8.891  -2.730  1.00  0.00           H
ATOM    291  CG2 ILE N  35      -1.217  -8.639  -4.397  1.00  0.00           C
ATOM    292  CG1 ILE N  35      -2.438  -6.780  -3.102  1.00  0.00           C
ATOM    293  CD  PRO N  36      -4.443 -11.058  -3.213  1.00  0.00           C
ATOM    294  HB1 PRO N  36      -6.946 -11.757  -1.047  1.00  0.00           H
ATOM    295  HB2 PRO N  36      -7.121 -12.007  -2.784  1.00  0.00           H
ATOM    296  CG  PRO N  36      -5.037 -11.985  -2.151  1.00  0.00           C
ATOM    297  HB1 TYR N  44       2.146  -2.523  -7.193  1.00  0.00           H
ATOM    298  HB2 TYR N  44       2.976  -3.535  -6.009  1.00  0.00           H
ATOM    299  CG  TYR N  44       3.666  -3.804  -8.048  1.00  0.00           C
ATOM    300  O   TYR N  44       2.656  -0.983  -4.830  1.00  0.00           O
ATOM    301  N   ALA N  45       4.357   0.343  -5.572  1.00  0.00           N
ATOM    302  HB1 ALA N   9       2.570   2.862 -13.789  1.00  0.00           H
ATOM    303  HB2 ALA N   9       1.985   2.959 -12.110  1.00  0.00           H
ATOM    304  HB3 ALA N   9       1.026   2.106 -13.358  1.00  0.00           H
ATOM    305  O   ALA N   9      -1.422   4.061 -13.372  1.00  0.00           O
ATOM    306  N   ARG N  10      -0.349   4.817 -11.517  1.00  0.00           N
ATOM    307  O   THR N  28      -1.711  -3.633 -18.795  1.00  0.00           O
ATOM    308  CA  THR N  28      -2.958  -4.954 -17.222  1.00  0.00           C
ATOM    309  CD1 TYR N  29      -5.050   0.659 -20.596  1.00  0.00           C
ATOM    310  CD2 TYR N  29      -4.771   1.989 -18.626  1.00  0.00           C
ATOM    311 HG21 ILE N  35      -0.296  -8.416  -3.840  1.00  0.00           H
ATOM    312 HG22 ILE N  35      -1.166  -8.101  -5.355  1.00  0.00           H
ATOM    313 HG23 ILE N  35      -1.217  -9.718  -4.621  1.00  0.00           H
ATOM    314 HG11 ILE N  35      -2.235  -6.101  -3.948  1.00  0.00           H
ATOM    315 HG12 ILE N  35      -3.436  -6.498  -2.726  1.00  0.00           H
ATOM    316  CD1 ILE N  35      -1.410  -6.522  -2.004  1.00  0.00           C
ATOM    317  HD1 PRO N  36      -3.368 -10.897  -3.063  1.00  0.00           H
ATOM    318  HD2 PRO N  36      -4.593 -11.452  -4.233  1.00  0.00           H
ATOM    319  HG1 PRO N  36      -4.950 -13.041  -2.436  1.00  0.00           H
ATOM    320  HG2 PRO N  36      -4.485 -11.848  -1.211  1.00  0.00           H
ATOM    321  CD1 TYR N  44       3.370  -3.510  -9.382  1.00  0.00           C
ATOM    322  CD2 TYR N  44       4.565  -4.848  -7.791  1.00  0.00           C
ATOM    323  H   ALA N  45       5.095   0.431  -6.265  1.00  0.00           H
ATOM    324  CA  ALA N  45       4.362   1.255  -4.455  1.00  0.00           C
ATOM    325  H   ARG N  10       0.546   5.022 -11.071  1.00  0.00           H
ATOM    326  CA  ARG N  10      -1.582   5.064 -10.785  1.00  0.00           C
ATOM    327  HA  THR N  28      -1.945  -5.297 -16.969  1.00  0.00           H
ATOM    328  N   THR N  28      -3.678  -4.675 -15.981  1.00  0.00           N
ATOM    329  CB  THR N  28      -3.628  -6.063 -18.044  1.00  0.00           C
ATOM    330  HD1 TYR N  29      -5.119  -0.309 -21.098  1.00  0.00           H
ATOM    331  CE1 TYR N  29      -5.206   1.817 -21.355  1.00  0.00           C
ATOM    332  HD2 TYR N  29      -4.614   2.077 -17.551  1.00  0.00           H
ATOM    333  CE2 TYR N  29      -4.923   3.160 -19.367  1.00  0.00           C
ATOM    334 HD11 ILE N  35      -1.364  -5.447  -1.786  1.00  0.00           H
ATOM    335 HD12 ILE N  35      -0.386  -6.804  -2.290  1.00  0.00           H
ATOM    336 HD13 ILE N  35      -1.659  -7.078  -1.083  1.00  0.00           H
ATOM    337  HD1 TYR N  44       2.676  -2.704  -9.616  1.00  0.00           H
ATOM    338  CE1 TYR N  44       3.909  -4.252 -10.433  1.00  0.00           C
ATOM    339  HD2 TYR N  44       4.819  -5.113  -6.767  1.00  0.00           H
ATOM    340  CE2 TYR N  44       5.150  -5.574  -8.826  1.00  0.00           C
ATOM    341  HA  ALA N  45       4.451   0.662  -3.538  1.00  0.00           H
ATOM    342  C   ALA N  45       3.089   2.073  -4.294  1.00  0.00           C
ATOM    343  CB  ALA N  45       5.559   2.210  -4.577  1.00  0.00           C
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ATOM    344  HA  ARG N  10      -2.199   4.160 -10.855  1.00  0.00           H
ATOM    345  CB  ARG N  10      -1.305   5.363  -9.300  1.00  0.00           C
ATOM    346  C   ARG N  10      -2.450   6.145 -11.463  1.00  0.00           C
ATOM    347  H   THR N  28      -4.647  -4.982 -15.876  1.00  0.00           H
ATOM    348  C   ALA N  27      -3.107  -3.861 -15.065  1.00  0.00           C
ATOM    349  HB  THR N  28      -3.072  -6.102 -18.998  1.00  0.00           H
ATOM    350  OG1 THR N  28      -4.973  -5.624 -18.286  1.00  0.00           O
ATOM    351  CG2 THR N  28      -3.568  -7.426 -17.369  1.00  0.00           C
ATOM    352  HE1 TYR N  29      -5.395   1.746 -22.428  1.00  0.00           H
ATOM    353  CZ  TYR N  29      -5.116   3.075 -20.747  1.00  0.00           C
ATOM    354  HE2 TYR N  29      -4.882   4.136 -18.879  1.00  0.00           H
ATOM    355  HE1 TYR N  44       3.588  -4.038 -11.456  1.00  0.00           H
ATOM    356  CZ  TYR N  44       4.802  -5.288 -10.148  1.00  0.00           C
ATOM    357  HE2 TYR N  44       5.859  -6.371  -8.601  1.00  0.00           H
ATOM    358  O   ALA N  45       2.831   2.503  -3.142  1.00  0.00           O
ATOM    359  N   ASN N  46       2.375   2.396  -5.368  1.00  0.00           N
ATOM    360  HB1 ALA N  45       5.630   2.845  -3.683  1.00  0.00           H
ATOM    361  HB2 ALA N  45       6.491   1.633  -4.675  1.00  0.00           H
ATOM    362  HB3 ALA N  45       5.454   2.863  -5.457  1.00  0.00           H
ATOM    363  HB1 ARG N  10      -0.721   4.528  -8.884  1.00  0.00           H
ATOM    364  HB2 ARG N  10      -0.668   6.257  -9.232  1.00  0.00           H
ATOM    365  CG  ARG N  10      -2.577   5.592  -8.471  1.00  0.00           C
ATOM    366  O   ARG N  10      -3.664   5.925 -11.606  1.00  0.00           O
ATOM    367  N   SER N  11      -1.879   7.285 -11.895  1.00  0.00           N
ATOM    368  O   ALA N  27      -1.983  -3.376 -15.232  1.00  0.00           O
ATOM    369  CA  ALA N  27      -3.899  -3.519 -13.788  1.00  0.00           C
ATOM    370  HG1 THR N  28      -5.391  -6.245 -18.903  1.00  0.00           H
ATOM    371 HG21 THR N  28      -2.533  -7.770 -17.246  1.00  0.00           H
ATOM    372 HG22 THR N  28      -4.052  -7.420 -16.381  1.00  0.00           H
ATOM    373 HG23 THR N  28      -4.088  -8.175 -17.990  1.00  0.00           H
ATOM    374  OH  TYR N  29      -5.222   4.242 -21.460  1.00  0.00           O
ATOM    375  OH  TYR N  44       5.363  -6.061 -11.142  1.00  0.00           O
ATOM    376  H   ASN N  46       2.589   1.920  -6.255  1.00  0.00           H
ATOM    377  CA  ASN N  46       1.468   3.539  -5.397  1.00  0.00           C
ATOM    378  HG1 ARG N  10      -3.166   6.389  -8.939  1.00  0.00           H
ATOM    379  HG2 ARG N  10      -2.287   5.982  -7.484  1.00  0.00           H
ATOM    380  CD  ARG N  10      -3.509   4.390  -8.278  1.00  0.00           C
ATOM    381  H   SER N  11      -0.900   7.487 -11.660  1.00  0.00           H
ATOM    382  CA  SER N  11      -2.657   8.268 -12.648  1.00  0.00           C
ATOM    383  HA  ALA N  27      -3.262  -2.787 -13.286  1.00  0.00           H
ATOM    384  N   ALA N  27      -5.167  -2.878 -14.122  1.00  0.00           N
ATOM    385  CB  ALA N  27      -4.133  -4.723 -12.874  1.00  0.00           C
ATOM    386  HH  TYR N  29      -5.017   4.054 -22.389  1.00  0.00           H
ATOM    387  HH  TYR N  44       4.934  -5.840 -11.983  1.00  0.00           H
ATOM    388  HA  ASN N  46       1.457   3.962  -4.386  1.00  0.00           H
ATOM    389  CB  ASN N  46       2.013   4.579  -6.393  1.00  0.00           C
ATOM    390  C   ASN N  46      -0.007   3.214  -5.708  1.00  0.00           C
ATOM    391  HD1 ARG N  10      -3.656   3.858  -9.232  1.00  0.00           H
ATOM    392  HD2 ARG N  10      -4.505   4.757  -7.978  1.00  0.00           H
ATOM    393  NE  ARG N  10      -2.981   3.472  -7.269  1.00  0.00           N
ATOM    394  HA  SER N  11      -3.438   8.700 -12.003  1.00  0.00           H
ATOM    395  CB  SER N  11      -1.777   9.401 -13.195  1.00  0.00           C
ATOM    396  C   SER N  11      -3.404   7.633 -13.841  1.00  0.00           C
ATOM    397  H   ALA N  27      -6.020  -3.397 -13.932  1.00  0.00           H
ATOM    398  C   CYS N  26      -5.276  -1.697 -14.747  1.00  0.00           C
ATOM    399  HB1 ALA N  27      -3.171  -5.196 -12.653  1.00  0.00           H
ATOM    400  HB2 ALA N  27      -4.797  -5.457 -13.349  1.00  0.00           H
ATOM    401  HB3 ALA N  27      -4.589  -4.390 -11.929  1.00  0.00           H
ATOM    402  HB1 ASN N  46       1.955   4.199  -7.422  1.00  0.00           H
ATOM    403  HB2 ASN N  46       1.380   5.476  -6.327  1.00  0.00           H
ATOM    404  CG  ASN N  46       3.469   4.938  -6.136  1.00  0.00           C
ATOM    405  OXT ASN N  46      -0.774   4.211  -5.764  1.00  0.00           O
ATOM    406  O   ASN N  46      -0.344   2.010  -5.899  1.00  0.00           O
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ATOM    407  HE  ARG N  10      -2.167   3.786  -6.691  1.00  0.00           H
ATOM    408  CZ  ARG N  10      -3.638   2.403  -6.798  1.00  0.00           C
ATOM    409  HB1 SER N  11      -1.044   8.986 -13.905  1.00  0.00           H
ATOM    410  HB2 SER N  11      -2.441  10.081 -13.757  1.00  0.00           H
ATOM    411  OG  SER N  11      -1.132  10.066 -12.123  1.00  0.00           O
ATOM    412  O   SER N  11      -4.600   7.885 -14.062  1.00  0.00           O
ATOM    413  N   ASN N  12      -2.642   6.856 -14.623  1.00  0.00           N
ATOM    414  O   CYS N  26      -4.323  -0.934 -14.976  1.00  0.00           O
ATOM    415  CA  CYS N  26      -6.677  -1.312 -15.248  1.00  0.00           C
ATOM    416  OD1 ASN N  46       4.341   4.771  -6.995  1.00  0.00           O
ATOM    417  ND2 ASN N  46       3.762   5.458  -4.920  1.00  0.00           N
ATOM    418  NH2 ARG N  10      -3.142   1.772  -5.723  1.00  0.00           N
ATOM    419  NH1 ARG N  10      -4.797   2.004  -7.349  1.00  0.00           N
ATOM    420  H   SER N  11      -0.958  11.001 -12.376  1.00  0.00           H
ATOM    421  H   ASN N  12      -1.642   6.781 -14.413  1.00  0.00           H
ATOM    422  CA  ASN N  12      -3.121   6.303 -15.882  1.00  0.00           C
ATOM    423  HA  CYS N  26      -6.485  -0.887 -16.242  1.00  0.00           H
ATOM    424  N   CYS N  26      -7.545  -2.456 -15.414  1.00  0.00           N
ATOM    425  CB  CYS N  26      -7.357  -0.244 -14.401  1.00  0.00           C
ATOM    426 HD21 ASN N  46       4.726   5.726  -4.756  1.00  0.00           H
ATOM    427 HD22 ASN N  46       3.099   5.574  -4.153  1.00  0.00           H
ATOM    428 HH21 ARG N  10      -3.544   0.876  -5.431  1.00  0.00           H
ATOM    429 HH22 ARG N  10      -2.125   1.894  -5.569  1.00  0.00           H
ATOM    430 HH11 ARG N  10      -5.087   2.399  -8.236  1.00  0.00           H
ATOM    431 HH12 ARG N  10      -5.243   1.112  -7.107  1.00  0.00           H
ATOM    432  HA  ASN N  12      -3.643   7.088 -16.445  1.00  0.00           H
ATOM    433  CB  ASN N  12      -1.926   5.789 -16.702  1.00  0.00           C
ATOM    434  C   ASN N  12      -4.184   5.214 -15.608  1.00  0.00           C
ATOM    435  H   CYS N  26      -8.316  -2.596 -14.764  1.00  0.00           H
ATOM    436  C   LEU N  25      -7.409  -3.270 -16.485  1.00  0.00           C
ATOM    437  HB1 CYS N  26      -6.704   0.626 -14.259  1.00  0.00           H
ATOM    438  HB2 CYS N  26      -7.619  -0.630 -13.404  1.00  0.00           H
ATOM    439  SG  CYS N  26      -8.961   0.281 -15.125  1.00  0.00           S
ATOM    440  HB1 ASN N  12      -2.297   5.288 -17.610  1.00  0.00           H
ATOM    441  HB2 ASN N  12      -1.371   5.031 -16.125  1.00  0.00           H
ATOM    442  CG  ASN N  12      -0.964   6.930 -17.094  1.00  0.00           C
ATOM    443  O   ASN N  12      -5.213   5.112 -16.295  1.00  0.00           O
ATOM    444  N   PHE N  13      -3.914   4.432 -14.550  1.00  0.00           N
ATOM    445  O   LEU N  25      -6.567  -3.080 -17.365  1.00  0.00           O
ATOM    446  CA  LEU N  25      -8.373  -4.458 -16.553  1.00  0.00           C
ATOM    447  SG  CYS N  16      -8.419   0.856 -17.056  1.00  0.00           S
ATOM    448  OD1 ASN N  12      -1.147   8.082 -16.693  1.00  0.00           O
ATOM    449  ND2 ASN N  12       0.077   6.604 -17.882  1.00  0.00           N
ATOM    450  H   PHE N  13      -3.024   4.556 -14.056  1.00  0.00           H
ATOM    451  CA  PHE N  13      -4.835   3.463 -13.984  1.00  0.00           C
ATOM    452  HA  LEU N  25      -7.817  -5.221 -17.110  1.00  0.00           H
ATOM    453  N   LEU N  25      -8.673  -4.980 -15.220  1.00  0.00           N
ATOM    454  CB  LEU N  25      -9.675  -4.076 -17.269  1.00  0.00           C
ATOM    455  CB  CYS N  16      -7.826   2.567 -16.817  1.00  0.00           C
ATOM    456 HD21 ASN N  12       0.272   5.681 -18.257  1.00  0.00           H
ATOM    457 HD22 ASN N  12       0.684   7.367 -18.189  1.00  0.00           H
ATOM    458  HA  PHE N  13      -5.105   2.703 -14.733  1.00  0.00           H
ATOM    459  C   PHE N  13      -6.152   4.128 -13.574  1.00  0.00           C
ATOM    460  CB  PHE N  13      -4.134   2.804 -12.773  1.00  0.00           C
ATOM    461  H   LEU N  25      -9.553  -4.710 -14.783  1.00  0.00           H
ATOM    462  C   ALA N  24      -7.680  -5.444 -14.426  1.00  0.00           C
ATOM    463  HB1 LEU N  25     -10.260  -3.457 -16.576  1.00  0.00           H
ATOM    464  HB2 LEU N  25      -9.425  -3.428 -18.125  1.00  0.00           H
ATOM    465  CG  LEU N  25     -10.528  -5.263 -17.753  1.00  0.00           C
ATOM    466  HB1 CYS N  16      -7.235   2.607 -15.893  1.00  0.00           H
ATOM    467  HB2 CYS N  16      -7.150   2.753 -17.664  1.00  0.00           H
ATOM    468  CA  CYS N  16      -8.910   3.649 -16.795  1.00  0.00           C
ATOM    469  O   PHE N  13      -7.237   3.579 -13.826  1.00  0.00           O
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ATOM    470  N   ASN N  14      -6.046   5.293 -12.919  1.00  0.00           N
ATOM    471  HB1 PHE N  13      -3.671   3.609 -12.195  1.00  0.00           H
ATOM    472  HB2 PHE N  13      -3.323   2.172 -13.152  1.00  0.00           H
ATOM    473  CG  PHE N  13      -5.034   2.009 -11.872  1.00  0.00           C
ATOM    474  O   ALA N  24      -6.510  -5.532 -14.804  1.00  0.00           O
ATOM    475  CA  ALA N  24      -8.085  -5.948 -13.033  1.00  0.00           C
ATOM    476  HG  LEU N  25     -10.658  -5.948 -16.901  1.00  0.00           H
ATOM    477  CD1 LEU N  25      -9.838  -6.038 -18.876  1.00  0.00           C
ATOM    478  CD2 LEU N  25     -11.923  -4.783 -18.177  1.00  0.00           C
ATOM    479  HA  CYS N  16      -9.364   3.734 -17.789  1.00  0.00           H
ATOM    480  N   CYS N  16      -8.265   4.900 -16.439  1.00  0.00           N
ATOM    481  C   CYS N  16     -10.115   3.340 -15.881  1.00  0.00           C
ATOM    482  H   ASN N  14      -5.116   5.628 -12.646  1.00  0.00           H
ATOM    483  CA  ASN N  14      -7.209   6.003 -12.421  1.00  0.00           C
ATOM    484  CD1 PHE N  13      -5.130   0.622 -12.016  1.00  0.00           C
ATOM    485  CD2 PHE N  13      -5.791   2.646 -10.875  1.00  0.00           C
ATOM    486  HA  ALA N  24      -7.147  -5.971 -12.460  1.00  0.00           H
ATOM    487  N   ALA N  24      -9.009  -5.040 -12.354  1.00  0.00           N
ATOM    488  CB  ALA N  24      -8.664  -7.357 -13.150  1.00  0.00           C
ATOM    489 HD11 LEU N  25      -8.869  -6.456 -18.569  1.00  0.00           H
ATOM    490 HD12 LEU N  25     -10.451  -6.884 -19.220  1.00  0.00           H
ATOM    491 HD13 LEU N  25      -9.656  -5.389 -19.746  1.00  0.00           H
ATOM    492 HD21 LEU N  25     -12.459  -4.295 -17.350  1.00  0.00           H
ATOM    493 HD22 LEU N  25     -12.550  -5.620 -18.521  1.00  0.00           H
ATOM    494 HD23 LEU N  25     -11.861  -4.050 -18.999  1.00  0.00           H
ATOM    495  H   CYS N  16      -7.275   4.900 -16.183  1.00  0.00           H
ATOM    496  C   VAL N  15      -8.971   6.052 -16.410  1.00  0.00           C
ATOM    497  O   CYS N  16     -11.188   2.966 -16.385  1.00  0.00           O
ATOM    498  N   ARG N  17      -9.977   3.500 -14.556  1.00  0.00           N
ATOM    499  HA  ASN N  14      -7.833   5.322 -11.824  1.00  0.00           H
ATOM    500  CB  ASN N  14      -6.783   7.188 -11.557  1.00  0.00           C
ATOM    501  C   ASN N  14      -8.107   6.495 -13.568  1.00  0.00           C
ATOM    502  HD1 PHE N  13      -4.534   0.132 -12.785  1.00  0.00           H
ATOM    503  CE1 PHE N  13      -5.984  -0.122 -11.203  1.00  0.00           C
ATOM    504  HD2 PHE N  13      -5.724   3.724 -10.728  1.00  0.00           H
ATOM    505  CE2 PHE N  13      -6.645   1.901 -10.064  1.00  0.00           C
ATOM    506  H   ALA N  24      -9.922  -5.378 -12.067  1.00  0.00           H
ATOM    507  C   GLU N  23      -8.607  -3.799 -11.966  1.00  0.00           C
ATOM    508  HB1 ALA N  24      -7.916  -8.018 -13.603  1.00  0.00           H
ATOM    509  HB2 ALA N  24      -9.556  -7.374 -13.785  1.00  0.00           H
ATOM    510  HB3 ALA N  24      -8.929  -7.767 -12.167  1.00  0.00           H
ATOM    511  O   VAL N  15     -10.145   6.126 -16.780  1.00  0.00           O
ATOM    512  CA  VAL N  15      -8.225   7.280 -15.881  1.00  0.00           C
ATOM    513  H   ARG N  17      -9.050   3.723 -14.179  1.00  0.00           H
ATOM    514  CA  ARG N  17     -11.083   3.166 -13.664  1.00  0.00           C
ATOM    515  HB1 ASN N  14      -6.121   7.853 -12.133  1.00  0.00           H
ATOM    516  HB2 ASN N  14      -7.690   7.758 -11.303  1.00  0.00           H
ATOM    517  CG  ASN N  14      -6.135   6.790 -10.229  1.00  0.00           C
ATOM    518  O   ASN N  14      -9.340   6.479 -13.445  1.00  0.00           O
ATOM    519  N   VAL N  15      -7.479   6.958 -14.668  1.00  0.00           N
ATOM    520  HE1 PHE N  13      -6.063  -1.202 -11.344  1.00  0.00           H
ATOM    521  CZ  PHE N  13      -6.750   0.519 -10.229  1.00  0.00           C
ATOM    522  HE2 PHE N  13      -7.235   2.406  -9.295  1.00  0.00           H
ATOM    523  O   GLU N  23      -7.506  -3.348 -12.290  1.00  0.00           O
ATOM    524  CA  GLU N  23      -9.515  -3.010 -11.008  1.00  0.00           C
ATOM    525  HA  VAL N  15      -9.026   7.990 -15.628  1.00  0.00           H
ATOM    526  CB  VAL N  15      -7.305   7.925 -16.943  1.00  0.00           C
ATOM    527  HA  ARG N  17     -11.483   2.177 -13.928  1.00  0.00           H
ATOM    528  C   ARG N  17     -12.267   4.129 -13.860  1.00  0.00           C
ATOM    529  CB  ARG N  17     -10.658   3.186 -12.181  1.00  0.00           C
ATOM    530  OD1 ASN N  14      -6.378   5.730  -9.659  1.00  0.00           O
ATOM    531  ND2 ASN N  14      -5.346   7.761  -9.704  1.00  0.00           N
ATOM    532  H   VAL N  15      -6.456   6.992 -14.681  1.00  0.00           H
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ATOM    533  HZ  PHE N  13      -7.422  -0.046  -9.590  1.00  0.00           H
ATOM    534  HA  GLU N  23      -9.031  -2.029 -10.908  1.00  0.00           H
ATOM    535  N   GLU N  23     -10.878  -2.855 -11.511  1.00  0.00           N
ATOM    536  CB  GLU N  23      -9.566  -3.715  -9.634  1.00  0.00           C
ATOM    537  HB  VAL N  15      -6.371   7.338 -16.968  1.00  0.00           H
ATOM    538  CG2 VAL N  15      -6.995   9.357 -16.515  1.00  0.00           C
ATOM    539  CG1 VAL N  15      -7.935   7.871 -18.337  1.00  0.00           C
ATOM    540  O   ARG N  17     -13.428   3.728 -13.686  1.00  0.00           O
ATOM    541  N   LEU N  18     -11.971   5.400 -14.194  1.00  0.00           N
ATOM    542  HB1 ARG N  17     -11.566   3.004 -11.583  1.00  0.00           H
ATOM    543  HB2 ARG N  17     -10.326   4.210 -11.940  1.00  0.00           H
ATOM    544  CG  ARG N  17      -9.540   2.209 -11.775  1.00  0.00           C
ATOM    545 HD21 ASN N  14      -5.060   8.542 -10.279  1.00  0.00           H
ATOM    546 HD22 ASN N  14      -4.848   7.637  -8.823  1.00  0.00           H
ATOM    547  H   GLU N  23     -11.583  -2.650 -10.808  1.00  0.00           H
ATOM    548  C   PRO N  22     -11.266  -2.748 -12.807  1.00  0.00           C
ATOM    549  HB1 GLU N  23      -8.548  -4.025  -9.366  1.00  0.00           H
ATOM    550  HB2 GLU N  23     -10.143  -4.644  -9.765  1.00  0.00           H
ATOM    551  CG  GLU N  23     -10.188  -2.918  -8.466  1.00  0.00           C
ATOM    552 HG21 VAL N  15      -6.391   9.888 -17.258  1.00  0.00           H
ATOM    553 HG22 VAL N  15      -6.442   9.398 -15.568  1.00  0.00           H
ATOM    554 HG23 VAL N  15      -7.933   9.920 -16.391  1.00  0.00           H
ATOM    555 HG11 VAL N  15      -7.344   8.448 -19.060  1.00  0.00           H
ATOM    556 HG12 VAL N  15      -8.001   6.838 -18.707  1.00  0.00           H
ATOM    557 HG13 VAL N  15      -8.953   8.291 -18.348  1.00  0.00           H
ATOM    558  H   LEU N  18     -10.988   5.681 -14.230  1.00  0.00           H
ATOM    559  CA  LEU N  18     -12.955   6.477 -14.196  1.00  0.00           C
ATOM    560  HG1 ARG N  17      -8.694   2.305 -12.471  1.00  0.00           H
ATOM    561  HG2 ARG N  17      -9.147   2.538 -10.803  1.00  0.00           H
ATOM    562  CD  ARG N  17      -9.886   0.713 -11.659  1.00  0.00           C
ATOM    563  O   PRO N  22     -10.497  -2.840 -13.767  1.00  0.00           O
ATOM    564  CA  PRO N  22     -12.790  -2.652 -12.951  1.00  0.00           C
ATOM    565  HG1 GLU N  23     -10.611  -3.644  -7.764  1.00  0.00           H
ATOM    566  HG2 GLU N  23     -11.016  -2.282  -8.815  1.00  0.00           H
ATOM    567  CD  GLU N  23      -9.173  -2.069  -7.678  1.00  0.00           C
ATOM    568  HA  LEU N  18     -13.198   6.717 -13.150  1.00  0.00           H
ATOM    569  C   LEU N  18     -14.314   6.107 -14.797  1.00  0.00           C
ATOM    570  CB  LEU N  18     -12.415   7.742 -14.913  1.00  0.00           C
ATOM    571  HD1 ARG N  17      -8.963   0.140 -11.806  1.00  0.00           H
ATOM    572  HD2 ARG N  17     -10.575   0.389 -12.450  1.00  0.00           H
ATOM    573  NE  ARG N  17     -10.395   0.297 -10.346  1.00  0.00           N
ATOM    574  HA  PRO N  22     -13.183  -2.006 -12.149  1.00  0.00           H
ATOM    575  N   PRO N  22     -13.195  -2.121 -14.246  1.00  0.00           N
ATOM    576  CB  PRO N  22     -13.433  -4.055 -12.892  1.00  0.00           C
ATOM    577  OE2 GLU N  23      -8.667  -2.593  -6.660  1.00  0.00           O
ATOM    578  OE1 GLU N  23      -8.875  -0.914  -8.148  1.00  0.00           O
ATOM    579  O   LEU N  18     -15.343   6.385 -14.141  1.00  0.00           O
ATOM    580  N   PRO N  19     -14.398   5.598 -16.037  1.00  0.00           N
ATOM    581  HB1 LEU N  18     -11.389   7.544 -15.249  1.00  0.00           H
ATOM    582  HB2 LEU N  18     -12.990   7.912 -15.838  1.00  0.00           H
ATOM    583  CG  LEU N  18     -12.458   9.033 -14.080  1.00  0.00           C
ATOM    584  HE  ARG N  17      -9.722   0.014  -9.617  1.00  0.00           H
ATOM    585  CZ  ARG N  17     -11.679   0.294  -9.955  1.00  0.00           C
ATOM    586  C   THR N  21     -12.955  -0.822 -14.526  1.00  0.00           C
ATOM    587  CD  PRO N  22     -14.097  -3.031 -14.968  1.00  0.00           C
ATOM    588  HB1 PRO N  22     -13.725  -4.340 -11.875  1.00  0.00           H
ATOM    589  HB2 PRO N  22     -12.717  -4.805 -13.260  1.00  0.00           H
ATOM    590  CG  PRO N  22     -14.617  -3.948 -13.858  1.00  0.00           C
ATOM    591  CA  PRO N  19     -15.720   5.360 -16.644  1.00  0.00           C
ATOM    592  CD  PRO N  19     -13.290   5.300 -16.984  1.00  0.00           C
ATOM    593  HG  LEU N  18     -11.788   8.886 -13.211  1.00  0.00           H
ATOM    594  CD1 LEU N  18     -11.902  10.181 -14.932  1.00  0.00           C
ATOM    595  CD2 LEU N  18     -13.857   9.382 -13.555  1.00  0.00           C
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ATOM    596  NH1 ARG N  17     -12.688   0.334 -10.835  1.00  0.00           N
ATOM    597  NH2 ARG N  17     -11.967   0.212  -8.650  1.00  0.00           N
ATOM    598  O   THR N  21     -12.370  -0.089 -13.712  1.00  0.00           O
ATOM    599  CA  THR N  21     -13.378  -0.259 -15.890  1.00  0.00           C
ATOM    600  HD1 PRO N  22     -14.900  -2.462 -15.446  1.00  0.00           H
ATOM    601  HD2 PRO N  22     -13.540  -3.594 -15.732  1.00  0.00           H
ATOM    602  HG1 PRO N  22     -14.932  -4.933 -14.237  1.00  0.00           H
ATOM    603  HG2 PRO N  22     -15.478  -3.475 -13.360  1.00  0.00           H
ATOM    604  HA  PRO N  19     -16.394   6.201 -16.437  1.00  0.00           H
ATOM    605  CB  PRO N  19     -15.384   5.212 -18.134  1.00  0.00           C
ATOM    606  C   PRO N  19     -16.440   4.099 -16.137  1.00  0.00           C
ATOM    607  HD1 PRO N  19     -12.508   4.705 -16.514  1.00  0.00           H
ATOM    608  HD2 PRO N  19     -12.832   6.240 -17.327  1.00  0.00           H
ATOM    609  CG  PRO N  19     -13.996   4.574 -18.129  1.00  0.00           C
ATOM    610 HD11 LEU N  18     -10.934   9.919 -15.383  1.00  0.00           H
ATOM    611 HD12 LEU N  18     -11.757  11.102 -14.346  1.00  0.00           H
ATOM    612 HD13 LEU N  18     -12.588  10.427 -15.760  1.00  0.00           H
ATOM    613 HD21 LEU N  18     -14.293   8.580 -12.943  1.00  0.00           H
ATOM    614 HD22 LEU N  18     -13.838  10.287 -12.932  1.00  0.00           H
ATOM    615 HD23 LEU N  18     -14.556   9.554 -14.390  1.00  0.00           H
ATOM    616 HH11 ARG N  17     -12.506   0.335 -11.840  1.00  0.00           H
ATOM    617 HH12 ARG N  17     -13.590   0.721 -10.504  1.00  0.00           H
ATOM    618 HH21 ARG N  17     -11.218   0.221  -7.965  1.00  0.00           H
ATOM    619 HH22 ARG N  17     -12.903  -0.100  -8.341  1.00  0.00           H
ATOM    620  HA  THR N  21     -13.962  -1.001 -16.452  1.00  0.00           H
ATOM    621  N   THR N  21     -14.199   0.906 -15.672  1.00  0.00           N
ATOM    622  CB  THR N  21     -12.125   0.111 -16.711  1.00  0.00           C
ATOM    623  HB1 PRO N  19     -16.139   4.640 -18.677  1.00  0.00           H
ATOM    624  HB2 PRO N  19     -15.318   6.207 -18.591  1.00  0.00           H
ATOM    625  O   PRO N  19     -17.608   3.903 -16.458  1.00  0.00           O
ATOM    626  N   GLY N  20     -15.679   3.220 -15.427  1.00  0.00           N
ATOM    627  HG1 PRO N  19     -13.484   4.702 -19.089  1.00  0.00           H
ATOM    628  HG2 PRO N  19     -14.054   3.494 -17.919  1.00  0.00           H
ATOM    629  H   THR N  21     -13.886   1.799 -16.035  1.00  0.00           H
ATOM    630  C   GLY N  20     -15.404   0.758 -15.092  1.00  0.00           C
ATOM    631  HB  THR N  21     -11.434   0.622 -16.030  1.00  0.00           H
ATOM    632  OG1 THR N  21     -12.489   1.015 -17.743  1.00  0.00           O
ATOM    633  CG2 THR N  21     -11.472  -1.146 -17.252  1.00  0.00           C
ATOM    634  H   GLY N  20     -14.832   3.563 -14.964  1.00  0.00           H
ATOM    635  CA  GLY N  20     -16.247   2.004 -14.888  1.00  0.00           C
ATOM    636  O   GLY N  20     -15.802  -0.350 -14.712  1.00  0.00           O
ATOM    637  HG1 THR N  21     -11.987   1.833 -17.545  1.00  0.00           H
ATOM    638 HG21 THR N  21     -11.151  -1.776 -16.412  1.00  0.00           H
ATOM    639 HG22 THR N  21     -10.590  -0.898 -17.855  1.00  0.00           H
ATOM    640 HG23 THR N  21     -12.166  -1.722 -17.879  1.00  0.00           H
ATOM    641  HA1 GLY N  20     -17.223   1.821 -15.358  1.00  0.00           H
ATOM    642  HA2 GLY N  20     -16.411   2.111 -13.805  1.00  0.00           H
END
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3) CRAMBIN – molecule as in the optimized 84W crystal

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COMPND    CRAMBIN OPTIMIZED CRYSTAL 84W GEOMETRY
AUTHOR    DELLE PIANE, CORNO, ORLANDO, DOVESI, UGLIENGO
ATOM      1  N   THR N   1      -7.330   3.687  -4.789  1.00  0.00           N
ATOM      2  H1  THR N   1      -7.752   2.757  -4.913  1.00  0.00           H
ATOM      3  H2  THR N   1      -6.627   3.803  -5.557  1.00  0.00           H
ATOM      4  H3  THR N   1      -8.043   4.470  -4.836  1.00  0.00           H
ATOM      5  CA  THR N   1      -6.680   3.696  -3.453  1.00  0.00           C
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ATOM      6  HA  THR N   1      -7.478   3.693  -2.697  1.00  0.00           H
ATOM      7  C   THR N   1      -5.830   4.954  -3.364  1.00  0.00           C
ATOM      8  CB  THR N   1      -5.817   2.413  -3.308  1.00  0.00           C
ATOM      9  O   THR N   1      -5.269   5.378  -4.383  1.00  0.00           O
ATOM     10  N   THR N   2      -5.708   5.501  -2.151  1.00  0.00           N
ATOM     11  HB  THR N   1      -4.968   2.514  -4.006  1.00  0.00           H
ATOM     12  OG1 THR N   1      -6.631   1.324  -3.713  1.00  0.00           O
ATOM     13  CG2 THR N   1      -5.286   2.221  -1.892  1.00  0.00           C
ATOM     14  H   THR N   2      -6.142   5.059  -1.322  1.00  0.00           H
ATOM     15  CA  THR N   2      -4.777   6.584  -1.921  1.00  0.00           C
ATOM     16  HG1 THR N   1      -6.142   0.904  -4.465  1.00  0.00           H
ATOM     17 HG21 THR N   1      -4.752   1.262  -1.834  1.00  0.00           H
ATOM     18 HG22 THR N   1      -4.582   3.016  -1.607  1.00  0.00           H
ATOM     19 HG23 THR N   1      -6.103   2.204  -1.154  1.00  0.00           H
ATOM     20  HA  THR N   2      -4.418   6.907  -2.903  1.00  0.00           H
ATOM     21  C   THR N   2      -3.548   6.115  -1.146  1.00  0.00           C
ATOM     22  CB  THR N   2      -5.465   7.817  -1.269  1.00  0.00           C
ATOM     23  O   THR N   2      -3.606   5.269  -0.228  1.00  0.00           O
ATOM     24  N   CYS N   3      -2.428   6.734  -1.541  1.00  0.00           N
ATOM     25  HB  THR N   2      -4.668   8.450  -0.842  1.00  0.00           H
ATOM     26  OG1 THR N   2      -6.308   7.424  -0.182  1.00  0.00           O
ATOM     27  CG2 THR N   2      -6.186   8.601  -2.355  1.00  0.00           C
ATOM     28  H   CYS N   3      -2.498   7.387  -2.333  1.00  0.00           H
ATOM     29  CA  CYS N   3      -1.096   6.499  -1.020  1.00  0.00           C
ATOM     30  HG1 THR N   2      -7.255   7.613  -0.399  1.00  0.00           H
ATOM     31 HG21 THR N   2      -6.673   9.485  -1.933  1.00  0.00           H
ATOM     32 HG22 THR N   2      -5.458   8.940  -3.103  1.00  0.00           H
ATOM     33 HG23 THR N   2      -6.945   7.987  -2.859  1.00  0.00           H
ATOM     34  HA  CYS N   3      -1.166   5.864  -0.130  1.00  0.00           H
ATOM     35  C   CYS N   3      -0.480   7.871  -0.707  1.00  0.00           C
ATOM     36  CB  CYS N   3      -0.187   5.827  -2.071  1.00  0.00           C
ATOM     37  O   CYS N   3      -0.670   8.807  -1.499  1.00  0.00           O
ATOM     38  N   CYS N   4       0.301   7.984   0.376  1.00  0.00           N
ATOM     39  HB1 CYS N   3       0.780   5.578  -1.615  1.00  0.00           H
ATOM     40  HB2 CYS N   3      -0.008   6.522  -2.903  1.00  0.00           H
ATOM     41  SG  CYS N   3      -0.874   4.341  -2.889  1.00  0.00           S
ATOM     42  H   CYS N   4       0.398   7.221   1.058  1.00  0.00           H
ATOM     43  CA  CYS N   4       0.852   9.279   0.732  1.00  0.00           C
ATOM     44  SG  CYS N  40      -0.642   2.875  -1.434  1.00  0.00           S
ATOM     45  HA  CYS N   4       0.601   9.947  -0.096  1.00  0.00           H
ATOM     46  C   CYS N   4       2.372   9.194   0.862  1.00  0.00           C
ATOM     47  CB  CYS N   4       0.216   9.836   2.014  1.00  0.00           C
ATOM     48  CB  CYS N  40       1.140   2.454  -1.626  1.00  0.00           C
ATOM     49  O   CYS N   4       2.923   8.200   1.355  1.00  0.00           O
ATOM     50  N   PRO N   5       3.069  10.269   0.445  1.00  0.00           N
ATOM     51  HB1 CYS N   4       0.237   9.091   2.821  1.00  0.00           H
ATOM     52  HB2 CYS N   4       0.749  10.721   2.386  1.00  0.00           H
ATOM     53  SG  CYS N   4      -1.556  10.271   1.813  1.00  0.00           S
ATOM     54  HB1 CYS N  40       1.750   3.364  -1.567  1.00  0.00           H
ATOM     55  HB2 CYS N  40       1.385   1.850  -0.739  1.00  0.00           H
ATOM     56  CA  CYS N  40       1.438   1.661  -2.901  1.00  0.00           C
ATOM     57  CA  PRO N   5       4.542  10.265   0.469  1.00  0.00           C
ATOM     58  CD  PRO N   5       2.525  11.485  -0.212  1.00  0.00           C
ATOM     59  SG  CYS N  32      -1.485  12.169   0.957  1.00  0.00           S
ATOM     60  HA  CYS N  40       1.092   2.219  -3.781  1.00  0.00           H
ATOM     61  N   CYS N  40       0.748   0.396  -2.846  1.00  0.00           N
ATOM     62  C   CYS N  40       2.953   1.422  -2.997  1.00  0.00           C
ATOM     63  HA  PRO N   5       4.937   9.295   0.150  1.00  0.00           H
ATOM     64  C   PRO N   5       5.129  10.510   1.855  1.00  0.00           C
ATOM     65  CB  PRO N   5       4.899  11.385  -0.516  1.00  0.00           C
ATOM     66  HD1 PRO N   5       1.732  11.945   0.393  1.00  0.00           H
ATOM     67  HD2 PRO N   5       2.109  11.221  -1.193  1.00  0.00           H
ATOM     68  CG  PRO N   5       3.751  12.381  -0.362  1.00  0.00           C
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ATOM     69  CB  CYS N  32      -1.904  11.894  -0.820  1.00  0.00           C
ATOM     70  H   CYS N  40       0.330   0.114  -1.950  1.00  0.00           H
ATOM     71  C   THR N  39       0.635  -0.424  -3.898  1.00  0.00           C
ATOM     72  O   CYS N  40       3.483   0.489  -2.371  1.00  0.00           O
ATOM     73  N   PRO N  41       3.664   2.274  -3.748  1.00  0.00           N
ATOM     74  O   PRO N   5       6.340  10.314   2.052  1.00  0.00           O
ATOM     75  N   SER N   6       4.293  10.984   2.790  1.00  0.00           N
ATOM     76  HB1 PRO N   5       5.886  11.812  -0.322  1.00  0.00           H
ATOM     77  HB2 PRO N   5       4.896  10.967  -1.528  1.00  0.00           H
ATOM     78  HG1 PRO N   5       3.660  13.066  -1.211  1.00  0.00           H
ATOM     79  HG2 PRO N   5       3.875  13.000   0.532  1.00  0.00           H
ATOM     80  HB1 CYS N  32      -2.298  10.875  -0.909  1.00  0.00           H
ATOM     81  HB2 CYS N  32      -2.728  12.589  -1.040  1.00  0.00           H
ATOM     82  CA  CYS N  32      -0.751  12.100  -1.810  1.00  0.00           C
ATOM     83  O   THR N  39       1.085  -0.168  -5.027  1.00  0.00           O
ATOM     84  CA  THR N  39      -0.173  -1.683  -3.597  1.00  0.00           C
ATOM     85  CA  PRO N  41       5.115   2.137  -3.847  1.00  0.00           C
ATOM     86  CD  PRO N  41       3.158   3.448  -4.489  1.00  0.00           C
ATOM     87  H   SER N   6       3.301  11.068   2.595  1.00  0.00           H
ATOM     88  CA  SER N   6       4.687  11.130   4.171  1.00  0.00           C
ATOM     89  HA  CYS N  32       0.045  11.376  -1.595  1.00  0.00           H
ATOM     90  N   CYS N  32      -0.218  13.450  -1.719  1.00  0.00           N
ATOM     91  C   CYS N  32      -1.226  11.808  -3.261  1.00  0.00           C
ATOM     92  HA  THR N  39      -0.205  -1.856  -2.515  1.00  0.00           H
ATOM     93  N   THR N  39      -1.542  -1.407  -4.008  1.00  0.00           N
ATOM     94  CB  THR N  39       0.380  -2.962  -4.254  1.00  0.00           C
ATOM     95  HA  PRO N  41       5.384   1.092  -4.042  1.00  0.00           H
ATOM     96  C   PRO N  41       5.784   2.584  -2.534  1.00  0.00           C
ATOM     97  CB  PRO N  41       5.470   3.072  -5.023  1.00  0.00           C
ATOM     98  HD1 PRO N  41       2.491   4.056  -3.862  1.00  0.00           H
ATOM     99  HD2 PRO N  41       2.591   3.116  -5.375  1.00  0.00           H
ATOM    100  CG  PRO N  41       4.433   4.190  -4.889  1.00  0.00           C
ATOM    101  HA  SER N   6       5.405  10.334   4.399  1.00  0.00           H
ATOM    102  C   SER N   6       3.462  10.940   5.051  1.00  0.00           C
ATOM    103  CB  SER N   6       5.355  12.466   4.469  1.00  0.00           C
ATOM    104  H   CYS N  32      -0.796  14.164  -1.262  1.00  0.00           H
ATOM    105  C   GLY N  31       0.864  13.846  -2.414  1.00  0.00           C
ATOM    106  O   CYS N  32      -1.251  12.708  -4.103  1.00  0.00           O
ATOM    107  N   ILE N  33      -1.604  10.542  -3.520  1.00  0.00           N
ATOM    108  H   THR N  39      -1.698  -1.126  -4.975  1.00  0.00           H
ATOM    109  C   ALA N  38      -2.607  -1.567  -3.195  1.00  0.00           C
ATOM    110  HB  THR N  39       0.385  -2.849  -5.346  1.00  0.00           H
ATOM    111  OG1 THR N  39      -0.477  -4.040  -3.891  1.00  0.00           O
ATOM    112  CG2 THR N  39       1.789  -3.294  -3.800  1.00  0.00           C
ATOM    113  O   PRO N  41       5.201   3.290  -1.702  1.00  0.00           O
ATOM    114  N   GLY N  42       7.078   2.214  -2.408  1.00  0.00           N
ATOM    115  HB1 PRO N  41       6.498   3.450  -4.994  1.00  0.00           H
ATOM    116  HB2 PRO N  41       5.338   2.531  -5.974  1.00  0.00           H
ATOM    117  HG1 PRO N  41       4.292   4.757  -5.812  1.00  0.00           H
ATOM    118  HG2 PRO N  41       4.742   4.878  -4.093  1.00  0.00           H
ATOM    119  O   SER N   6       2.306  11.046   4.605  1.00  0.00           O
ATOM    120  N   ILE N   7       3.758  10.679   6.329  1.00  0.00           N
ATOM    121  HB1 SER N   6       5.848  12.406   5.443  1.00  0.00           H
ATOM    122  HB2 SER N   6       6.142  12.621   3.724  1.00  0.00           H
ATOM    123  OG  SER N   6       4.405  13.524   4.450  1.00  0.00           O
ATOM    124  O   GLY N  31       1.598  13.050  -3.028  1.00  0.00           O
ATOM    125  CA  GLY N  31       1.204  15.338  -2.451  1.00  0.00           C
ATOM    126  H   ILE N  33      -1.442   9.819  -2.814  1.00  0.00           H
ATOM    127  CA  ILE N  33      -1.872  10.088  -4.879  1.00  0.00           C
ATOM    128  O   ALA N  38      -2.518  -1.960  -2.022  1.00  0.00           O
ATOM    129  CA  ALA N  38      -3.968  -1.174  -3.802  1.00  0.00           C
ATOM    130  HG1 THR N  39      -1.353  -3.907  -4.321  1.00  0.00           H
ATOM    131 HG21 THR N  39       2.490  -2.506  -4.108  1.00  0.00           H
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ATOM    132 HG22 THR N  39       2.109  -4.233  -4.270  1.00  0.00           H
ATOM    133 HG23 THR N  39       1.834  -3.386  -2.704  1.00  0.00           H
ATOM    134  H   GLY N  42       7.484   1.614  -3.131  1.00  0.00           H
ATOM    135  CA  GLY N  42       7.853   2.541  -1.224  1.00  0.00           C
ATOM    136  H   ILE N   7       4.750  10.596   6.595  1.00  0.00           H
ATOM    137  CA  ILE N   7       2.749  10.553   7.363  1.00  0.00           C
ATOM    138  H   SER N   6       4.823  14.251   4.957  1.00  0.00           H
ATOM    139  HA1 GLY N  31       1.359  15.576  -3.512  1.00  0.00           H
ATOM    140  HA2 GLY N  31       2.160  15.482  -1.926  1.00  0.00           H
ATOM    141  N   GLY N  31       0.196  16.216  -1.904  1.00  0.00           N
ATOM    142  HA  ILE N  33      -2.189  10.960  -5.464  1.00  0.00           H
ATOM    143  C   ILE N  33      -2.985   9.049  -4.861  1.00  0.00           C
ATOM    144  CB  ILE N  33      -0.598   9.504  -5.576  1.00  0.00           C
ATOM    145  HA  ALA N  38      -4.101  -0.107  -3.566  1.00  0.00           H
ATOM    146  N   ALA N  38      -3.916  -1.278  -5.257  1.00  0.00           N
ATOM    147  CB  ALA N  38      -5.113  -1.972  -3.178  1.00  0.00           C
ATOM    148  HA1 GLY N  42       8.828   2.040  -1.306  1.00  0.00           H
ATOM    149  HA2 GLY N  42       7.376   2.139  -0.319  1.00  0.00           H
ATOM    150  C   GLY N  42       8.110   4.028  -0.984  1.00  0.00           C
ATOM    151  HA  ILE N   7       2.005   9.801   7.058  1.00  0.00           H
ATOM    152  C   ILE N   7       1.929  11.841   7.524  1.00  0.00           C
ATOM    153  CB  ILE N   7       3.420  10.115   8.679  1.00  0.00           C
ATOM    154  H   GLY N  31      -0.621  16.403  -2.490  1.00  0.00           H
ATOM    155  C   THR N  30       0.193  16.648  -0.633  1.00  0.00           C
ATOM    156  O   ILE N  33      -3.104   8.253  -3.912  1.00  0.00           O
ATOM    157  N   ILE N  34      -3.750   9.001  -5.965  1.00  0.00           N
ATOM    158  HB  ILE N  33      -0.903   9.302  -6.613  1.00  0.00           H
ATOM    159  CG2 ILE N  33       0.488  10.578  -5.598  1.00  0.00           C
ATOM    160  CG1 ILE N  33      -0.105   8.178  -4.961  1.00  0.00           C
ATOM    161  H   ALA N  38      -3.570  -2.190  -5.588  1.00  0.00           H
ATOM    162  C   GLY N  37      -4.464  -0.382  -6.101  1.00  0.00           C
ATOM    163  HB1 ALA N  38      -6.075  -1.600  -3.555  1.00  0.00           H
ATOM    164  HB2 ALA N  38      -5.098  -1.860  -2.086  1.00  0.00           H
ATOM    165  HB3 ALA N  38      -5.014  -3.041  -3.416  1.00  0.00           H
ATOM    166  O   GLY N  42       8.478   4.392   0.142  1.00  0.00           O
ATOM    167  N   ASP N  43       7.932   4.869  -2.026  1.00  0.00           N
ATOM    168  O   ILE N   7       0.693  11.766   7.610  1.00  0.00           O
ATOM    169  N   VAL N   8       2.591  13.008   7.578  1.00  0.00           N
ATOM    170  HB  ILE N   7       4.225  10.841   8.892  1.00  0.00           H
ATOM    171  CG2 ILE N   7       2.427  10.182   9.831  1.00  0.00           C
ATOM    172  CG1 ILE N   7       4.073   8.727   8.535  1.00  0.00           C
ATOM    173  O   THR N  30       1.108  16.437   0.182  1.00  0.00           O
ATOM    174  CA  THR N  30      -1.074  17.314  -0.118  1.00  0.00           C
ATOM    175  H   ILE N  34      -3.692   9.750  -6.668  1.00  0.00           H
ATOM    176  CA  ILE N  34      -4.645   7.891  -6.245  1.00  0.00           C
ATOM    177 HG21 ILE N  33       1.419  10.176  -5.992  1.00  0.00           H
ATOM    178 HG22 ILE N  33       0.715  10.953  -4.594  1.00  0.00           H
ATOM    179 HG23 ILE N  33       0.187  11.431  -6.221  1.00  0.00           H
ATOM    180 HG11 ILE N  33      -0.950   7.473  -4.901  1.00  0.00           H
ATOM    181 HG12 ILE N  33       0.214   8.359  -3.921  1.00  0.00           H
ATOM    182  CD1 ILE N  33       1.034   7.500  -5.733  1.00  0.00           C
ATOM    183  O   GLY N  37      -5.052   0.640  -5.725  1.00  0.00           O
ATOM    184  CA  GLY N  37      -4.301  -0.686  -7.601  1.00  0.00           C
ATOM    185  H   ASP N  43       7.652   4.524  -2.943  1.00  0.00           H
ATOM    186  CA  ASP N  43       8.021   6.314  -1.910  1.00  0.00           C
ATOM    187  H   VAL N   8       3.620  13.011   7.607  1.00  0.00           H
ATOM    188  CA  VAL N   8       1.842  14.254   7.709  1.00  0.00           C
ATOM    189 HG21 ILE N   7       2.909   9.876  10.766  1.00  0.00           H
ATOM    190 HG22 ILE N   7       2.056  11.203   9.985  1.00  0.00           H
ATOM    191 HG23 ILE N   7       1.555   9.531   9.656  1.00  0.00           H
ATOM    192 HG11 ILE N   7       4.743   8.724   7.663  1.00  0.00           H
ATOM    193 HG12 ILE N   7       3.292   7.974   8.320  1.00  0.00           H
ATOM    194  CD1 ILE N   7       4.876   8.325   9.766  1.00  0.00           C
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ATOM    195  HA  THR N  30      -0.740  18.152   0.510  1.00  0.00           H
ATOM    196  N   THR N  30      -1.967  17.834  -1.133  1.00  0.00           N
ATOM    197  CB  THR N  30      -1.768  16.253   0.782  1.00  0.00           C
ATOM    198  HA  ILE N  34      -4.852   7.380  -5.299  1.00  0.00           H
ATOM    199  C   ILE N  34      -3.966   6.923  -7.215  1.00  0.00           C
ATOM    200  CB  ILE N  34      -5.974   8.340  -6.910  1.00  0.00           C
ATOM    201 HD11 ILE N  33       1.966   8.080  -5.690  1.00  0.00           H
ATOM    202 HD12 ILE N  33       0.757   7.356  -6.790  1.00  0.00           H
ATOM    203 HD13 ILE N  33       1.255   6.510  -5.302  1.00  0.00           H
ATOM    204  HA1 GLY N  37      -3.258  -0.967  -7.806  1.00  0.00           H
ATOM    205  HA2 GLY N  37      -4.950  -1.540  -7.851  1.00  0.00           H
ATOM    206  N   GLY N  37      -4.657   0.445  -8.410  1.00  0.00           N
ATOM    207  HA  ASP N  43       8.591   6.521  -0.997  1.00  0.00           H
ATOM    208  CB  ASP N  43       8.797   6.931  -3.078  1.00  0.00           C
ATOM    209  C   ASP N  43       6.660   6.985  -1.651  1.00  0.00           C
ATOM    210  HA  VAL N   8       0.988  14.045   8.366  1.00  0.00           H
ATOM    211  C   VAL N   8       1.161  14.658   6.399  1.00  0.00           C
ATOM    212  CB  VAL N   8       2.688  15.352   8.395  1.00  0.00           C
ATOM    213 HD11 ILE N   7       5.485   7.432   9.593  1.00  0.00           H
ATOM    214 HD12 ILE N   7       5.554   9.137  10.060  1.00  0.00           H
ATOM    215 HD13 ILE N   7       4.233   8.115  10.631  1.00  0.00           H
ATOM    216  H   THR N  30      -2.764  17.265  -1.418  1.00  0.00           H
ATOM    217  C   TYR N  29      -1.931  19.143  -1.521  1.00  0.00           C
ATOM    218  HB  THR N  30      -1.025  15.920   1.515  1.00  0.00           H
ATOM    219  OG1 THR N  30      -2.093  15.082   0.014  1.00  0.00           O
ATOM    220  CG2 THR N  30      -2.962  16.813   1.537  1.00  0.00           C
ATOM    221  O   ILE N  34      -3.439   7.348  -8.272  1.00  0.00           O
ATOM    222  N   ILE N  35      -4.076   5.628  -6.918  1.00  0.00           N
ATOM    223  HB  ILE N  34      -5.696   8.781  -7.880  1.00  0.00           H
ATOM    224  CG1 ILE N  34      -6.712   9.425  -6.109  1.00  0.00           C
ATOM    225  CG2 ILE N  34      -6.902   7.140  -7.162  1.00  0.00           C
ATOM    226  H   GLY N  37      -3.894   1.057  -8.712  1.00  0.00           H
ATOM    227  C   PRO N  36      -5.947   0.722  -8.706  1.00  0.00           C
ATOM    228  HB1 ASP N  43       8.832   8.024  -2.981  1.00  0.00           H
ATOM    229  HB2 ASP N  43       9.845   6.600  -3.012  1.00  0.00           H
ATOM    230  CG  ASP N  43       8.287   6.619  -4.491  1.00  0.00           C
ATOM    231  O   ASP N  43       6.610   8.212  -1.434  1.00  0.00           O
ATOM    232  N   TYR N  44       5.578   6.195  -1.608  1.00  0.00           N
ATOM    233  O   VAL N   8       0.096  15.290   6.456  1.00  0.00           O
ATOM    234  N   ALA N   9       1.682  14.253   5.226  1.00  0.00           N
ATOM    235  HB  VAL N   8       3.710  15.279   7.985  1.00  0.00           H
ATOM    236  CG1 VAL N   8       2.192  16.774   8.116  1.00  0.00           C
ATOM    237  CG2 VAL N   8       2.724  15.040   9.898  1.00  0.00           C
ATOM    238  O   TYR N  29      -1.020  19.905  -1.220  1.00  0.00           O
ATOM    239  CA  TYR N  29      -3.167  19.609  -2.319  1.00  0.00           C
ATOM    240  HG1 THR N  30      -2.898  15.278  -0.517  1.00  0.00           H
ATOM    241 HG21 THR N  30      -3.291  16.082   2.277  1.00  0.00           H
ATOM    242 HG22 THR N  30      -3.803  17.053   0.872  1.00  0.00           H
ATOM    243 HG23 THR N  30      -2.662  17.721   2.080  1.00  0.00           H
ATOM    244  H   ILE N  35      -4.547   5.369  -6.045  1.00  0.00           H
ATOM    245  CA  ILE N  35      -3.750   4.570  -7.857  1.00  0.00           C
ATOM    246 HG11 ILE N  34      -5.988  10.089  -5.613  1.00  0.00           H
ATOM    247 HG12 ILE N  34      -7.308   8.952  -5.311  1.00  0.00           H
ATOM    248  CD1 ILE N  34      -7.613  10.260  -7.012  1.00  0.00           C
ATOM    249 HG21 ILE N  34      -7.865   7.480  -7.568  1.00  0.00           H
ATOM    250 HG22 ILE N  34      -7.114   6.606  -6.225  1.00  0.00           H
ATOM    251 HG23 ILE N  34      -6.483   6.402  -7.864  1.00  0.00           H
ATOM    252  O   PRO N  36      -6.884  -0.044  -8.480  1.00  0.00           O
ATOM    253  CA  PRO N  36      -6.239   2.078  -9.379  1.00  0.00           C
ATOM    254  OD2 ASP N  43       7.283   5.863  -4.631  1.00  0.00           O
ATOM    255  OD1 ASP N  43       8.940   7.166  -5.429  1.00  0.00           O
ATOM    256  H   TYR N  44       5.689   5.188  -1.744  1.00  0.00           H
ATOM    257  CA  TYR N  44       4.260   6.646  -1.176  1.00  0.00           C
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ATOM    258  H   ALA N   9       2.572  13.755   5.179  1.00  0.00           H
ATOM    259  CA  ALA N   9       0.878  14.396   4.014  1.00  0.00           C
ATOM    260 HG11 VAL N   8       2.813  17.499   8.658  1.00  0.00           H
ATOM    261 HG12 VAL N   8       2.252  17.028   7.048  1.00  0.00           H
ATOM    262 HG13 VAL N   8       1.146  16.926   8.424  1.00  0.00           H
ATOM    263 HG21 VAL N   8       3.291  15.802  10.443  1.00  0.00           H
ATOM    264 HG22 VAL N   8       3.189  14.063  10.102  1.00  0.00           H
ATOM    265 HG23 VAL N   8       1.707  15.020  10.318  1.00  0.00           H
ATOM    266  HA  TYR N  29      -2.913  20.618  -2.673  1.00  0.00           H
ATOM    267  N   TYR N  29      -3.413  18.734  -3.464  1.00  0.00           N
ATOM    268  CB  TYR N  29      -4.430  19.663  -1.425  1.00  0.00           C
ATOM    269  HA  ILE N  35      -3.516   5.062  -8.807  1.00  0.00           H
ATOM    270  C   ILE N  35      -4.994   3.686  -8.026  1.00  0.00           C
ATOM    271  CB  ILE N  35      -2.496   3.752  -7.430  1.00  0.00           C
ATOM    272 HD11 ILE N  34      -8.249  10.922  -6.422  1.00  0.00           H
ATOM    273 HD12 ILE N  34      -7.011  10.871  -7.702  1.00  0.00           H
ATOM    274 HD13 ILE N  34      -8.295   9.642  -7.615  1.00  0.00           H
ATOM    275  HA  PRO N  36      -7.153   2.431  -8.885  1.00  0.00           H
ATOM    276  N   PRO N  36      -5.161   3.063  -9.213  1.00  0.00           N
ATOM    277  CB  PRO N  36      -6.412   1.980 -10.907  1.00  0.00           C
ATOM    278  HA  TYR N  44       4.409   7.602  -0.659  1.00  0.00           H
ATOM    279  C   TYR N  44       3.745   5.643  -0.138  1.00  0.00           C
ATOM    280  CB  TYR N  44       3.267   6.867  -2.324  1.00  0.00           C
ATOM    281  HA  ALA N   9       0.558  15.440   3.918  1.00  0.00           H
ATOM    282  CB  ALA N   9       1.660  14.018   2.758  1.00  0.00           C
ATOM    283  C   ALA N   9      -0.436  13.607   4.171  1.00  0.00           C
ATOM    284  H   TYR N  29      -4.321  18.268  -3.540  1.00  0.00           H
ATOM    285  C   THR N  28      -2.584  18.733  -4.528  1.00  0.00           C
ATOM    286  HB1 TYR N  29      -4.586  18.678  -0.963  1.00  0.00           H
ATOM    287  HB2 TYR N  29      -5.297  19.818  -2.084  1.00  0.00           H
ATOM    288  CG  TYR N  29      -4.393  20.739  -0.365  1.00  0.00           C
ATOM    289  O   ILE N  35      -5.793   3.512  -7.091  1.00  0.00           O
ATOM    290  HB  ILE N  35      -2.386   2.968  -8.193  1.00  0.00           H
ATOM    291  CG2 ILE N  35      -1.251   4.647  -7.492  1.00  0.00           C
ATOM    292  CG1 ILE N  35      -2.684   3.061  -6.063  1.00  0.00           C
ATOM    293  CD  PRO N  36      -4.493   3.406 -10.490  1.00  0.00           C
ATOM    294  HB1 PRO N  36      -6.745   0.977 -11.206  1.00  0.00           H
ATOM    295  HB2 PRO N  36      -7.180   2.702 -11.230  1.00  0.00           H
ATOM    296  CG  PRO N  36      -5.032   2.356 -11.468  1.00  0.00           C
ATOM    297  O   TYR N  44       2.682   5.015  -0.291  1.00  0.00           O
ATOM    298  N   ALA N  45       4.564   5.490   0.913  1.00  0.00           N
ATOM    299  HB1 TYR N  44       2.296   7.086  -1.864  1.00  0.00           H
ATOM    300  HB2 TYR N  44       3.150   5.930  -2.886  1.00  0.00           H
ATOM    301  CG  TYR N  44       3.669   8.014  -3.211  1.00  0.00           C
ATOM    302  HB1 ALA N   9       2.510  14.699   2.618  1.00  0.00           H
ATOM    303  HB2 ALA N   9       1.010  14.109   1.877  1.00  0.00           H
ATOM    304  HB3 ALA N   9       2.050  12.993   2.816  1.00  0.00           H
ATOM    305  O   ALA N   9      -1.509  14.115   3.816  1.00  0.00           O
ATOM    306  N   ARG N  10      -0.365  12.374   4.723  1.00  0.00           N
ATOM    307  O   THR N  28      -1.608  19.488  -4.627  1.00  0.00           O
ATOM    308  CA  THR N  28      -2.852  17.722  -5.657  1.00  0.00           C
ATOM    309  CD1 TYR N  29      -4.596  22.083  -0.704  1.00  0.00           C
ATOM    310  CD2 TYR N  29      -4.154  20.444   0.983  1.00  0.00           C
ATOM    311 HG21 ILE N  35      -0.341   4.079  -7.248  1.00  0.00           H
ATOM    312 HG22 ILE N  35      -1.106   5.070  -8.498  1.00  0.00           H
ATOM    313 HG23 ILE N  35      -1.313   5.488  -6.783  1.00  0.00           H
ATOM    314 HG11 ILE N  35      -3.658   2.552  -6.053  1.00  0.00           H
ATOM    315 HG12 ILE N  35      -2.722   3.825  -5.267  1.00  0.00           H
ATOM    316  CD1 ILE N  35      -1.604   2.028  -5.731  1.00  0.00           C
ATOM    317  HD1 PRO N  36      -3.407   3.333 -10.387  1.00  0.00           H
ATOM    318  HD2 PRO N  36      -4.771   4.432 -10.782  1.00  0.00           H
ATOM    319  HG1 PRO N  36      -4.380   1.473 -11.479  1.00  0.00           H
ATOM    320  HG2 PRO N  36      -5.080   2.750 -12.493  1.00  0.00           H
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ATOM    321  H   ALA N  45       5.333   6.170   1.057  1.00  0.00           H
ATOM    322  CA  ALA N  45       4.414   4.427   1.884  1.00  0.00           C
ATOM    323  CD2 TYR N  44       3.017   9.244  -3.099  1.00  0.00           C
ATOM    324  CD1 TYR N  44       4.750   7.918  -4.100  1.00  0.00           C
ATOM    325  H   ARG N  10       0.548  11.991   4.971  1.00  0.00           H
ATOM    326  CA  ARG N  10      -1.562  11.627   5.095  1.00  0.00           C
ATOM    327  HA  THR N  28      -1.844  17.409  -5.959  1.00  0.00           H
ATOM    328  N   THR N  28      -3.579  16.544  -5.188  1.00  0.00           N
ATOM    329  CB  THR N  28      -3.511  18.393  -6.873  1.00  0.00           C
ATOM    330  HD1 TYR N  29      -4.776  22.357  -1.744  1.00  0.00           H
ATOM    331  CE1 TYR N  29      -4.564  23.092   0.253  1.00  0.00           C
ATOM    332  HD2 TYR N  29      -3.992  19.408   1.282  1.00  0.00           H
ATOM    333  CE2 TYR N  29      -4.115  21.442   1.956  1.00  0.00           C
ATOM    334 HD11 ILE N  35      -0.600   2.474  -5.658  1.00  0.00           H
ATOM    335 HD12 ILE N  35      -1.550   1.233  -6.491  1.00  0.00           H
ATOM    336 HD13 ILE N  35      -1.807   1.547  -4.760  1.00  0.00           H
ATOM    337  HA  ALA N  45       4.014   3.551   1.352  1.00  0.00           H
ATOM    338  C   ALA N  45       3.403   4.750   2.986  1.00  0.00           C
ATOM    339  CB  ALA N  45       5.786   4.103   2.495  1.00  0.00           C
ATOM    340  HD2 TYR N  44       2.167   9.341  -2.419  1.00  0.00           H
ATOM    341  CE2 TYR N  44       3.410  10.353  -3.848  1.00  0.00           C
ATOM    342  HD1 TYR N  44       5.304   6.988  -4.213  1.00  0.00           H
ATOM    343  CE1 TYR N  44       5.169   9.019  -4.836  1.00  0.00           C
ATOM    344  HA  ARG N  10      -2.195  11.530   4.206  1.00  0.00           H
ATOM    345  C   ARG N  10      -2.434  12.384   6.105  1.00  0.00           C
ATOM    346  CB  ARG N  10      -1.189  10.228   5.619  1.00  0.00           C
ATOM    347  H   THR N  28      -4.569  16.433  -5.421  1.00  0.00           H
ATOM    348  C   ALA N  27      -2.962  15.703  -4.337  1.00  0.00           C
ATOM    349  HB  THR N  28      -2.907  19.300  -7.062  1.00  0.00           H
ATOM    350  OG1 THR N  28      -4.834  18.757  -6.496  1.00  0.00           O
ATOM    351  CG2 THR N  28      -3.480  17.526  -8.128  1.00  0.00           C
ATOM    352  HE1 TYR N  29      -4.710  24.130  -0.038  1.00  0.00           H
ATOM    353  CZ  TYR N  29      -4.315  22.782   1.599  1.00  0.00           C
ATOM    354  HE2 TYR N  29      -3.919  21.200   3.002  1.00  0.00           H
ATOM    355  O   ALA N  45       3.039   3.850   3.778  1.00  0.00           O
ATOM    356  N   ASN N  46       2.986   6.007   3.080  1.00  0.00           N
ATOM    357  HB1 ALA N  45       5.720   3.248   3.177  1.00  0.00           H
ATOM    358  HB2 ALA N  45       6.506   3.875   1.698  1.00  0.00           H
ATOM    359  HB3 ALA N  45       6.171   4.968   3.055  1.00  0.00           H
ATOM    360  HE2 TYR N  44       2.874  11.292  -3.742  1.00  0.00           H
ATOM    361  CZ  TYR N  44       4.487  10.238  -4.731  1.00  0.00           C
ATOM    362  HE1 TYR N  44       6.036   8.939  -5.490  1.00  0.00           H
ATOM    363  O   ARG N  10      -3.672  12.383   5.963  1.00  0.00           O
ATOM    364  N   SER N  11      -1.823  13.017   7.117  1.00  0.00           N
ATOM    365  HB1 ARG N  10      -0.521  10.348   6.481  1.00  0.00           H
ATOM    366  HB2 ARG N  10      -0.606   9.714   4.844  1.00  0.00           H
ATOM    367  CG  ARG N  10      -2.387   9.376   6.054  1.00  0.00           C
ATOM    368  O   ALA N  27      -1.766  15.853  -4.029  1.00  0.00           O
ATOM    369  CA  ALA N  27      -3.752  14.511  -3.766  1.00  0.00           C
ATOM    370  HG1 THR N  28      -5.131  19.467  -7.115  1.00  0.00           H
ATOM    371 HG21 THR N  28      -2.451  17.342  -8.466  1.00  0.00           H
ATOM    372 HG22 THR N  28      -3.986  18.058  -8.945  1.00  0.00           H
ATOM    373 HG23 THR N  28      -4.002  16.573  -7.973  1.00  0.00           H
ATOM    374  OH  TYR N  29      -4.238  23.733   2.564  1.00  0.00           O
ATOM    375  H   ASN N  46       3.224   6.689   2.355  1.00  0.00           H
ATOM    376  CA  ASN N  46       2.187   6.486   4.188  1.00  0.00           C
ATOM    377  OH  TYR N  44       4.912  11.262  -5.521  1.00  0.00           O
ATOM    378  H   SER N  11      -0.833  12.818   7.299  1.00  0.00           H
ATOM    379  CA  SER N  11      -2.612  13.751   8.094  1.00  0.00           C
ATOM    380  HG1 ARG N  10      -2.963   9.916   6.817  1.00  0.00           H
ATOM    381  HG2 ARG N  10      -2.004   8.479   6.565  1.00  0.00           H
ATOM    382  CD  ARG N  10      -3.355   8.952   4.953  1.00  0.00           C
ATOM    383  HA  ALA N  27      -3.106  14.130  -2.966  1.00  0.00           H
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ATOM    384  N   ALA N  27      -5.037  14.924  -3.208  1.00  0.00           N
ATOM    385  CB  ALA N  27      -3.980  13.432  -4.829  1.00  0.00           C
ATOM    386  HH  TYR N  29      -4.426  24.633   2.172  1.00  0.00           H
ATOM    387  HA  ASN N  46       2.167   5.687   4.936  1.00  0.00           H
ATOM    388  CB  ASN N  46       2.873   7.713   4.815  1.00  0.00           C
ATOM    389  C   ASN N  46       0.717   6.734   3.795  1.00  0.00           C
ATOM    390  HH  TYR N  44       4.419  12.101  -5.333  1.00  0.00           H
ATOM    391  HA  SER N  11      -3.360  13.077   8.522  1.00  0.00           H
ATOM    392  CB  SER N  11      -1.759  14.339   9.221  1.00  0.00           C
ATOM    393  C   SER N  11      -3.389  14.885   7.404  1.00  0.00           C
ATOM    394  HD1 ARG N  10      -4.258   8.530   5.407  1.00  0.00           H
ATOM    395  HD2 ARG N  10      -3.682   9.813   4.348  1.00  0.00           H
ATOM    396  NE  ARG N  10      -2.743   7.950   4.075  1.00  0.00           N
ATOM    397  H   ALA N  27      -5.883  14.557  -3.654  1.00  0.00           H
ATOM    398  C   CYS N  26      -5.176  15.649  -2.100  1.00  0.00           C
ATOM    399  HB1 ALA N  27      -4.764  13.743  -5.522  1.00  0.00           H
ATOM    400  HB2 ALA N  27      -3.055  13.255  -5.386  1.00  0.00           H
ATOM    401  HB3 ALA N  27      -4.288  12.490  -4.353  1.00  0.00           H
ATOM    402  HB1 ASN N  46       2.783   8.578   4.151  1.00  0.00           H
ATOM    403  HB2 ASN N  46       2.382   7.957   5.766  1.00  0.00           H
ATOM    404  CG  ASN N  46       4.361   7.444   5.021  1.00  0.00           C
ATOM    405  OXT ASN N  46       0.008   7.360   4.630  1.00  0.00           O
ATOM    406  O   ASN N  46       0.302   6.296   2.681  1.00  0.00           O
ATOM    407  HB1 SER N  11      -2.449  14.869   9.900  1.00  0.00           H
ATOM    408  HB2 SER N  11      -1.056  15.080   8.803  1.00  0.00           H
ATOM    409  OG  SER N  11      -1.075  13.305   9.904  1.00  0.00           O
ATOM    410  O   SER N  11      -4.611  15.066   7.616  1.00  0.00           O
ATOM    411  N   ASN N  12      -2.673  15.657   6.591  1.00  0.00           N
ATOM    412  HE  ARG N  10      -1.767   7.674   4.267  1.00  0.00           H
ATOM    413  CZ  ARG N  10      -3.288   7.481   2.948  1.00  0.00           C
ATOM    414  O   CYS N  26      -4.225  15.989  -1.367  1.00  0.00           O
ATOM    415  CA  CYS N  26      -6.587  16.137  -1.733  1.00  0.00           C
ATOM    416  OD1 ASN N  46       5.216   8.052   4.363  1.00  0.00           O
ATOM    417  ND2 ASN N  46       4.688   6.490   5.914  1.00  0.00           N
ATOM    418  H   SER N  11      -0.639  13.719  10.691  1.00  0.00           H
ATOM    419  H   ASN N  12      -1.664  15.476   6.492  1.00  0.00           H
ATOM    420  CA  ASN N  12      -3.253  16.786   5.880  1.00  0.00           C
ATOM    421  NH2 ARG N  10      -4.572   7.728   2.654  1.00  0.00           N
ATOM    422  NH1 ARG N  10      -2.507   6.805   2.086  1.00  0.00           N
ATOM    423  HA  CYS N  26      -6.403  17.141  -1.322  1.00  0.00           H
ATOM    424  N   CYS N  26      -7.439  16.256  -2.893  1.00  0.00           N
ATOM    425  CB  CYS N  26      -7.238  15.288  -0.644  1.00  0.00           C
ATOM    426 HD21 ASN N  46       5.677   6.316   6.066  1.00  0.00           H
ATOM    427 HD22 ASN N  46       4.001   5.962   6.465  1.00  0.00           H
ATOM    428  HA  ASN N  12      -3.753  17.446   6.600  1.00  0.00           H
ATOM    429  CB  ASN N  12      -2.149  17.570   5.162  1.00  0.00           C
ATOM    430  C   ASN N  12      -4.352  16.296   4.922  1.00  0.00           C
ATOM    431 HH21 ARG N  10      -4.948   7.439   1.754  1.00  0.00           H
ATOM    432 HH22 ARG N  10      -5.263   7.849   3.419  1.00  0.00           H
ATOM    433 HH11 ARG N  10      -2.951   6.109   1.488  1.00  0.00           H
ATOM    434 HH12 ARG N  10      -1.551   6.564   2.380  1.00  0.00           H
ATOM    435  H   CYS N  26      -8.265  15.654  -2.988  1.00  0.00           H
ATOM    436  C   LEU N  25      -7.166  17.207  -3.808  1.00  0.00           C
ATOM    437  HB1 CYS N  26      -6.549  15.157   0.199  1.00  0.00           H
ATOM    438  HB2 CYS N  26      -7.507  14.288  -1.017  1.00  0.00           H
ATOM    439  SG  CYS N  26      -8.824  15.999  -0.041  1.00  0.00           S
ATOM    440  HB1 ASN N  12      -1.598  16.930   4.457  1.00  0.00           H
ATOM    441  HB2 ASN N  12      -2.618  18.370   4.566  1.00  0.00           H
ATOM    442  CG  ASN N  12      -1.173  18.222   6.164  1.00  0.00           C
ATOM    443  O   ASN N  12      -5.412  16.928   4.786  1.00  0.00           O
ATOM    444  N   PHE N  13      -4.086  15.147   4.276  1.00  0.00           N
ATOM    445  O   LEU N  25      -6.247  18.023  -3.664  1.00  0.00           O
ATOM    446  CA  LEU N  25      -8.055  17.241  -5.051  1.00  0.00           C
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ATOM    447  SG  CYS N  16      -8.233  17.870   0.666  1.00  0.00           S
ATOM    448  OD1 ASN N  12      -1.437  18.284   7.364  1.00  0.00           O
ATOM    449  ND2 ASN N  12      -0.054  18.735   5.611  1.00  0.00           N
ATOM    450  H   PHE N  13      -3.154  14.725   4.356  1.00  0.00           H
ATOM    451  CA  PHE N  13      -5.030  14.496   3.384  1.00  0.00           C
ATOM    452  HA  LEU N  25      -7.437  17.732  -5.812  1.00  0.00           H
ATOM    453  N   LEU N  25      -8.385  15.894  -5.520  1.00  0.00           N
ATOM    454  CB  LEU N  25      -9.341  18.037  -4.769  1.00  0.00           C
ATOM    455  CB  CYS N  16      -7.726  17.511   2.388  1.00  0.00           C
ATOM    456 HD21 ASN N  12       0.160  18.589   4.627  1.00  0.00           H
ATOM    457 HD22 ASN N  12       0.654  19.136   6.226  1.00  0.00           H
ATOM    458  HA  PHE N  13      -5.355  15.198   2.601  1.00  0.00           H
ATOM    459  C   PHE N  13      -6.316  14.106   4.114  1.00  0.00           C
ATOM    460  CB  PHE N  13      -4.330  13.279   2.745  1.00  0.00           C
ATOM    461  H   LEU N  25      -9.241  15.472  -5.156  1.00  0.00           H
ATOM    462  C   ALA N  24      -7.446  15.056  -6.000  1.00  0.00           C
ATOM    463  HB1 LEU N  25     -10.014  17.388  -4.187  1.00  0.00           H
ATOM    464  HB2 LEU N  25      -9.088  18.885  -4.110  1.00  0.00           H
ATOM    465  CG  LEU N  25     -10.059  18.554  -6.026  1.00  0.00           C
ATOM    466  HB1 CYS N  16      -7.274  16.511   2.420  1.00  0.00           H
ATOM    467  HB2 CYS N  16      -6.941  18.243   2.629  1.00  0.00           H
ATOM    468  CA  CYS N  16      -8.845  17.605   3.438  1.00  0.00           C
ATOM    469  O   PHE N  13      -7.419  14.385   3.621  1.00  0.00           O
ATOM    470  N   ASN N  14      -6.184  13.446   5.279  1.00  0.00           N
ATOM    471  HB1 PHE N  13      -3.514  13.655   2.116  1.00  0.00           H
ATOM    472  HB2 PHE N  13      -3.866  12.704   3.555  1.00  0.00           H
ATOM    473  CG  PHE N  13      -5.235  12.379   1.949  1.00  0.00           C
ATOM    474  O   ALA N  24      -6.270  15.412  -6.188  1.00  0.00           O
ATOM    475  CA  ALA N  24      -7.901  13.634  -6.379  1.00  0.00           C
ATOM    476  HG  LEU N  25     -10.101  17.719  -6.739  1.00  0.00           H
ATOM    477  CD1 LEU N  25      -9.312  19.703  -6.699  1.00  0.00           C
ATOM    478  CD2 LEU N  25     -11.502  18.955  -5.700  1.00  0.00           C
ATOM    479  HA  CYS N  16      -9.220  18.636   3.494  1.00  0.00           H
ATOM    480  N   CYS N  16      -8.261  17.203   4.711  1.00  0.00           N
ATOM    481  C   CYS N  16     -10.093  16.760   3.097  1.00  0.00           C
ATOM    482  H   ASN N  14      -5.249  13.195   5.627  1.00  0.00           H
ATOM    483  CA  ASN N  14      -7.372  13.013   5.992  1.00  0.00           C
ATOM    484  CD1 PHE N  13      -5.420  12.578   0.575  1.00  0.00           C
ATOM    485  CD2 PHE N  13      -5.907  11.317   2.574  1.00  0.00           C
ATOM    486  HA  ALA N  24      -6.978  13.044  -6.436  1.00  0.00           H
ATOM    487  N   ALA N  24      -8.771  13.075  -5.350  1.00  0.00           N
ATOM    488  CB  ALA N  24      -8.587  13.631  -7.744  1.00  0.00           C
ATOM    489 HD11 LEU N  25      -8.277  19.443  -6.962  1.00  0.00           H
ATOM    490 HD12 LEU N  25      -9.811  20.004  -7.631  1.00  0.00           H
ATOM    491 HD13 LEU N  25      -9.280  20.590  -6.047  1.00  0.00           H
ATOM    492 HD21 LEU N  25     -12.094  18.091  -5.371  1.00  0.00           H
ATOM    493 HD22 LEU N  25     -12.009  19.381  -6.580  1.00  0.00           H
ATOM    494 HD23 LEU N  25     -11.538  19.709  -4.894  1.00  0.00           H
ATOM    495  H   CYS N  16      -7.265  16.954   4.735  1.00  0.00           H
ATOM    496  C   VAL N  15      -9.003  17.113   5.829  1.00  0.00           C
ATOM    497  O   CYS N  16     -11.099  17.276   2.580  1.00  0.00           O
ATOM    498  N   ARG N  17     -10.034  15.461   3.420  1.00  0.00           N
ATOM    499  HA  ASN N  14      -8.023  12.466   5.297  1.00  0.00           H
ATOM    500  CB  ASN N  14      -7.042  12.096   7.172  1.00  0.00           C
ATOM    501  C   ASN N  14      -8.219  14.208   6.453  1.00  0.00           C
ATOM    502  HD1 PHE N  13      -4.884  13.392   0.082  1.00  0.00           H
ATOM    503  CE1 PHE N  13      -6.271  11.749  -0.160  1.00  0.00           C
ATOM    504  HD2 PHE N  13      -5.777  11.144   3.643  1.00  0.00           H
ATOM    505  CE2 PHE N  13      -6.746  10.480   1.843  1.00  0.00           C
ATOM    506  H   ALA N  24      -9.610  12.551  -5.640  1.00  0.00           H
ATOM    507  C   GLU N  23      -8.290  12.896  -4.100  1.00  0.00           C
ATOM    508  HB1 ALA N  24      -7.907  14.046  -8.496  1.00  0.00           H
ATOM    509  HB2 ALA N  24      -9.503  14.232  -7.735  1.00  0.00           H
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ATOM    510  HB3 ALA N  24      -8.856  12.609  -8.040  1.00  0.00           H
ATOM    511  O   VAL N  15     -10.198  17.443   5.864  1.00  0.00           O
ATOM    512  CA  VAL N  15      -8.308  16.569   7.081  1.00  0.00           C
ATOM    513  H   ARG N  17      -9.140  15.071   3.737  1.00  0.00           H
ATOM    514  CA  ARG N  17     -11.127  14.541   3.168  1.00  0.00           C
ATOM    515  HB1 ASN N  14      -6.360  12.573   7.888  1.00  0.00           H
ATOM    516  HB2 ASN N  14      -7.986  11.903   7.707  1.00  0.00           H
ATOM    517  CG  ASN N  14      -6.535  10.725   6.750  1.00  0.00           C
ATOM    518  O   ASN N  14      -9.458  14.111   6.491  1.00  0.00           O
ATOM    519  N   VAL N  15      -7.576  15.336   6.798  1.00  0.00           N
ATOM    520  HE1 PHE N  13      -6.402  11.920  -1.232  1.00  0.00           H
ATOM    521  CZ  PHE N  13      -6.937  10.699   0.478  1.00  0.00           C
ATOM    522  HE2 PHE N  13      -7.259   9.655   2.340  1.00  0.00           H
ATOM    523  O   GLU N  23      -7.140  13.222  -3.773  1.00  0.00           O
ATOM    524  CA  GLU N  23      -9.216  12.270  -3.056  1.00  0.00           C
ATOM    525  HA  VAL N  15      -9.137  16.331   7.759  1.00  0.00           H
ATOM    526  CB  VAL N  15      -7.387  17.607   7.759  1.00  0.00           C
ATOM    527  HA  ARG N  17     -11.563  14.762   2.180  1.00  0.00           H
ATOM    528  C   ARG N  17     -12.301  14.698   4.131  1.00  0.00           C
ATOM    529  CB  ARG N  17     -10.605  13.094   3.213  1.00  0.00           C
ATOM    530  OD1 ASN N  14      -6.986  10.175   5.719  1.00  0.00           O
ATOM    531  ND2 ASN N  14      -5.666  10.124   7.561  1.00  0.00           N
ATOM    532  H   VAL N  15      -6.554  15.358   6.770  1.00  0.00           H
ATOM    533  HZ  PHE N  13      -7.591  10.033  -0.078  1.00  0.00           H
ATOM    534  HA  GLU N  23      -8.816  12.634  -2.097  1.00  0.00           H
ATOM    535  N   GLU N  23     -10.584  12.717  -3.208  1.00  0.00           N
ATOM    536  CB  GLU N  23      -9.095  10.740  -3.100  1.00  0.00           C
ATOM    537  HB  VAL N  15      -6.429  17.606   7.211  1.00  0.00           H
ATOM    538  CG2 VAL N  15      -7.142  17.167   9.200  1.00  0.00           C
ATOM    539  CG1 VAL N  15      -7.968  19.021   7.683  1.00  0.00           C
ATOM    540  O   ARG N  17     -13.397  14.177   3.818  1.00  0.00           O
ATOM    541  N   LEU N  18     -12.155  15.365   5.278  1.00  0.00           N
ATOM    542  HB1 ARG N  17     -10.043  12.965   4.144  1.00  0.00           H
ATOM    543  HB2 ARG N  17     -11.461  12.408   3.274  1.00  0.00           H
ATOM    544  CG  ARG N  17      -9.722  12.725   2.020  1.00  0.00           C
ATOM    545 HD21 ASN N  14      -5.413   9.154   7.366  1.00  0.00           H
ATOM    546 HD22 ASN N  14      -5.221  10.582   8.375  1.00  0.00           H
ATOM    547  H   GLU N  23     -11.317  12.009  -3.457  1.00  0.00           H
ATOM    548  C   PRO N  22     -10.874  14.021  -3.295  1.00  0.00           C
ATOM    549  HB1 GLU N  23      -9.497  10.370  -4.050  1.00  0.00           H
ATOM    550  HB2 GLU N  23      -8.020  10.514  -3.108  1.00  0.00           H
ATOM    551  CG  GLU N  23      -9.780  10.027  -1.924  1.00  0.00           C
ATOM    552 HG21 VAL N  15      -6.499  17.866   9.744  1.00  0.00           H
ATOM    553 HG22 VAL N  15      -6.655  16.187   9.243  1.00  0.00           H
ATOM    554 HG23 VAL N  15      -8.099  17.091   9.741  1.00  0.00           H
ATOM    555 HG11 VAL N  15      -7.311  19.722   8.210  1.00  0.00           H
ATOM    556 HG12 VAL N  15      -8.056  19.367   6.643  1.00  0.00           H
ATOM    557 HG13 VAL N  15      -8.967  19.081   8.140  1.00  0.00           H
ATOM    558  H   LEU N  18     -11.278  15.846   5.495  1.00  0.00           H
ATOM    559  CA  LEU N  18     -13.256  15.461   6.230  1.00  0.00           C
ATOM    560  HG1 ARG N  17      -9.180  11.802   2.265  1.00  0.00           H
ATOM    561  HG2 ARG N  17      -8.949  13.488   1.856  1.00  0.00           H
ATOM    562  CD  ARG N  17     -10.497  12.542   0.720  1.00  0.00           C
ATOM    563  O   PRO N  22     -10.024  14.930  -3.199  1.00  0.00           O
ATOM    564  CA  PRO N  22     -12.314  14.322  -3.674  1.00  0.00           C
ATOM    565  HG1 GLU N  23      -9.553  10.537  -0.982  1.00  0.00           H
ATOM    566  HG2 GLU N  23     -10.870  10.060  -2.068  1.00  0.00           H
ATOM    567  CD  GLU N  23      -9.385   8.556  -1.794  1.00  0.00           C
ATOM    568  HA  LEU N  18     -13.598  14.441   6.455  1.00  0.00           H
ATOM    569  CB  LEU N  18     -12.826  16.158   7.521  1.00  0.00           C
ATOM    570  C   LEU N  18     -14.507  16.125   5.651  1.00  0.00           C
ATOM    571  HD1 ARG N  17     -11.104  13.428   0.502  1.00  0.00           H
ATOM    572  HD2 ARG N  17      -9.786  12.445  -0.119  1.00  0.00           H
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ATOM    573  NE  ARG N  17     -11.353  11.357   0.791  1.00  0.00           N
ATOM    574  HA  PRO N  22     -12.948  13.447  -3.475  1.00  0.00           H
ATOM    575  N   PRO N  22     -12.848  15.490  -2.966  1.00  0.00           N
ATOM    576  CB  PRO N  22     -12.429  14.728  -5.149  1.00  0.00           C
ATOM    577  OE1 GLU N  23      -9.436   7.852  -2.839  1.00  0.00           O
ATOM    578  OE2 GLU N  23      -9.023   8.122  -0.649  1.00  0.00           O
ATOM    579  HB1 LEU N  18     -12.321  17.102   7.268  1.00  0.00           H
ATOM    580  HB2 LEU N  18     -13.738  16.427   8.074  1.00  0.00           H
ATOM    581  CG  LEU N  18     -11.911  15.339   8.445  1.00  0.00           C
ATOM    582  O   LEU N  18     -15.626  15.630   5.919  1.00  0.00           O
ATOM    583  N   PRO N  19     -14.411  17.209   4.864  1.00  0.00           N
ATOM    584  HE  ARG N  17     -10.941  10.544   1.270  1.00  0.00           H
ATOM    585  CZ  ARG N  17     -12.382  11.092  -0.033  1.00  0.00           C
ATOM    586  C   THR N  21     -12.707  15.586  -1.639  1.00  0.00           C
ATOM    587  CD  PRO N  22     -13.694  16.330  -3.836  1.00  0.00           C
ATOM    588  HB1 PRO N  22     -12.491  13.852  -5.804  1.00  0.00           H
ATOM    589  HB2 PRO N  22     -11.556  15.339  -5.425  1.00  0.00           H
ATOM    590  CG  PRO N  22     -13.705  15.568  -5.166  1.00  0.00           C
ATOM    591  HG  LEU N  18     -10.988  15.100   7.895  1.00  0.00           H
ATOM    592  CD2 LEU N  18     -11.548  16.249   9.620  1.00  0.00           C
ATOM    593  CD1 LEU N  18     -12.547  14.018   8.895  1.00  0.00           C
ATOM    594  CA  PRO N  19     -15.617  17.740   4.209  1.00  0.00           C
ATOM    595  CD  PRO N  19     -13.288  18.189   4.811  1.00  0.00           C
ATOM    596  NH1 ARG N  17     -12.936  12.036  -0.790  1.00  0.00           N
ATOM    597  NH2 ARG N  17     -12.869   9.844  -0.084  1.00  0.00           N
ATOM    598  O   THR N  21     -12.119  14.721  -0.967  1.00  0.00           O
ATOM    599  CA  THR N  21     -13.202  16.847  -0.921  1.00  0.00           C
ATOM    600  HD1 PRO N  22     -14.702  16.426  -3.413  1.00  0.00           H
ATOM    601  HD2 PRO N  22     -13.255  17.334  -3.928  1.00  0.00           H
ATOM    602  HG1 PRO N  22     -13.773  16.241  -6.025  1.00  0.00           H
ATOM    603  HG2 PRO N  22     -14.573  14.903  -5.183  1.00  0.00           H
ATOM    604 HD21 LEU N  18     -10.868  15.763  10.330  1.00  0.00           H
ATOM    605 HD22 LEU N  18     -11.053  17.165   9.261  1.00  0.00           H
ATOM    606 HD23 LEU N  18     -12.444  16.560  10.180  1.00  0.00           H
ATOM    607 HD11 LEU N  18     -13.522  14.184   9.374  1.00  0.00           H
ATOM    608 HD12 LEU N  18     -11.906  13.494   9.619  1.00  0.00           H
ATOM    609 HD13 LEU N  18     -12.692  13.326   8.051  1.00  0.00           H
ATOM    610  HA  PRO N  19     -16.512  17.533   4.810  1.00  0.00           H
ATOM    611  CB  PRO N  19     -15.335  19.233   4.104  1.00  0.00           C
ATOM    612  C   PRO N  19     -15.882  17.087   2.847  1.00  0.00           C
ATOM    613  HD1 PRO N  19     -12.370  17.734   4.436  1.00  0.00           H
ATOM    614  HD2 PRO N  19     -13.106  18.566   5.828  1.00  0.00           H
ATOM    615  CG  PRO N  19     -13.825  19.293   3.899  1.00  0.00           C
ATOM    616 HH11 ARG N  17     -12.590  13.001  -0.805  1.00  0.00           H
ATOM    617 HH12 ARG N  17     -13.616  11.772  -1.516  1.00  0.00           H
ATOM    618 HH21 ARG N  17     -12.364   9.045   0.309  1.00  0.00           H
ATOM    619 HH22 ARG N  17     -13.674   9.637  -0.685  1.00  0.00           H
ATOM    620  HA  THR N  21     -13.820  17.480  -1.573  1.00  0.00           H
ATOM    621  N   THR N  21     -13.981  16.445   0.230  1.00  0.00           N
ATOM    622  CB  THR N  21     -11.964  17.635  -0.441  1.00  0.00           C
ATOM    623  HB1 PRO N  19     -15.907  19.725   3.319  1.00  0.00           H
ATOM    624  HB2 PRO N  19     -15.600  19.707   5.050  1.00  0.00           H
ATOM    625  O   PRO N  19     -16.666  17.641   2.047  1.00  0.00           O
ATOM    626  N   GLY N  20     -15.279  15.920   2.583  1.00  0.00           N
ATOM    627  HG1 PRO N  19     -13.419  20.279   4.151  1.00  0.00           H
ATOM    628  HG2 PRO N  19     -13.572  19.080   2.853  1.00  0.00           H
ATOM    629  H   THR N  21     -13.714  16.817   1.135  1.00  0.00           H
ATOM    630  C   GLY N  20     -14.934  15.502   0.144  1.00  0.00           C
ATOM    631  HB  THR N  21     -11.302  16.907   0.046  1.00  0.00           H
ATOM    632  OG1 THR N  21     -12.369  18.584   0.549  1.00  0.00           O
ATOM    633  CG2 THR N  21     -11.232  18.291  -1.600  1.00  0.00           C
ATOM    634  H   GLY N  20     -14.628  15.500   3.251  1.00  0.00           H
ATOM    635  CA  GLY N  20     -15.621  15.103   1.434  1.00  0.00           C
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ATOM    636  O   GLY N  20     -15.233  14.957  -0.922  1.00  0.00           O
ATOM    637  HG1 THR N  21     -11.845  18.372   1.353  1.00  0.00           H
ATOM    638 HG21 THR N  21     -10.815  17.518  -2.258  1.00  0.00           H
ATOM    639 HG22 THR N  21     -10.402  18.902  -1.222  1.00  0.00           H
ATOM    640 HG23 THR N  21     -11.898  18.941  -2.186  1.00  0.00           H
ATOM    641  HA1 GLY N  20     -16.700  15.141   1.242  1.00  0.00           H
ATOM    642  HA2 GLY N  20     -15.327  14.067   1.647  1.00  0.00           H
END
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4) CRAMBIN – molecule as in the optimized 172W crystal

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COMPND    CRAMBIN OPTIMIZED CRYSTAL 172W GEOMETRY
AUTHOR    DELLE PIANE, CORNO, ORLANDO, DOVESI, UGLIENGO
ATOM      1  N   THR N   1      -6.981  -4.273  -2.053  1.00  0.00           N
ATOM      2  H1  THR N   1      -6.366  -5.104  -2.013  1.00  0.00           H
ATOM      3  H2  THR N   1      -7.626  -4.384  -2.862  1.00  0.00           H
ATOM      4  H3  THR N   1      -7.578  -4.181  -1.184  1.00  0.00           H
ATOM      5  CA  THR N   1      -6.209  -3.015  -2.242  1.00  0.00           C
ATOM      6  HA  THR N   1      -6.902  -2.179  -2.074  1.00  0.00           H
ATOM      7  C   THR N   1      -5.659  -3.012  -3.656  1.00  0.00           C
ATOM      8  CB  THR N   1      -5.097  -2.937  -1.169  1.00  0.00           C
ATOM      9  O   THR N   1      -5.157  -4.037  -4.136  1.00  0.00           O
ATOM     10  N   THR N   2      -5.741  -1.835  -4.296  1.00  0.00           N
ATOM     11  HB  THR N   1      -4.492  -3.855  -1.261  1.00  0.00           H
ATOM     12  OG1 THR N   1      -5.747  -2.931   0.090  1.00  0.00           O
ATOM     13  CG2 THR N   1      -4.187  -1.732  -1.308  1.00  0.00           C
ATOM     14  H   THR N   2      -6.101  -1.014  -3.798  1.00  0.00           H
ATOM     15  CA  THR N   2      -5.062  -1.600  -5.559  1.00  0.00           C
ATOM     16  HG1 THR N   1      -5.694  -3.860   0.443  1.00  0.00           H
ATOM     17 HG21 THR N   1      -4.742  -0.798  -1.179  1.00  0.00           H
ATOM     18 HG22 THR N   1      -3.696  -1.712  -2.287  1.00  0.00           H
ATOM     19 HG23 THR N   1      -3.410  -1.777  -0.535  1.00  0.00           H
ATOM     20  HA  THR N   2      -4.867  -2.578  -6.015  1.00  0.00           H
ATOM     21  C   THR N   2      -3.725  -0.926  -5.260  1.00  0.00           C
ATOM     22  CB  THR N   2      -5.940  -0.775  -6.535  1.00  0.00           C
ATOM     23  O   THR N   2      -3.636   0.012  -4.433  1.00  0.00           O
ATOM     24  N   CYS N   3      -2.679  -1.411  -5.929  1.00  0.00           N
ATOM     25  HB  THR N   2      -5.389  -0.716  -7.489  1.00  0.00           H
ATOM     26  OG1 THR N   2      -6.095   0.559  -6.075  1.00  0.00           O
ATOM     27  CG2 THR N   2      -7.272  -1.482  -6.757  1.00  0.00           C
ATOM     28  H   CYS N   3      -2.825  -2.235  -6.533  1.00  0.00           H
ATOM     29  CA  CYS N   3      -1.310  -0.994  -5.669  1.00  0.00           C
ATOM     30  HG1 THR N   2      -6.964   0.684  -5.607  1.00  0.00           H
ATOM     31 HG21 THR N   2      -7.960  -0.833  -7.308  1.00  0.00           H
ATOM     32 HG22 THR N   2      -7.750  -1.746  -5.806  1.00  0.00           H
ATOM     33 HG23 THR N   2      -7.130  -2.411  -7.328  1.00  0.00           H
ATOM     34  HA  CYS N   3      -1.338  -0.095  -5.040  1.00  0.00           H
ATOM     35  C   CYS N   3      -0.662  -0.709  -7.023  1.00  0.00           C
ATOM     36  CB  CYS N   3      -0.512  -2.104  -4.968  1.00  0.00           C
ATOM     37  O   CYS N   3      -0.690  -1.584  -7.904  1.00  0.00           O
ATOM     38  N   CYS N   4      -0.075   0.479  -7.208  1.00  0.00           N
ATOM     39  HB1 CYS N   3       0.510  -1.753  -4.785  1.00  0.00           H
ATOM     40  HB2 CYS N   3      -0.469  -2.995  -5.609  1.00  0.00           H
ATOM     41  SG  CYS N   3      -1.226  -2.706  -3.398  1.00  0.00           S
ATOM     42  H   CYS N   4      -0.046   1.199  -6.479  1.00  0.00           H
ATOM     43  CA  CYS N   4       0.416   0.827  -8.528  1.00  0.00           C
ATOM     44  SG  CYS N  40      -0.820  -1.125  -2.107  1.00  0.00           S
ATOM     45  HA  CYS N   4       0.126  -0.001  -9.178  1.00  0.00           H
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ATOM     46  C   CYS N   4       1.939   0.916  -8.521  1.00  0.00           C
ATOM     47  CB  CYS N   4      -0.255   2.101  -9.050  1.00  0.00           C
ATOM     48  CB  CYS N  40       0.921  -1.474  -1.645  1.00  0.00           C
ATOM     49  O   CYS N   4       2.563   1.414  -7.570  1.00  0.00           O
ATOM     50  N   PRO N   5       2.575   0.437  -9.605  1.00  0.00           N
ATOM     51  HB1 CYS N   4       0.222   2.474  -9.965  1.00  0.00           H
ATOM     52  HB2 CYS N   4      -0.205   2.912  -8.311  1.00  0.00           H
ATOM     53  SG  CYS N   4      -2.046   1.849  -9.375  1.00  0.00           S
ATOM     54  HB1 CYS N  40       1.549  -1.517  -2.545  1.00  0.00           H
ATOM     55  HB2 CYS N  40       1.246  -0.591  -1.073  1.00  0.00           H
ATOM     56  CA  CYS N  40       1.075  -2.741  -0.801  1.00  0.00           C
ATOM     57  CA  PRO N   5       4.046   0.443  -9.656  1.00  0.00           C
ATOM     58  CD  PRO N   5       1.975  -0.229 -10.790  1.00  0.00           C
ATOM     59  SG  CYS N  32      -2.058   0.916 -11.241  1.00  0.00           S
ATOM     60  HA  CYS N  40       0.639  -3.595  -1.332  1.00  0.00           H
ATOM     61  N   CYS N  40       0.402  -2.581   0.462  1.00  0.00           N
ATOM     62  C   CYS N  40       2.571  -2.985  -0.593  1.00  0.00           C
ATOM     63  HA  PRO N   5       4.471   0.091  -8.710  1.00  0.00           H
ATOM     64  C   PRO N   5       4.631   1.837  -9.876  1.00  0.00           C
ATOM     65  CB  PRO N   5       4.348  -0.520 -10.812  1.00  0.00           C
ATOM     66  HD1 PRO N   5       1.147   0.359 -11.204  1.00  0.00           H
ATOM     67  HD2 PRO N   5       1.596  -1.219 -10.504  1.00  0.00           H
ATOM     68  CG  PRO N   5       3.154  -0.357 -11.749  1.00  0.00           C
ATOM     69  CB  CYS N  32      -2.384  -0.863 -10.866  1.00  0.00           C
ATOM     70  H   CYS N  40       0.018  -1.659   0.693  1.00  0.00           H
ATOM     71  C   THR N  39       0.323  -3.584   1.354  1.00  0.00           C
ATOM     72  O   CYS N  40       3.194  -2.409   0.317  1.00  0.00           O
ATOM     73  N   PRO N  41       3.175  -3.780  -1.485  1.00  0.00           N
ATOM     74  O   PRO N   5       5.836   2.032  -9.650  1.00  0.00           O
ATOM     75  N   SER N   6       3.795   2.768 -10.365  1.00  0.00           N
ATOM     76  HB1 PRO N   5       5.317  -0.329 -11.282  1.00  0.00           H
ATOM     77  HB2 PRO N   5       4.368  -1.540 -10.414  1.00  0.00           H
ATOM     78  HG1 PRO N   5       3.036  -1.193 -12.446  1.00  0.00           H
ATOM     79  HG2 PRO N   5       3.239   0.552 -12.357  1.00  0.00           H
ATOM     80  HB1 CYS N  32      -2.654  -0.929  -9.806  1.00  0.00           H
ATOM     81  HB2 CYS N  32      -3.274  -1.131 -11.451  1.00  0.00           H
ATOM     82  CA  CYS N  32      -1.238  -1.843 -11.165  1.00  0.00           C
ATOM     83  O   THR N  39       0.778  -4.717   1.156  1.00  0.00           O
ATOM     84  CA  THR N  39      -0.437  -3.215   2.626  1.00  0.00           C
ATOM     85  CA  PRO N  41       4.624  -3.949  -1.455  1.00  0.00           C
ATOM     86  CD  PRO N  41       2.538  -4.512  -2.606  1.00  0.00           C
ATOM     87  H   SER N   6       2.810   2.554 -10.481  1.00  0.00           H
ATOM     88  CA  SER N   6       4.181   4.146 -10.560  1.00  0.00           C
ATOM     89  HA  CYS N  32      -0.391  -1.626 -10.505  1.00  0.00           H
ATOM     90  N   CYS N  32      -0.808  -1.774 -12.548  1.00  0.00           N
ATOM     91  C   CYS N  32      -1.711  -3.276 -10.827  1.00  0.00           C
ATOM     92  HA  THR N  39      -0.504  -2.123   2.722  1.00  0.00           H
ATOM     93  N   THR N  39      -1.795  -3.714   2.510  1.00  0.00           N
ATOM     94  CB  THR N  39       0.232  -3.793   3.894  1.00  0.00           C
ATOM     95  HA  PRO N  41       4.956  -4.207  -0.440  1.00  0.00           H
ATOM     96  CB  PRO N  41       4.847  -5.111  -2.443  1.00  0.00           C
ATOM     97  C   PRO N  41       5.313  -2.637  -1.883  1.00  0.00           C
ATOM     98  HD1 PRO N  41       1.833  -3.870  -3.151  1.00  0.00           H
ATOM     99  HD2 PRO N  41       1.987  -5.383  -2.219  1.00  0.00           H
ATOM    100  CG  PRO N  41       3.724  -4.949  -3.459  1.00  0.00           C
ATOM    101  HA  SER N   6       4.943   4.384  -9.810  1.00  0.00           H
ATOM    102  C   SER N   6       2.974   5.047 -10.328  1.00  0.00           C
ATOM    103  CB  SER N   6       4.783   4.402 -11.937  1.00  0.00           C
ATOM    104  H   CYS N  32      -1.475  -1.383 -13.218  1.00  0.00           H
ATOM    105  C   GLY N  31       0.220  -2.509 -13.020  1.00  0.00           C
ATOM    106  O   CYS N  32      -1.912  -4.107 -11.718  1.00  0.00           O
ATOM    107  N   ILE N  33      -1.907  -3.522  -9.524  1.00  0.00           N
ATOM    108  H   THR N  39      -1.893  -4.738   2.549  1.00  0.00           H
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ATOM    109  C   ALA N  38      -2.879  -2.923   2.442  1.00  0.00           C
ATOM    110  HB  THR N  39       0.420  -4.866   3.733  1.00  0.00           H
ATOM    111  OG1 THR N  39      -0.649  -3.628   5.001  1.00  0.00           O
ATOM    112  CG2 THR N  39       1.549  -3.110   4.215  1.00  0.00           C
ATOM    113  HB1 PRO N  41       5.838  -5.087  -2.887  1.00  0.00           H
ATOM    114  HB2 PRO N  41       4.746  -6.061  -1.896  1.00  0.00           H
ATOM    115  O   PRO N  41       4.727  -1.770  -2.543  1.00  0.00           O
ATOM    116  N   GLY N  42       6.616  -2.517  -1.519  1.00  0.00           N
ATOM    117  HG1 PRO N  41       3.521  -5.874  -4.007  1.00  0.00           H
ATOM    118  HG2 PRO N  41       3.993  -4.157  -4.172  1.00  0.00           H
ATOM    119  O   SER N   6       1.811   4.608 -10.369  1.00  0.00           O
ATOM    120  N   ILE N   7       3.282   6.333 -10.111  1.00  0.00           N
ATOM    121  HB1 SER N   6       5.301   5.365 -11.917  1.00  0.00           H
ATOM    122  HB2 SER N   6       5.540   3.633 -12.128  1.00  0.00           H
ATOM    123  OG  SER N   6       3.776   4.396 -12.945  1.00  0.00           O
ATOM    124  O   GLY N  31       1.007  -3.124 -12.278  1.00  0.00           O
ATOM    125  CA  GLY N  31       0.424  -2.558 -14.535  1.00  0.00           C
ATOM    126  H   ILE N  33      -1.614  -2.824  -8.835  1.00  0.00           H
ATOM    127  CA  ILE N  33      -2.190  -4.860  -9.045  1.00  0.00           C
ATOM    128  O   ALA N  38      -2.827  -1.694   2.236  1.00  0.00           O
ATOM    129  CA  ALA N  38      -4.224  -3.601   2.746  1.00  0.00           C
ATOM    130  HG1 THR N  39      -1.361  -4.311   4.940  1.00  0.00           H
ATOM    131 HG21 THR N  39       2.264  -3.233   3.390  1.00  0.00           H
ATOM    132 HG22 THR N  39       1.986  -3.551   5.124  1.00  0.00           H
ATOM    133 HG23 THR N  39       1.403  -2.028   4.366  1.00  0.00           H
ATOM    134  H   GLY N  42       7.086  -3.306  -1.085  1.00  0.00           H
ATOM    135  CA  GLY N  42       7.403  -1.326  -1.795  1.00  0.00           C
ATOM    136  H   ILE N   7       4.275   6.607 -10.065  1.00  0.00           H
ATOM    137  CA  ILE N   7       2.262   7.357  -9.959  1.00  0.00           C
ATOM    138  H   SER N   6       4.194   4.838 -13.710  1.00  0.00           H
ATOM    139  HA1 GLY N  31       0.524  -3.613 -14.820  1.00  0.00           H
ATOM    140  HA2 GLY N  31       1.375  -2.056 -14.768  1.00  0.00           H
ATOM    141  N   GLY N  31      -0.650  -1.971 -15.301  1.00  0.00           N
ATOM    142  HA  ILE N  33      -2.575  -5.434  -9.896  1.00  0.00           H
ATOM    143  C   ILE N  33      -3.277  -4.788  -7.981  1.00  0.00           C
ATOM    144  CB  ILE N  33      -0.907  -5.586  -8.545  1.00  0.00           C
ATOM    145  HA  ALA N  38      -4.925  -3.273   1.985  1.00  0.00           H
ATOM    146  N   ALA N  38      -4.144  -5.058   2.692  1.00  0.00           N
ATOM    147  CB  ALA N  38      -4.718  -3.089   4.109  1.00  0.00           C
ATOM    148  HA1 GLY N  42       8.334  -1.369  -1.222  1.00  0.00           H
ATOM    149  HA2 GLY N  42       6.865  -0.434  -1.442  1.00  0.00           H
ATOM    150  C   GLY N  42       7.757  -1.056  -3.253  1.00  0.00           C
ATOM    151  HA  ILE N   7       1.515   7.000  -9.235  1.00  0.00           H
ATOM    152  C   ILE N   7       1.427   7.554 -11.232  1.00  0.00           C
ATOM    153  CB  ILE N   7       2.897   8.654  -9.409  1.00  0.00           C
ATOM    154  H   GLY N  31      -1.448  -2.568 -15.512  1.00  0.00           H
ATOM    155  C   THR N  30      -0.734  -0.660 -15.569  1.00  0.00           C
ATOM    156  O   ILE N  33      -3.483  -3.756  -7.318  1.00  0.00           O
ATOM    157  N   ILE N  34      -3.963  -5.932  -7.800  1.00  0.00           N
ATOM    158  HB  ILE N  33      -1.210  -6.611  -8.296  1.00  0.00           H
ATOM    159  CG2 ILE N  33       0.099  -5.653  -9.696  1.00  0.00           C
ATOM    160  CG1 ILE N  33      -0.324  -4.968  -7.261  1.00  0.00           C
ATOM    161  H   ALA N  38      -3.641  -5.487   3.479  1.00  0.00           H
ATOM    162  C   GLY N  37      -4.583  -5.842   1.689  1.00  0.00           C
ATOM    163  HB1 ALA N  38      -5.708  -3.502   4.336  1.00  0.00           H
ATOM    164  HB2 ALA N  38      -4.026  -3.365   4.915  1.00  0.00           H
ATOM    165  HB3 ALA N  38      -4.801  -1.994   4.074  1.00  0.00           H
ATOM    166  O   GLY N  42       8.312   0.007  -3.562  1.00  0.00           O
ATOM    167  N   ASP N  43       7.372  -1.991  -4.145  1.00  0.00           N
ATOM    168  O   ILE N   7       0.196   7.663 -11.118  1.00  0.00           O
ATOM    169  N   VAL N   8       2.046   7.582 -12.425  1.00  0.00           N
ATOM    170  HB  ILE N   7       3.833   8.833  -9.969  1.00  0.00           H
ATOM    171  CG2 ILE N   7       1.990   9.858  -9.628  1.00  0.00           C
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ATOM    172  CG1 ILE N   7       3.238   8.442  -7.920  1.00  0.00           C
ATOM    173  O   THR N  30       0.137   0.170 -15.256  1.00  0.00           O
ATOM    174  CA  THR N  30      -2.048  -0.155 -16.154  1.00  0.00           C
ATOM    175  H   ILE N  34      -3.720  -6.734  -8.387  1.00  0.00           H
ATOM    176  CA  ILE N  34      -4.896  -6.102  -6.699  1.00  0.00           C
ATOM    177 HG21 ILE N  33       1.059  -6.031  -9.349  1.00  0.00           H
ATOM    178 HG22 ILE N  33       0.294  -4.668 -10.135  1.00  0.00           H
ATOM    179 HG23 ILE N  33      -0.259  -6.319 -10.494  1.00  0.00           H
ATOM    180 HG11 ILE N  33       0.036  -3.948  -7.467  1.00  0.00           H
ATOM    181 HG12 ILE N  33      -1.135  -4.867  -6.519  1.00  0.00           H
ATOM    182  CD1 ILE N  33       0.806  -5.788  -6.634  1.00  0.00           C
ATOM    183  O   GLY N  37      -5.192  -5.439   0.685  1.00  0.00           O
ATOM    184  CA  GLY N  37      -4.277  -7.340   1.876  1.00  0.00           C
ATOM    185  H   ASP N  43       7.115  -2.921  -3.822  1.00  0.00           H
ATOM    186  CA  ASP N  43       7.540  -1.865  -5.575  1.00  0.00           C
ATOM    187  H   VAL N   8       3.075   7.571 -12.474  1.00  0.00           H
ATOM    188  CA  VAL N   8       1.231   7.642 -13.635  1.00  0.00           C
ATOM    189 HG21 ILE N   7       2.486  10.761  -9.261  1.00  0.00           H
ATOM    190 HG22 ILE N   7       1.774  10.026 -10.692  1.00  0.00           H
ATOM    191 HG23 ILE N   7       1.030   9.743  -9.102  1.00  0.00           H
ATOM    192 HG11 ILE N   7       3.912   7.578  -7.833  1.00  0.00           H
ATOM    193 HG12 ILE N   7       2.305   8.163  -7.398  1.00  0.00           H
ATOM    194  CD1 ILE N   7       3.882   9.623  -7.203  1.00  0.00           C
ATOM    195  HA  THR N  30      -1.784   0.506 -16.991  1.00  0.00           H
ATOM    196  N   THR N  30      -2.922  -1.203 -16.648  1.00  0.00           N
ATOM    197  CB  THR N  30      -2.743   0.671 -15.042  1.00  0.00           C
ATOM    198  HA  ILE N  34      -4.968  -5.129  -6.201  1.00  0.00           H
ATOM    199  C   ILE N  34      -4.312  -7.131  -5.740  1.00  0.00           C
ATOM    200  CB  ILE N  34      -6.308  -6.589  -7.113  1.00  0.00           C
ATOM    201 HD11 ILE N  33       1.699  -5.811  -7.274  1.00  0.00           H
ATOM    202 HD12 ILE N  33       1.115  -5.356  -5.670  1.00  0.00           H
ATOM    203 HD13 ILE N  33       0.476  -6.826  -6.460  1.00  0.00           H
ATOM    204  HA1 GLY N  37      -3.203  -7.445   2.083  1.00  0.00           H
ATOM    205  HA2 GLY N  37      -4.844  -7.699   2.749  1.00  0.00           H
ATOM    206  N   GLY N  37      -4.587  -8.140   0.714  1.00  0.00           N
ATOM    207  HA  ASP N  43       8.092  -0.928  -5.740  1.00  0.00           H
ATOM    208  CB  ASP N  43       8.362  -3.012  -6.185  1.00  0.00           C
ATOM    209  C   ASP N  43       6.188  -1.674  -6.293  1.00  0.00           C
ATOM    210  HA  VAL N   8       0.474   8.427 -13.495  1.00  0.00           H
ATOM    211  C   VAL N   8       0.386   6.376 -13.797  1.00  0.00           C
ATOM    212  CB  VAL N   8       2.063   7.992 -14.894  1.00  0.00           C
ATOM    213 HD11 ILE N   7       4.830   9.910  -7.679  1.00  0.00           H
ATOM    214 HD12 ILE N   7       4.099   9.366  -6.157  1.00  0.00           H
ATOM    215 HD13 ILE N   7       3.236  10.512  -7.188  1.00  0.00           H
ATOM    216  H   THR N  30      -3.621  -1.601 -16.018  1.00  0.00           H
ATOM    217  C   TYR N  29      -3.032  -1.494 -17.965  1.00  0.00           C
ATOM    218  HB  THR N  30      -2.024   1.426 -14.698  1.00  0.00           H
ATOM    219  OG1 THR N  30      -2.982  -0.172 -13.904  1.00  0.00           O
ATOM    220  CG2 THR N  30      -4.002   1.378 -15.522  1.00  0.00           C
ATOM    221  O   ILE N  34      -3.969  -8.261  -6.165  1.00  0.00           O
ATOM    222  N   ILE N  35      -4.250  -6.788  -4.452  1.00  0.00           N
ATOM    223  HB  ILE N  34      -6.201  -7.637  -7.440  1.00  0.00           H
ATOM    224  CG1 ILE N  34      -6.892  -5.815  -8.301  1.00  0.00           C
ATOM    225  CG2 ILE N  34      -7.240  -6.541  -5.895  1.00  0.00           C
ATOM    226  H   GLY N  37      -3.784  -8.445   0.152  1.00  0.00           H
ATOM    227  C   PRO N  36      -5.817  -8.596   0.446  1.00  0.00           C
ATOM    228  HB1 ASP N  43       8.484  -2.856  -7.262  1.00  0.00           H
ATOM    229  HB2 ASP N  43       9.363  -2.978  -5.733  1.00  0.00           H
ATOM    230  CG  ASP N  43       7.824  -4.422  -5.959  1.00  0.00           C
ATOM    231  O   ASP N  43       6.149  -1.501  -7.525  1.00  0.00           O
ATOM    232  N   TYR N  44       5.089  -1.662  -5.524  1.00  0.00           N
ATOM    233  O   VAL N   8      -0.765   6.476 -14.243  1.00  0.00           O
ATOM    234  N   ALA N   9       0.912   5.191 -13.434  1.00  0.00           N
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ATOM    235  HB  VAL N   8       3.046   7.497 -14.789  1.00  0.00           H
ATOM    236  CG1 VAL N   8       1.426   7.475 -16.191  1.00  0.00           C
ATOM    237  CG2 VAL N   8       2.274   9.512 -14.939  1.00  0.00           C
ATOM    238  O   TYR N  29      -2.303  -1.017 -18.833  1.00  0.00           O
ATOM    239  CA  TYR N  29      -4.204  -2.404 -18.355  1.00  0.00           C
ATOM    240  HG1 THR N  30      -3.774  -0.727 -14.089  1.00  0.00           H
ATOM    241 HG21 THR N  30      -4.356   2.054 -14.738  1.00  0.00           H
ATOM    242 HG22 THR N  30      -4.803   0.669 -15.770  1.00  0.00           H
ATOM    243 HG23 THR N  30      -3.776   1.981 -16.412  1.00  0.00           H
ATOM    244  H   ILE N  35      -4.581  -5.860  -4.169  1.00  0.00           H
ATOM    245  CA  ILE N  35      -3.826  -7.743  -3.443  1.00  0.00           C
ATOM    246 HG11 ILE N  34      -6.137  -5.758  -9.097  1.00  0.00           H
ATOM    247 HG12 ILE N  34      -7.123  -4.780  -7.991  1.00  0.00           H
ATOM    248  CD1 ILE N  34      -8.139  -6.496  -8.862  1.00  0.00           C
ATOM    249 HG21 ILE N  34      -8.233  -6.922  -6.162  1.00  0.00           H
ATOM    250 HG22 ILE N  34      -6.879  -7.150  -5.055  1.00  0.00           H
ATOM    251 HG23 ILE N  34      -7.354  -5.508  -5.529  1.00  0.00           H
ATOM    252  O   PRO N  36      -6.810  -8.400   1.168  1.00  0.00           O
ATOM    253  CA  PRO N  36      -6.044  -9.432  -0.815  1.00  0.00           C
ATOM    254  OD2 ASP N  43       7.101  -4.644  -4.943  1.00  0.00           O
ATOM    255  OD1 ASP N  43       8.161  -5.311  -6.808  1.00  0.00           O
ATOM    256  H   TYR N  44       5.196  -1.753  -4.510  1.00  0.00           H
ATOM    257  CA  TYR N  44       3.775  -1.270  -6.020  1.00  0.00           C
ATOM    258  H   ALA N   9       1.867   5.122 -13.077  1.00  0.00           H
ATOM    259  CA  ALA N   9       0.073   3.995 -13.471  1.00  0.00           C
ATOM    260 HG11 VAL N   8       2.055   7.744 -17.049  1.00  0.00           H
ATOM    261 HG12 VAL N   8       1.319   6.380 -16.193  1.00  0.00           H
ATOM    262 HG13 VAL N   8       0.420   7.892 -16.353  1.00  0.00           H
ATOM    263 HG21 VAL N   8       2.835   9.804 -15.835  1.00  0.00           H
ATOM    264 HG22 VAL N   8       2.824   9.876 -14.059  1.00  0.00           H
ATOM    265 HG23 VAL N   8       1.303  10.033 -14.967  1.00  0.00           H
ATOM    266  HA  TYR N  29      -3.902  -2.810 -19.329  1.00  0.00           H
ATOM    267  N   TYR N  29      -4.407  -3.515 -17.429  1.00  0.00           N
ATOM    268  CB  TYR N  29      -5.489  -1.558 -18.523  1.00  0.00           C
ATOM    269  HA  ILE N  35      -3.648  -8.672  -3.990  1.00  0.00           H
ATOM    270  C   ILE N  35      -4.960  -7.961  -2.446  1.00  0.00           C
ATOM    271  CB  ILE N  35      -2.493  -7.342  -2.747  1.00  0.00           C
ATOM    272 HD11 ILE N  34      -8.495  -5.981  -9.756  1.00  0.00           H
ATOM    273 HD12 ILE N  34      -8.976  -6.511  -8.152  1.00  0.00           H
ATOM    274 HD13 ILE N  34      -7.915  -7.535  -9.145  1.00  0.00           H
ATOM    275  HA  PRO N  36      -7.053  -9.177  -1.156  1.00  0.00           H
ATOM    276  N   PRO N  36      -5.062  -9.177  -1.879  1.00  0.00           N
ATOM    277  CB  PRO N  36      -5.973 -10.957  -0.565  1.00  0.00           C
ATOM    278  HA  TYR N  44       3.938  -0.794  -6.995  1.00  0.00           H
ATOM    279  CB  TYR N  44       2.815  -2.446  -6.211  1.00  0.00           C
ATOM    280  C   TYR N  44       3.235  -0.200  -5.067  1.00  0.00           C
ATOM    281  HA  ALA N   9      -0.320   3.873 -14.489  1.00  0.00           H
ATOM    282  CB  ALA N   9       0.872   2.740 -13.121  1.00  0.00           C
ATOM    283  C   ALA N   9      -1.174   4.191 -12.584  1.00  0.00           C
ATOM    284  H   TYR N  29      -5.325  -3.628 -16.986  1.00  0.00           H
ATOM    285  C   THR N  28      -3.537  -4.542 -17.426  1.00  0.00           C
ATOM    286  HB1 TYR N  29      -5.759  -1.112 -17.555  1.00  0.00           H
ATOM    287  HB2 TYR N  29      -6.313  -2.239 -18.786  1.00  0.00           H
ATOM    288  CG  TYR N  29      -5.292  -0.491 -19.575  1.00  0.00           C
ATOM    289  O   ILE N  35      -5.720  -7.017  -2.136  1.00  0.00           O
ATOM    290  HB  ILE N  35      -2.276  -8.158  -2.040  1.00  0.00           H
ATOM    291  CG2 ILE N  35      -1.366  -7.297  -3.789  1.00  0.00           C
ATOM    292  CG1 ILE N  35      -2.628  -6.041  -1.932  1.00  0.00           C
ATOM    293  CD  PRO N  36      -4.429 -10.420  -2.370  1.00  0.00           C
ATOM    294  HB1 PRO N  36      -5.980 -11.179   0.509  1.00  0.00           H
ATOM    295  HB2 PRO N  36      -6.865 -11.420  -1.009  1.00  0.00           H
ATOM    296  CG  PRO N  36      -4.681 -11.427  -1.248  1.00  0.00           C
ATOM    297  HB1 TYR N  44       1.834  -2.023  -6.455  1.00  0.00           H
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ATOM    298  HB2 TYR N  44       2.702  -2.983  -5.260  1.00  0.00           H
ATOM    299  CG  TYR N  44       3.240  -3.355  -7.331  1.00  0.00           C
ATOM    300  O   TYR N  44       2.169  -0.335  -4.443  1.00  0.00           O
ATOM    301  N   ALA N  45       4.050   0.858  -4.931  1.00  0.00           N
ATOM    302  HB1 ALA N   9       0.215   1.862 -13.147  1.00  0.00           H
ATOM    303  HB2 ALA N   9       1.673   2.580 -13.856  1.00  0.00           H
ATOM    304  HB3 ALA N   9       1.330   2.825 -12.127  1.00  0.00           H
ATOM    305  O   ALA N   9      -2.279   3.795 -12.985  1.00  0.00           O
ATOM    306  N   ARG N  10      -1.010   4.807 -11.394  1.00  0.00           N
ATOM    307  O   THR N  28      -2.536  -4.556 -18.164  1.00  0.00           O
ATOM    308  CA  THR N  28      -3.762  -5.720 -16.464  1.00  0.00           C
ATOM    309  CD1 TYR N  29      -5.055  -0.861 -20.904  1.00  0.00           C
ATOM    310  CD2 TYR N  29      -5.213   0.870 -19.257  1.00  0.00           C
ATOM    311 HG21 ILE N  35      -0.376  -7.209  -3.324  1.00  0.00           H
ATOM    312 HG22 ILE N  35      -1.343  -8.212  -4.401  1.00  0.00           H
ATOM    313 HG23 ILE N  35      -1.489  -6.451  -4.484  1.00  0.00           H
ATOM    314 HG11 ILE N  35      -3.509  -6.115  -1.276  1.00  0.00           H
ATOM    315 HG12 ILE N  35      -2.827  -5.200  -2.621  1.00  0.00           H
ATOM    316  CD1 ILE N  35      -1.414  -5.709  -1.066  1.00  0.00           C
ATOM    317  HD1 PRO N  36      -3.361 -10.264  -2.536  1.00  0.00           H
ATOM    318  HD2 PRO N  36      -4.908 -10.711  -3.320  1.00  0.00           H
ATOM    319  HG1 PRO N  36      -3.855 -11.401  -0.530  1.00  0.00           H
ATOM    320  HG2 PRO N  36      -4.763 -12.455  -1.629  1.00  0.00           H
ATOM    321  CD1 TYR N  44       2.664  -3.183  -8.592  1.00  0.00           C
ATOM    322  CD2 TYR N  44       4.223  -4.344  -7.182  1.00  0.00           C
ATOM    323  H   ALA N  45       4.840   0.978  -5.579  1.00  0.00           H
ATOM    324  CA  ALA N  45       3.945   1.800  -3.839  1.00  0.00           C
ATOM    325  H   ARG N  10      -0.067   5.076 -11.110  1.00  0.00           H
ATOM    326  CA  ARG N  10      -2.135   5.212 -10.551  1.00  0.00           C
ATOM    327  HA  THR N  28      -2.738  -6.005 -16.187  1.00  0.00           H
ATOM    328  N   THR N  28      -4.470  -5.307 -15.261  1.00  0.00           N
ATOM    329  CB  THR N  28      -4.390  -6.938 -17.163  1.00  0.00           C
ATOM    330  HD1 TYR N  29      -5.086  -1.913 -21.185  1.00  0.00           H
ATOM    331  CE1 TYR N  29      -4.737   0.074 -21.881  1.00  0.00           C
ATOM    332  HD2 TYR N  29      -5.391   1.193 -18.229  1.00  0.00           H
ATOM    333  CE2 TYR N  29      -4.889   1.824 -20.222  1.00  0.00           C
ATOM    334 HD11 ILE N  35      -0.502  -5.564  -1.663  1.00  0.00           H
ATOM    335 HD12 ILE N  35      -1.206  -6.505  -0.336  1.00  0.00           H
ATOM    336 HD13 ILE N  35      -1.586  -4.783  -0.498  1.00  0.00           H
ATOM    337  HD1 TYR N  44       1.888  -2.427  -8.724  1.00  0.00           H
ATOM    338  CE1 TYR N  44       3.028  -3.972  -9.678  1.00  0.00           C
ATOM    339  HD2 TYR N  44       4.703  -4.507  -6.218  1.00  0.00           H
ATOM    340  CE2 TYR N  44       4.594  -5.150  -8.254  1.00  0.00           C
ATOM    341  HA  ALA N  45       3.505   1.267  -2.983  1.00  0.00           H
ATOM    342  C   ALA N  45       3.025   2.978  -4.134  1.00  0.00           C
ATOM    343  CB  ALA N  45       5.343   2.326  -3.501  1.00  0.00           C
ATOM    344  HA  ARG N  10      -2.747   4.328 -10.340  1.00  0.00           H
ATOM    345  C   ARG N  10      -3.086   6.191 -11.248  1.00  0.00           C
ATOM    346  CB  ARG N  10      -1.615   5.831  -9.242  1.00  0.00           C
ATOM    347  H   THR N  28      -5.450  -5.571 -15.129  1.00  0.00           H
ATOM    348  C   ALA N  27      -3.856  -4.419 -14.449  1.00  0.00           C
ATOM    349  HB  THR N  28      -3.822  -7.046 -18.107  1.00  0.00           H
ATOM    350  OG1 THR N  28      -5.749  -6.635 -17.442  1.00  0.00           O
ATOM    351  CG2 THR N  28      -4.246  -8.241 -16.381  1.00  0.00           C
ATOM    352  HE1 TYR N  29      -4.548  -0.248 -22.902  1.00  0.00           H
ATOM    353  CZ  TYR N  29      -4.624   1.433 -21.543  1.00  0.00           C
ATOM    354  HE2 TYR N  29      -4.809   2.881 -19.963  1.00  0.00           H
ATOM    355  HE1 TYR N  44       2.548  -3.819 -10.640  1.00  0.00           H
ATOM    356  CZ  TYR N  44       3.983  -4.980  -9.504  1.00  0.00           C
ATOM    357  HE2 TYR N  44       5.355  -5.920  -8.129  1.00  0.00           H
ATOM    358  O   ALA N  45       2.772   3.797  -3.219  1.00  0.00           O
ATOM    359  N   ASN N  46       2.587   3.118  -5.376  1.00  0.00           N
ATOM    360  HB1 ALA N  45       5.357   2.881  -2.562  1.00  0.00           H
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ATOM    361  HB2 ALA N  45       5.687   3.008  -4.288  1.00  0.00           H
ATOM    362  HB3 ALA N  45       6.056   1.495  -3.422  1.00  0.00           H
ATOM    363  O   ARG N  10      -4.316   6.018 -11.172  1.00  0.00           O
ATOM    364  N   SER N  11      -2.540   7.241 -11.882  1.00  0.00           N
ATOM    365  HB1 ARG N  10      -1.054   5.063  -8.693  1.00  0.00           H
ATOM    366  HB2 ARG N  10      -0.895   6.620  -9.499  1.00  0.00           H
ATOM    367  CG  ARG N  10      -2.694   6.456  -8.349  1.00  0.00           C
ATOM    368  O   ALA N  27      -2.691  -4.047 -14.667  1.00  0.00           O
ATOM    369  CA  ALA N  27      -4.626  -3.892 -13.226  1.00  0.00           C
ATOM    370  HG1 THR N  28      -6.009  -7.269 -18.155  1.00  0.00           H
ATOM    371 HG21 THR N  28      -4.661  -9.068 -16.975  1.00  0.00           H
ATOM    372 HG22 THR N  28      -3.191  -8.493 -16.202  1.00  0.00           H
ATOM    373 HG23 THR N  28      -4.786  -8.196 -15.425  1.00  0.00           H
ATOM    374  OH  TYR N  29      -4.247   2.373 -22.441  1.00  0.00           O
ATOM    375  OH  TYR N  44       4.345  -5.824 -10.507  1.00  0.00           O
ATOM    376  H   ASN N  46       2.736   2.374  -6.067  1.00  0.00           H
ATOM    377  CA  ASN N  46       1.877   4.292  -5.837  1.00  0.00           C
ATOM    378  H   SER N  11      -1.529   7.409 -11.832  1.00  0.00           H
ATOM    379  CA  SER N  11      -3.399   8.175 -12.593  1.00  0.00           C
ATOM    380  HG1 ARG N  10      -2.188   6.966  -7.517  1.00  0.00           H
ATOM    381  HG2 ARG N  10      -3.221   7.255  -8.892  1.00  0.00           H
ATOM    382  CD  ARG N  10      -3.751   5.513  -7.782  1.00  0.00           C
ATOM    383  HA  ALA N  27      -3.995  -3.081 -12.845  1.00  0.00           H
ATOM    384  N   ALA N  27      -5.933  -3.360 -13.611  1.00  0.00           N
ATOM    385  CB  ALA N  27      -4.789  -4.978 -12.158  1.00  0.00           C
ATOM    386  HH  TYR N  29      -4.351   2.018 -23.368  1.00  0.00           H
ATOM    387  HH  TYR N  44       3.841  -5.627 -11.336  1.00  0.00           H
ATOM    388  HA  ASN N  46       1.963   5.059  -5.064  1.00  0.00           H
ATOM    389  CB  ASN N  46       2.560   4.826  -7.105  1.00  0.00           C
ATOM    390  C   ASN N  46       0.366   4.035  -5.977  1.00  0.00           C
ATOM    391  HA  SER N  11      -4.129   8.593 -11.890  1.00  0.00           H
ATOM    392  CB  SER N  11      -2.602   9.316 -13.231  1.00  0.00           C
ATOM    393  C   SER N  11      -4.219   7.423 -13.662  1.00  0.00           C
ATOM    394  HD1 ARG N  10      -4.481   6.108  -7.215  1.00  0.00           H
ATOM    395  HD2 ARG N  10      -4.308   5.004  -8.584  1.00  0.00           H
ATOM    396  NE  ARG N  10      -3.134   4.515  -6.906  1.00  0.00           N
ATOM    397  H   ALA N  27      -6.769  -3.795 -13.204  1.00  0.00           H
ATOM    398  C   CYS N  26      -6.086  -2.275 -14.369  1.00  0.00           C
ATOM    399  HB1 ALA N  27      -5.501  -5.743 -12.480  1.00  0.00           H
ATOM    400  HB2 ALA N  27      -3.820  -5.454 -11.972  1.00  0.00           H
ATOM    401  HB3 ALA N  27      -5.152  -4.537 -11.218  1.00  0.00           H
ATOM    402  HB1 ASN N  46       2.403   4.142  -7.942  1.00  0.00           H
ATOM    403  HB2 ASN N  46       2.126   5.799  -7.363  1.00  0.00           H
ATOM    404  CG  ASN N  46       4.066   4.934  -6.865  1.00  0.00           C
ATOM    405  O   ASN N  46      -0.337   4.977  -6.432  1.00  0.00           O
ATOM    406  OXT ASN N  46      -0.093   2.909  -5.621  1.00  0.00           O
ATOM    407  HB1 SER N  11      -3.327   9.978 -13.729  1.00  0.00           H
ATOM    408  HB2 SER N  11      -1.919   8.905 -13.994  1.00  0.00           H
ATOM    409  OG  SER N  11      -1.878  10.024 -12.237  1.00  0.00           O
ATOM    410  O   SER N  11      -5.448   7.626 -13.806  1.00  0.00           O
ATOM    411  N   ASN N  12      -3.552   6.548 -14.409  1.00  0.00           N
ATOM    412  HE  ARG N  10      -2.146   4.659  -6.648  1.00  0.00           H
ATOM    413  CZ  ARG N  10      -3.684   3.345  -6.567  1.00  0.00           C
ATOM    414  O   CYS N  26      -5.133  -1.574 -14.768  1.00  0.00           O
ATOM    415  CA  CYS N  26      -7.506  -1.891 -14.823  1.00  0.00           C
ATOM    416  OD1 ASN N  46       4.849   4.176  -7.465  1.00  0.00           O
ATOM    417  ND2 ASN N  46       4.480   5.829  -5.957  1.00  0.00           N
ATOM    418  H   SER N  11      -1.438  10.800 -12.679  1.00  0.00           H
ATOM    419  H   ASN N  12      -2.535   6.446 -14.290  1.00  0.00           H
ATOM    420  CA  ASN N  12      -4.225   5.761 -15.431  1.00  0.00           C
ATOM    421  NH1 ARG N  10      -4.978   3.099  -6.809  1.00  0.00           N
ATOM    422  NH2 ARG N  10      -2.901   2.393  -6.032  1.00  0.00           N
ATOM    423  HA  CYS N  26      -7.335  -1.462 -15.821  1.00  0.00           H
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ATOM    424  N   CYS N  26      -8.369  -3.043 -14.955  1.00  0.00           N
ATOM    425  CB  CYS N  26      -8.132  -0.814 -13.941  1.00  0.00           C
ATOM    426 HD21 ASN N  46       3.830   6.466  -5.486  1.00  0.00           H
ATOM    427 HD22 ASN N  46       5.490   5.950  -5.792  1.00  0.00           H
ATOM    428  HA  ASN N  12      -4.766   6.438 -16.105  1.00  0.00           H
ATOM    429  CB  ASN N  12      -3.213   4.964 -16.247  1.00  0.00           C
ATOM    430  C   ASN N  12      -5.277   4.835 -14.817  1.00  0.00           C
ATOM    431 HH11 ARG N  10      -5.349   2.163  -6.604  1.00  0.00           H
ATOM    432 HH12 ARG N  10      -5.646   3.880  -6.770  1.00  0.00           H
ATOM    433 HH21 ARG N  10      -3.335   1.688  -5.438  1.00  0.00           H
ATOM    434 HH22 ARG N  10      -1.934   2.640  -5.785  1.00  0.00           H
ATOM    435  H   CYS N  26      -9.167  -3.159 -14.325  1.00  0.00           H
ATOM    436  C   LEU N  25      -8.125  -3.933 -15.939  1.00  0.00           C
ATOM    437  HB1 CYS N  26      -7.416  -0.003 -13.762  1.00  0.00           H
ATOM    438  HB2 CYS N  26      -8.429  -1.218 -12.962  1.00  0.00           H
ATOM    439  SG  CYS N  26      -9.688  -0.129 -14.642  1.00  0.00           S
ATOM    440  HB1 ASN N  12      -2.593   4.327 -15.599  1.00  0.00           H
ATOM    441  HB2 ASN N  12      -3.772   4.292 -16.918  1.00  0.00           H
ATOM    442  CG  ASN N  12      -2.348   5.877 -17.131  1.00  0.00           C
ATOM    443  O   ASN N  12      -6.363   4.657 -15.392  1.00  0.00           O
ATOM    444  N   PHE N  13      -4.951   4.232 -13.663  1.00  0.00           N
ATOM    445  O   LEU N  25      -7.233  -3.763 -16.779  1.00  0.00           O
ATOM    446  CA  LEU N  25      -8.993  -5.193 -15.973  1.00  0.00           C
ATOM    447  SG  CYS N  16      -9.064   0.644 -16.475  1.00  0.00           S
ATOM    448  OD1 ASN N  12      -2.702   7.028 -17.391  1.00  0.00           O
ATOM    449  ND2 ASN N  12      -1.237   5.286 -17.602  1.00  0.00           N
ATOM    450  H   PHE N  13      -3.990   4.301 -13.305  1.00  0.00           H
ATOM    451  CA  PHE N  13      -5.873   3.355 -12.962  1.00  0.00           C
ATOM    452  HA  LEU N  25      -8.343  -5.940 -16.447  1.00  0.00           H
ATOM    453  N   LEU N  25      -9.310  -5.666 -14.626  1.00  0.00           N
ATOM    454  CB  LEU N  25     -10.277  -4.981 -16.788  1.00  0.00           C
ATOM    455  CB  CYS N  16      -8.578   2.362 -16.060  1.00  0.00           C
ATOM    456 HD21 ASN N  12      -1.001   4.335 -17.319  1.00  0.00           H
ATOM    457 HD22 ASN N  12      -0.686   5.756 -18.331  1.00  0.00           H
ATOM    458  HA  PHE N  13      -6.181   2.529 -13.621  1.00  0.00           H
ATOM    459  C   PHE N  13      -7.163   4.097 -12.615  1.00  0.00           C
ATOM    460  CB  PHE N  13      -5.193   2.780 -11.701  1.00  0.00           C
ATOM    461  H   LEU N  25     -10.163  -5.321 -14.184  1.00  0.00           H
ATOM    462  C   ALA N  24      -8.344  -6.148 -13.822  1.00  0.00           C
ATOM    463  HB1 LEU N  25     -10.999  -4.442 -16.154  1.00  0.00           H
ATOM    464  HB2 LEU N  25     -10.047  -4.308 -17.631  1.00  0.00           H
ATOM    465  CG  LEU N  25     -10.902  -6.281 -17.326  1.00  0.00           C
ATOM    466  HB1 CYS N  16      -8.146   2.372 -15.050  1.00  0.00           H
ATOM    467  HB2 CYS N  16      -7.778   2.627 -16.768  1.00  0.00           H
ATOM    468  CA  CYS N  16      -9.702   3.408 -16.156  1.00  0.00           C
ATOM    469  O   PHE N  13      -8.271   3.608 -12.872  1.00  0.00           O
ATOM    470  N   ASN N  14      -7.016   5.290 -12.001  1.00  0.00           N
ATOM    471  HB1 PHE N  13      -4.220   2.376 -12.005  1.00  0.00           H
ATOM    472  HB2 PHE N  13      -4.993   3.603 -11.001  1.00  0.00           H
ATOM    473  CG  PHE N  13      -6.013   1.695 -11.050  1.00  0.00           C
ATOM    474  O   ALA N  24      -7.181  -6.319 -14.231  1.00  0.00           O
ATOM    475  CA  ALA N  24      -8.740  -6.528 -12.387  1.00  0.00           C
ATOM    476  HG  LEU N  25     -10.953  -6.995 -16.488  1.00  0.00           H
ATOM    477  CD1 LEU N  25     -10.043  -6.912 -18.427  1.00  0.00           C
ATOM    478  CD2 LEU N  25     -12.340  -6.034 -17.802  1.00  0.00           C
ATOM    479  HA  CYS N  16     -10.060   3.478 -17.192  1.00  0.00           H
ATOM    480  N   CYS N  16      -9.135   4.681 -15.733  1.00  0.00           N
ATOM    481  C   CYS N  16     -10.956   3.033 -15.341  1.00  0.00           C
ATOM    482  H   ASN N  14      -6.077   5.657 -11.807  1.00  0.00           H
ATOM    483  CA  ASN N  14      -8.202   6.023 -11.599  1.00  0.00           C
ATOM    484  CD2 PHE N  13      -6.975   1.984 -10.072  1.00  0.00           C
ATOM    485  CD1 PHE N  13      -5.842   0.364 -11.460  1.00  0.00           C
ATOM    486  HA  ALA N  24      -7.796  -6.550 -11.828  1.00  0.00           H
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ATOM    487  N   ALA N  24      -9.628  -5.528 -11.806  1.00  0.00           N
ATOM    488  CB  ALA N  24      -9.387  -7.913 -12.325  1.00  0.00           C
ATOM    489 HD11 LEU N  25     -10.492  -7.841 -18.803  1.00  0.00           H
ATOM    490 HD12 LEU N  25      -9.031  -7.165 -18.081  1.00  0.00           H
ATOM    491 HD13 LEU N  25      -9.932  -6.231 -19.286  1.00  0.00           H
ATOM    492 HD21 LEU N  25     -12.986  -5.698 -16.977  1.00  0.00           H
ATOM    493 HD22 LEU N  25     -12.792  -6.949 -18.214  1.00  0.00           H
ATOM    494 HD23 LEU N  25     -12.377  -5.258 -18.587  1.00  0.00           H
ATOM    495  H   CYS N  16      -8.144   4.702 -15.461  1.00  0.00           H
ATOM    496  C   VAL N  15      -9.865   5.810 -15.687  1.00  0.00           C
ATOM    497  O   CYS N  16     -11.927   2.475 -15.875  1.00  0.00           O
ATOM    498  N   ARG N  17     -10.930   3.365 -14.040  1.00  0.00           N
ATOM    499  HA  ASN N  14      -8.851   5.341 -11.035  1.00  0.00           H
ATOM    500  CB  ASN N  14      -7.874   7.238 -10.729  1.00  0.00           C
ATOM    501  C   ASN N  14      -9.052   6.432 -12.814  1.00  0.00           C
ATOM    502  HD2 PHE N  13      -7.134   3.015  -9.746  1.00  0.00           H
ATOM    503  CE2 PHE N  13      -7.754   0.963  -9.524  1.00  0.00           C
ATOM    504  HD1 PHE N  13      -5.097   0.143 -12.227  1.00  0.00           H
ATOM    505  CE1 PHE N  13      -6.616  -0.659 -10.913  1.00  0.00           C
ATOM    506  H   ALA N  24     -10.452  -5.869 -11.276  1.00  0.00           H
ATOM    507  C   GLU N  23      -9.180  -4.275 -11.592  1.00  0.00           C
ATOM    508  HB1 ALA N  24      -8.727  -8.655 -12.787  1.00  0.00           H
ATOM    509  HB2 ALA N  24      -9.555  -8.197 -11.278  1.00  0.00           H
ATOM    510  HB3 ALA N  24     -10.355  -7.932 -12.841  1.00  0.00           H
ATOM    511  O   VAL N  15     -11.053   5.854 -16.039  1.00  0.00           O
ATOM    512  CA  VAL N  15      -9.155   7.071 -15.167  1.00  0.00           C
ATOM    513  H   ARG N  17     -10.060   3.724 -13.637  1.00  0.00           H
ATOM    514  CA  ARG N  17     -12.041   3.089 -13.150  1.00  0.00           C
ATOM    515  HB1 ASN N  14      -7.230   7.954 -11.258  1.00  0.00           H
ATOM    516  HB2 ASN N  14      -8.830   7.748 -10.522  1.00  0.00           H
ATOM    517  CG  ASN N  14      -7.293   6.896  -9.362  1.00  0.00           C
ATOM    518  O   ASN N  14     -10.293   6.410 -12.737  1.00  0.00           O
ATOM    519  N   VAL N  15      -8.413   6.802 -13.936  1.00  0.00           N
ATOM    520  HE2 PHE N  13      -8.506   1.204  -8.769  1.00  0.00           H
ATOM    521  CZ  PHE N  13      -7.581  -0.355  -9.951  1.00  0.00           C
ATOM    522  HE1 PHE N  13      -6.492  -1.692 -11.246  1.00  0.00           H
ATOM    523  O   GLU N  23      -8.052  -3.892 -11.937  1.00  0.00           O
ATOM    524  CA  GLU N  23     -10.113  -3.301 -10.863  1.00  0.00           C
ATOM    525  HA  VAL N  15      -9.978   7.759 -14.933  1.00  0.00           H
ATOM    526  CB  VAL N  15      -8.237   7.726 -16.224  1.00  0.00           C
ATOM    527  HA  ARG N  17     -12.470   2.108 -13.412  1.00  0.00           H
ATOM    528  C   ARG N  17     -13.210   4.059 -13.323  1.00  0.00           C
ATOM    529  CB  ARG N  17     -11.564   3.087 -11.688  1.00  0.00           C
ATOM    530  OD1 ASN N  14      -7.650   5.854  -8.756  1.00  0.00           O
ATOM    531  ND2 ASN N  14      -6.466   7.789  -8.835  1.00  0.00           N
ATOM    532  H   VAL N  15      -7.390   6.798 -13.962  1.00  0.00           H
ATOM    533  HZ  PHE N  13      -8.192  -1.152  -9.531  1.00  0.00           H
ATOM    534  HA  GLU N  23      -9.744  -2.305 -11.152  1.00  0.00           H
ATOM    535  N   GLU N  23     -11.489  -3.450 -11.301  1.00  0.00           N
ATOM    536  CB  GLU N  23      -9.956  -3.480  -9.342  1.00  0.00           C
ATOM    537  HB  VAL N  15      -7.303   7.139 -16.254  1.00  0.00           H
ATOM    538  CG2 VAL N  15      -7.910   9.158 -15.801  1.00  0.00           C
ATOM    539  CG1 VAL N  15      -8.864   7.687 -17.619  1.00  0.00           C
ATOM    540  O   ARG N  17     -14.324   3.736 -12.851  1.00  0.00           O
ATOM    541  N   LEU N  18     -13.037   5.221 -13.961  1.00  0.00           N
ATOM    542  HB1 ARG N  17     -11.080   4.048 -11.480  1.00  0.00           H
ATOM    543  HB2 ARG N  17     -12.444   3.044 -11.030  1.00  0.00           H
ATOM    544  CG  ARG N  17     -10.601   1.944 -11.360  1.00  0.00           C
ATOM    545 HD21 ASN N  14      -6.183   7.683  -7.858  1.00  0.00           H
ATOM    546 HD22 ASN N  14      -6.118   8.622  -9.359  1.00  0.00           H
ATOM    547  H   GLU N  23     -12.214  -3.697 -10.603  1.00  0.00           H
ATOM    548  C   PRO N  22     -11.794  -3.470 -12.610  1.00  0.00           C
ATOM    549  HB1 GLU N  23     -10.331  -4.471  -9.063  1.00  0.00           H
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ATOM    552 HG21 VAL N  15      -7.435   9.191 -14.815  1.00  0.00           H
ATOM    553 HG22 VAL N  15      -7.223   9.645 -16.503  1.00  0.00           H
ATOM    554 HG23 VAL N  15      -8.829   9.765 -15.750  1.00  0.00           H
ATOM    555 HG11 VAL N  15      -8.228   8.221 -18.335  1.00  0.00           H
ATOM    556 HG12 VAL N  15      -8.989   6.656 -17.983  1.00  0.00           H
ATOM    557 HG13 VAL N  15      -9.858   8.162 -17.634  1.00  0.00           H
ATOM    558  H   LEU N  18     -12.139   5.444 -14.396  1.00  0.00           H
ATOM    559  CA  LEU N  18     -14.128   6.182 -14.096  1.00  0.00           C
ATOM    560  HG1 ARG N  17      -9.809   1.869 -12.117  1.00  0.00           H
ATOM    561  HG2 ARG N  17     -10.087   2.206 -10.424  1.00  0.00           H
ATOM    562  CD  ARG N  17     -11.274   0.581 -11.219  1.00  0.00           C
ATOM    563  O   PRO N  22     -10.949  -3.338 -13.516  1.00  0.00           O
ATOM    564  CA  PRO N  22     -13.242  -3.821 -12.914  1.00  0.00           C
ATOM    565  HG1 GLU N  23     -10.332  -1.399  -8.786  1.00  0.00           H
ATOM    566  HG2 GLU N  23     -11.729  -2.454  -8.622  1.00  0.00           H
ATOM    567  CD  GLU N  23     -10.382  -2.546  -6.985  1.00  0.00           C
ATOM    568  HA  LEU N  18     -14.506   6.409 -13.089  1.00  0.00           H
ATOM    569  CB  LEU N  18     -13.668   7.476 -14.776  1.00  0.00           C
ATOM    570  C   LEU N  18     -15.369   5.618 -14.803  1.00  0.00           C
ATOM    571  HD1 ARG N  17     -11.907   0.356 -12.086  1.00  0.00           H
ATOM    572  HD2 ARG N  17     -10.501  -0.208 -11.188  1.00  0.00           H
ATOM    573  NE  ARG N  17     -12.067   0.542  -9.997  1.00  0.00           N
ATOM    574  HA  PRO N  22     -13.874  -3.601 -12.043  1.00  0.00           H
ATOM    575  N   PRO N  22     -13.767  -3.116 -14.091  1.00  0.00           N
ATOM    576  CB  PRO N  22     -13.375  -5.302 -13.297  1.00  0.00           C
ATOM    577  OE2 GLU N  23     -10.531  -1.496  -6.287  1.00  0.00           O
ATOM    578  OE1 GLU N  23     -10.066  -3.678  -6.501  1.00  0.00           O
ATOM    579  HB1 LEU N  18     -14.571   8.034 -15.058  1.00  0.00           H
ATOM    580  HB2 LEU N  18     -13.145   7.223 -15.710  1.00  0.00           H
ATOM    581  CG  LEU N  18     -12.774   8.406 -13.935  1.00  0.00           C
ATOM    582  O   LEU N  18     -16.498   5.929 -14.362  1.00  0.00           O
ATOM    583  N   PRO N  19     -15.259   4.807 -15.872  1.00  0.00           N
ATOM    584  HE  ARG N  17     -11.615   0.879  -9.135  1.00  0.00           H
ATOM    585  CZ  ARG N  17     -13.204  -0.131  -9.764  1.00  0.00           C
ATOM    586  C   THR N  21     -13.628  -1.786 -14.191  1.00  0.00           C
ATOM    587  CD  PRO N  22     -14.570  -4.007 -14.955  1.00  0.00           C
ATOM    588  HB1 PRO N  22     -13.456  -5.939 -12.410  1.00  0.00           H
ATOM    589  HB2 PRO N  22     -12.499  -5.604 -13.894  1.00  0.00           H
ATOM    590  CG  PRO N  22     -14.638  -5.311 -14.154  1.00  0.00           C
ATOM    591  HG  LEU N  18     -11.847   7.867 -13.682  1.00  0.00           H
ATOM    592  CD1 LEU N  18     -12.407   9.606 -14.817  1.00  0.00           C
ATOM    593  CD2 LEU N  18     -13.440   8.839 -12.624  1.00  0.00           C
ATOM    594  CA  PRO N  19     -16.468   4.173 -16.423  1.00  0.00           C
ATOM    595  CD  PRO N  19     -14.109   4.716 -16.813  1.00  0.00           C
ATOM    596  NH1 ARG N  17     -13.874  -0.775 -10.716  1.00  0.00           N
ATOM    597  NH2 ARG N  17     -13.676  -0.116  -8.506  1.00  0.00           N
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ATOM    599  CA  THR N  21     -14.110  -1.066 -15.459  1.00  0.00           C
ATOM    600  HD1 PRO N  22     -15.565  -3.581 -15.131  1.00  0.00           H
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ATOM    602  HG1 PRO N  22     -14.721  -6.188 -14.802  1.00  0.00           H
ATOM    603  HG2 PRO N  22     -15.517  -5.282 -13.501  1.00  0.00           H
ATOM    604 HD11 LEU N  18     -11.735  10.305 -14.299  1.00  0.00           H
ATOM    605 HD12 LEU N  18     -11.901   9.279 -15.738  1.00  0.00           H
ATOM    606 HD13 LEU N  18     -13.303  10.172 -15.119  1.00  0.00           H
ATOM    607 HD21 LEU N  18     -12.826   9.581 -12.093  1.00  0.00           H
ATOM    608 HD22 LEU N  18     -13.578   7.994 -11.932  1.00  0.00           H
ATOM    609 HD23 LEU N  18     -14.426   9.295 -12.802  1.00  0.00           H
ATOM    610  HA  PRO N  19     -17.311   4.878 -16.413  1.00  0.00           H
ATOM    611  C   PRO N  19     -16.945   2.943 -15.646  1.00  0.00           C
ATOM    612  CB  PRO N  19     -16.067   3.769 -17.850  1.00  0.00           C
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ATOM    616 HH11 ARG N  17     -13.497  -0.887 -11.664  1.00  0.00           H
ATOM    617 HH12 ARG N  17     -14.640  -1.403 -10.448  1.00  0.00           H
ATOM    618 HH21 ARG N  17     -13.100   0.340  -7.795  1.00  0.00           H
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ATOM    621  N   THR N  21     -14.893   0.096 -15.087  1.00  0.00           N
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ATOM    626  HB2 PRO N  19     -16.568   2.847 -18.156  1.00  0.00           H
ATOM    627  HG1 PRO N  19     -14.099   3.791 -18.792  1.00  0.00           H
ATOM    628  HG2 PRO N  19     -14.246   2.649 -17.437  1.00  0.00           H
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ATOM    630  C   GLY N  20     -15.853   0.056 -14.148  1.00  0.00           C
ATOM    631  HB  THR N  21     -12.221  -0.074 -15.488  1.00  0.00           H
ATOM    632  OG1 THR N  21     -13.238   0.349 -17.221  1.00  0.00           O
ATOM    633  CG2 THR N  21     -12.077  -1.769 -16.807  1.00  0.00           C
ATOM    634  H   GLY N  20     -15.418   3.072 -14.277  1.00  0.00           H
ATOM    635  CA  GLY N  20     -16.561   1.360 -13.811  1.00  0.00           C
ATOM    636  O   GLY N  20     -16.140  -0.980 -13.537  1.00  0.00           O
ATOM    637  HG1 THR N  21     -12.708   1.157 -17.050  1.00  0.00           H
ATOM    638 HG21 THR N  21     -11.237  -1.400 -17.411  1.00  0.00           H
ATOM    639 HG22 THR N  21     -11.670  -2.388 -15.997  1.00  0.00           H
ATOM    640 HG23 THR N  21     -12.713  -2.394 -17.452  1.00  0.00           H
ATOM    641  HA1 GLY N  20     -17.638   1.168 -13.902  1.00  0.00           H
ATOM    642  HA2 GLY N  20     -16.322   1.586 -12.763  1.00  0.00           H
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OPTIMIZED GEOMETRIES (CIF files)

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H101	H	0.104163449761	0.423402585249	0.587439632723
H102	H	0.895836550239	0.923402585245	0.412560367277

H103	H	0.140638780199	0.512600437362	0.576963966090
H104	H	0.859361219801	0.012600437359	0.423036033910
H105	H	0.062644732347	0.510227448076	0.594822082703
H106	H	0.937355267653	0.010227448072	0.405177917297
H107	H	0.191543650423	0.594947921766	0.623596426576
H108	H	0.808456349577	0.094947921763	0.376403573423
H109	H	0.178069110771	0.573484287874	0.668287627242
H110	H	0.821930889229	0.073484287870	0.331712372758
H111	H	0.114945158135	0.609132284720	0.642257965030
H112	H	0.885054841865	0.109132284717	0.357742034970
H113	H	0.125174424110	0.305991167845	0.667633687597
H114	H	0.874825575891	0.805991167842	0.332366312403
H115	H	0.030903432326	0.244736039723	0.621186744036
H116	H	0.969096567674	0.744736039719	0.378813255964
H117	H	0.119422216164	0.164909971009	0.641535389225
H118	H	0.880577783836	0.664909971006	0.358464610774
H119	H	0.046058826510	0.121357120856	0.653166555703
H120	H	0.953941173490	0.621357120853	0.346833444297
H121	H	0.091944772063	0.170509468476	0.685249923936
H122	H	0.908055227937	0.670509468472	0.314750076064
H123	H	0.023692944137	0.289348644076	0.712622862684
H124	H	0.976307055863	0.789348644073	0.287377137316
H125	H	0.893211960804	0.239683540478	0.719020461573
H126	H	0.106788039196	0.739683540475	0.280979538427
H127	H	0.963899380691	0.260877233203	0.769745507524
H128	H	0.036100619309	0.760877233200	0.230254492476
H129	H	0.966374106096	0.360512514649	0.760696662762
H130	H	0.033625893904	0.860512514645	0.239303337238
H131	H	0.889690098968	0.344687057343	0.806511383447
H132	H	0.110309901032	0.844687057340	0.193488616553
H133	H	0.847589207723	0.368149567019	0.769015323359
H134	H	0.152410792277	0.868149567015	0.230984676641
H135	H	0.784107676478	0.274081350096	0.794338437348
H136	H	0.215892323522	0.774081350093	0.205661562651
H137	H	0.824223388556	0.222314823815	0.761547274469
H138	H	0.175776611445	0.722314823811	0.238452725531
H139	H	0.895591025170	0.218146776067	0.827047797167
H140	H	0.104408974830	0.718146776064	0.172952202833
H141	H	0.756379572214	0.138198254347	0.787803504591
H142	H	0.243620427786	0.638198254343	0.212196495409
H143	H	0.749196218990	0.064056315557	0.817147464323
H144	H	0.250803781010	0.564056315554	0.182852535676
H145	H	0.897813261864	0.109123819253	0.856143562278
H146	H	0.102186738136	0.609123819249	0.143856437722
H147	H	0.830339907935	0.050498538679	0.860130809014
H148	H	0.169660092065	0.550498538675	0.139869190986
H149	H	0.954810921853	0.431384814413	0.697761301870
H150	H	0.045189078147	0.931384814409	0.302238698130
H151	H	0.834042504403	0.501307395242	0.689614982396
H152	H	0.165957495597	0.001307395239	0.310385017604
H153	H	0.947515215526	0.517741149688	0.639556148517
H154	H	0.052484784474	0.017741149684	0.360443851483
H155	H	0.881122828810	0.580834483583	0.643798884235
H156	H	0.118877171190	0.080834483580	0.356201115764
H157	H	0.951897250758	0.633838060959	0.679211446136
H158	H	0.048102749242	0.133838060956	0.320788553864
H159	H	0.918994404562	0.390690595287	0.626554086753
H160	H	0.081005595438	0.890690595284	0.373445913247
H161	H	0.823374968718	0.408404720217	0.574426467183
H162	H	0.176625031282	0.908404720214	0.425573532817
H163	H	0.931532680371	0.289871653959	0.582078515213
H164	H	0.068467319629	0.789871653955	0.417921484786
H165	H	0.887176070637	0.304667032293	0.543812149247

H166	H	0.112823929363	0.804667032289	0.456187850753
H167	H	0.009205384875	0.327335424546	0.526288338213
H168	H	0.990794615125	0.827335424543	0.473711661787
H169	H	0.028823239962	0.424469738552	0.527935641126
H170	H	0.971176760038	0.924469738549	0.472064358874
H171	H	0.853319668200	0.262514464115	0.636234035306
H172	H	0.146680331800	0.762514464112	0.363765964694
H173	H	0.754235852973	0.155740124899	0.619257647801
H174	H	0.245764147027	0.655740124896	0.380742352199
H175	H	0.839303716742	0.125118638563	0.659751886373
H176	H	0.160696283258	0.625118638560	0.340248113626
H177	H	0.822938014508	0.207955358405	0.684675708807
H178	H	0.177061985492	0.707955358402	0.315324291193
H179	H	0.725598322178	0.214587222078	0.723340359041
H180	H	0.274401677822	0.714587222075	0.276659640959
H181	H	0.781756496304	0.007589499088	0.669634861993
H182	H	0.218243503696	0.507589499084	0.330365138007
H183	H	0.654008785195	0.138615020539	0.760952076937
H184	H	0.345991214805	0.638615020535	0.239047923063
H185	H	0.709360788195	0.930760755967	0.707453709023
H186	H	0.290639211805	0.430760755964	0.292546290977
H187	H	0.645042206972	0.997360922450	0.753354491205
H188	H	0.354957793028	0.497360922446	0.246645508795
H189	H	0.754111381818	0.324276541397	0.673413152833
H190	H	0.245888618182	0.824276541394	0.326586847166
H191	H	0.625079887691	0.306669145418	0.695520701385
H192	H	0.374920112309	0.806669145415	0.304479298614
H193	H	0.706421118992	0.452448653786	0.686999144362
H194	H	0.293578881008	0.952448653782	0.313000855637
H195	H	0.631985640108	0.447023581105	0.708984797948
H196	H	0.368014359892	0.947023581102	0.291015202052
H197	H	0.757242606889	0.492179351419	0.734789580988
H198	H	0.242757393111	0.992179351415	0.265210419011
H199	H	0.767655172401	0.440009533064	0.772502401551
H200	H	0.232344827599	0.940009533060	0.227497598448
H201	H	0.689966213570	0.402895835563	0.620988293766
H202	H	0.310033786430	0.902895835560	0.379011706234
H203	H	0.567529210028	0.460351574962	0.597161686743
H204	H	0.432470789972	0.960351574958	0.402838313256
H205	H	0.693568706287	0.422800039752	0.561637753045
H206	H	0.306431293713	0.922800039749	0.438362246955
H207	H	0.646832550591	0.486764366993	0.507652923770
H208	H	0.353167449409	0.986764366989	0.492347076230
H209	H	0.570487012537	0.477689239277	0.526585312900
H210	H	0.429512987463	0.977689239273	0.473414687100
H211	H	0.615677738562	0.393987930453	0.516993160375
H212	H	0.384322261439	0.893987930450	0.483006839624
H213	H	0.692546455193	0.569750271850	0.554122764690
H214	H	0.307453544807	0.069750271846	0.445877235310
H215	H	0.690442956252	0.541490531661	0.597992079903
H216	H	0.309557043748	0.041490531657	0.402007920097
H217	H	0.619387920795	0.571560547056	0.577060406387
H218	H	0.380612079205	0.071560547053	0.422939593612
H219	H	0.650706692105	0.282314858861	0.582269344542
H220	H	0.349293307895	0.782314858857	0.417730655458
H221	H	0.551048575817	0.215138540030	0.541202917003
H222	H	0.448951424183	0.715138540027	0.458797082997
H223	H	0.656335765881	0.158631870002	0.543802605932
H224	H	0.343664234119	0.658631869998	0.456197394068
H225	H	0.652657884974	0.150203088987	0.589772616683
H226	H	0.347342115026	0.650203088983	0.410227383317
H227	H	0.566690679527	0.214517579829	0.634777566117
H228	H	0.433309320473	0.714517579825	0.365222433883

H229	H	0.451029637069	0.125411308853	0.641979867974
H230	H	0.548970362931	0.625411308850	0.358020132026
H231	H	0.506494087572	0.242580576794	0.693236806439
H232	H	0.493505912428	0.742580576791	0.306763193561
H233	H	0.447579327725	0.173071090630	0.702835040372
H234	H	0.552420672275	0.673071090627	0.297164959628
H235	H	0.583970553920	0.132816652057	0.678990280944
H236	H	0.416029446080	0.632816652054	0.321009719056
H237	H	0.562773750728	0.146246375135	0.722373370999
H238	H	0.437226249272	0.646246375132	0.277626629001
H239	H	0.494510482811	0.022405940312	0.680072040544
H240	H	0.505489517189	0.522405940309	0.319927959456
H241	H	0.571319259494	0.008047852375	0.696308688571
H242	H	0.428680740506	0.508047852372	0.303691311428
H243	H	0.535663904166	0.000813633897	0.753327437867
H244	H	0.464336095835	0.500813633893	0.246672562133
H245	H	0.402829783518	0.019325511888	0.696442319154
H246	H	0.597170216482	0.519325511885	0.303557680846
H247	H	0.351512244426	0.041516643797	0.731427523717
H248	H	0.648487755574	0.541516643794	0.268572476283
H249	H	0.464878672375	0.012705545566	0.796597530100
H250	H	0.535121327625	0.512705545562	0.203402469900
H251	H	0.384653729660	0.994253583287	0.787342737086
H252	H	0.615346270340	0.494253583284	0.212657262914
H253	H	0.474508366571	0.327350559847	0.634018951030
H254	H	0.525491633429	0.827350559843	0.365981048970
H255	H	0.369619805396	0.387040343567	0.662675450879
H256	H	0.630380194604	0.887040343564	0.337324549121
H257	H	0.455230371642	0.434646790014	0.607698905629
H258	H	0.544769628358	0.934646790010	0.392301094371
H259	H	0.378984793966	0.455869615765	0.592861662842
H260	H	0.621015206034	0.955869615762	0.407138337157
H261	H	0.436694160365	0.512021692036	0.660685967799
H262	H	0.563305839635	0.012021692033	0.339314032201
H263	H	0.476861834945	0.571507728548	0.604084183725
H264	H	0.523138165056	0.071507728545	0.395915816275
H265	H	0.437915909607	0.639691617064	0.631226566104
H266	H	0.562084090393	0.139691617060	0.368773433896
H267	H	0.398103086433	0.600758927392	0.594778504610
H268	H	0.601896913567	0.100758927388	0.405221495390
H269	H	0.339265988767	0.592716619867	0.668517725214
H270	H	0.660734011233	0.092716619864	0.331482274786
H271	H	0.317591699946	0.494386897207	0.668350974035
H272	H	0.682408300054	0.994386897203	0.331649025965
H273	H	0.304790612688	0.550512046170	0.630887504918
H274	H	0.695209387312	0.050512046167	0.369112495082
H275	H	0.216982633862	0.357280646586	0.578314163426
H276	H	0.783017366138	0.857280646582	0.421685836573
H277	H	0.228619328549	0.267344661382	0.520138382835
H278	H	0.771380671451	0.767344661378	0.479861617165
H279	H	0.267707958702	0.357661587877	0.522127646730
H280	H	0.732292041298	0.857661587873	0.477872353269
H281	H	0.327937236504	0.201313813361	0.539192886785
H282	H	0.672062763496	0.701313813358	0.460807113214
H283	H	0.354844607179	0.270917848120	0.508668932493
H284	H	0.645155392821	0.770917848117	0.491331067507
H285	H	0.401788313999	0.271065990641	0.575201762653
H286	H	0.598211686001	0.771065990638	0.424798237346
H287	H	0.386172250095	0.359535145817	0.554191508634
H288	H	0.613827749905	0.859535145813	0.445808491366
H289	H	0.291546732708	0.205272453633	0.616083801839
H290	H	0.708453267292	0.705272453629	0.383916198161
H291	H	0.216719421965	0.121626067824	0.646592485724

H292	H	0.783280578035	0.621626067821	0.353407514276
H293	H	0.177749095842	0.104920925537	0.606535622996
H294	H	0.822250904158	0.604920925533	0.393464377004
H295	H	0.336333195248	0.103650422716	0.588028238448
H296	H	0.663666804752	0.603650422713	0.411971761552
H297	H	0.332651781228	0.942345742172	0.577220006402
H298	H	0.667348218772	0.442345742169	0.422779993598
H299	H	0.452959896653	0.035849669008	0.587448441270
H300	H	0.547040103347	0.535849669004	0.412551558730
H301	H	0.426340519817	0.105589538688	0.548289943764
H302	H	0.573659480183	0.605589538685	0.451710056236
H303	H	0.466311151328	0.897684660328	0.577453303353
H304	H	0.533688848672	0.397684660325	0.422546696646
H305	H	0.492738152669	0.948269361141	0.539858079402
H306	H	0.507261847331	0.448269361138	0.460141920598
H307	H	0.417773004075	0.900752669432	0.539688983338
H308	H	0.582226995925	0.400752669429	0.460311016662
H309	H	0.370569044263	0.884438334640	0.688616816098
H310	H	0.629430955738	0.384438334637	0.311383183902
H311	H	0.392507508647	0.723142381681	0.659664403036
H312	H	0.607492491353	0.223142381677	0.340335596964
H313	H	0.344838645785	0.749918207854	0.695892824843
H314	H	0.655161354215	0.249918207851	0.304107175157
H315	H	0.286961427393	0.715782048113	0.634969557259
H316	H	0.713038572607	0.215782048110	0.365030442741
H317	H	0.261141669870	0.799785304403	0.657864561948
H318	H	0.738858330130	0.299785304400	0.342135438052
H319	H	0.352870840809	0.792909948404	0.595766304371
H320	H	0.647129159191	0.292909948401	0.404233695629
H321	H	0.288240343389	0.858165041623	0.603603930992
H322	H	0.711759656611	0.358165041619	0.396396069008
H323	H	0.446936676864	0.847334896733	0.722961381641
H324	H	0.553063323137	0.347334896729	0.277038618359
H325	H	0.568250850817	0.883114517139	0.719626082982
H326	H	0.431749149183	0.383114517135	0.280373917018
H327	H	0.515625215454	0.732408904278	0.749607515616
H328	H	0.484374784546	0.232408904275	0.250392484384
H329	H	0.591546667402	0.768112657230	0.759485860689
H330	H	0.408453332598	0.268112657227	0.240514139311
H331	H	0.474313449549	0.868535718664	0.774502279857
H332	H	0.525686550451	0.368535718661	0.225497720143
H333	H	0.493756881282	0.790030153925	0.801645105697
H334	H	0.506243118718	0.290030153921	0.198354894303
H335	H	0.525665637060	0.690126435242	0.689804797377
H336	H	0.474334362940	0.190126435239	0.310195202623
H337	H	0.657555791096	0.655971712518	0.678808114843
H338	H	0.342444208904	0.155971712515	0.321191885157
H339	H	0.572864891833	0.552459453886	0.686934998444
H340	H	0.427135108167	0.052459453882	0.313065001556
H341	H	0.620766288282	0.538013402480	0.649388238060
H342	H	0.379233711718	0.038013402476	0.350611761940
H343	H	0.542705900821	0.575148802615	0.645141333201
H344	H	0.457294099179	0.075148802612	0.354858666799
H345	H	0.542642373571	0.728601668040	0.619244866901
H346	H	0.457357626429	0.228601668037	0.380755133099
H347	H	0.624748495275	0.699175375848	0.558367640391
H348	H	0.375251504725	0.199175375845	0.441632359609
H349	H	0.508661286699	0.800830654327	0.572945157893
H350	H	0.491338713302	0.300830654323	0.427054842107
H351	H	0.548054389731	0.802479402190	0.532521380159
H352	H	0.451945610269	0.302479402186	0.467478619841
H353	H	0.489657942082	0.657269987207	0.564618731054
H354	H	0.510342057919	0.157269987203	0.435381268946

H355	H	0.403912959467	0.752554913411	0.553495987965
H356	H	0.596087040534	0.252554913408	0.446504012035
H357	H	0.399386359923	0.676165954751	0.523150378403
H358	H	0.600613640077	0.176165954747	0.476849621597
H359	H	0.432058273096	0.766622069179	0.510544413641
H360	H	0.567941726904	0.266622069176	0.489455586358
H361	H	0.499039195318	0.603380933551	0.504406070925
H362	H	0.500960804682	0.103380933548	0.495593929075
H363	H	0.574401097157	0.628001074138	0.520820453507
H364	H	0.425598902843	0.128001074135	0.479179546493
H365	H	0.536760595589	0.689516859859	0.490517175637
H366	H	0.463239404411	0.189516859856	0.509482824363
H367	H	0.601485906625	0.850427376642	0.619394132198
H368	H	0.398514093375	0.350427376638	0.380605867802
H369	H	0.688252042503	0.948892899529	0.580508429915
H370	H	0.311747957497	0.448892899525	0.419491570085
H371	H	0.634930354506	0.963677599734	0.654454291533
H372	H	0.365069645494	0.463677599731	0.345545708467
H373	H	0.678254351218	0.036048005995	0.632008651158
H374	H	0.321745648782	0.536048005992	0.367991348842
H375	H	0.710846249446	0.804243471993	0.640292016279
H376	H	0.289153750554	0.304243471990	0.359707983721
H377	H	0.842163172011	0.839437654197	0.656275572625
H378	H	0.157836827989	0.339437654193	0.343724427375
H379	H	0.779339108041	0.747041257048	0.691858915730
H380	H	0.220660891959	0.247041257045	0.308141084270
H381	H	0.846599763012	0.700630554402	0.672664459426
H382	H	0.153400236988	0.200630554399	0.327335540574
H383	H	0.769148556224	0.685593843906	0.655081247891
H384	H	0.230851443776	0.185593843903	0.344918752108
H385	H	0.775761328229	0.712944587543	0.589471772729
H386	H	0.224238671771	0.212944587539	0.410528227271
H387	H	0.904028857344	0.694810132940	0.560334366699
H388	H	0.095971142656	0.194810132937	0.439665633300
H389	H	0.850018974823	0.648428207063	0.508024082590
H390	H	0.149981025177	0.148428207060	0.491975917410
H391	H	0.739766280451	0.640173021868	0.511158894275
H392	H	0.260233719549	0.140173021865	0.488841105725
H393	H	0.876019643694	0.552316654676	0.553319710579
H394	H	0.123980356306	0.052316654673	0.446680289421
H395	H	0.801930224909	0.528995861136	0.534469694265
H396	H	0.198069775091	0.028995861133	0.465530305735
H397	H	0.803968884943	0.572468111043	0.576197753843
H398	H	0.196031115057	0.072468111040	0.423802246157
H399	H	0.781398646902	0.833791908700	0.545879567127
H400	H	0.218601353098	0.333791908697	0.454120432873
H401	H	0.834175752263	0.904493598807	0.487554514534
H402	H	0.165824247737	0.404493598803	0.512445485466
H403	H	0.731691623562	0.933657938697	0.521765767534
H404	H	0.268308376438	0.433657938693	0.478234232466
H405	H	0.777450295445	0.984553907553	0.551959700475
H406	H	0.222549704556	0.484553907550	0.448040299525
H407	H	0.752256099154	0.982211418466	0.454142542537
H408	H	0.247743900846	0.482211418463	0.545857457463
H409	H	0.777011204366	0.119693217808	0.546002634135
H410	H	0.222988795634	0.619693217805	0.453997365865
H411	H	0.738872463698	0.100627748576	0.419708543514
H412	H	0.261127536302	0.600627748573	0.580291456486
H413	H	0.763993622193	0.238283026341	0.511631415691
H414	H	0.236006377807	0.738283026337	0.488368584309
H415	H	0.756857508358	0.233556959866	0.420620459252
H416	H	0.243142491642	0.733556959863	0.579379540747
H417	H	0.894213877786	0.914338331793	0.572121894610

H418	H	0.105786122214	0.414338331789	0.427878105389
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H420	H	0.012770308409	0.533282174189	0.451581452343
H421	H	0.979436568506	0.080394295641	0.610406995221
H422	H	0.020563431494	0.580394295638	0.389593004779
H423	H	0.870808432487	0.984121865889	0.619242106078
H424	H	0.129191567513	0.484121865885	0.380757893922
H425	H	0.908322825874	0.135512310712	0.561552034570
H426	H	0.091677174126	0.635512310709	0.438447965430
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H428	H	0.118983414454	0.649478051405	0.395138637988
H429	H	0.846554262849	0.076319037813	0.578455965771
H430	H	0.153445737151	0.576319037810	0.421544034229
H431	H	0.981614778581	0.850513928402	0.583247357622
H432	H	0.018385221419	0.350513928398	0.416752642378
H433	H	0.065571520647	0.777780921987	0.607296788423
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H435	H	0.112739844708	0.862665547030	0.610624283032
H436	H	0.887260155292	0.362665547027	0.389375716968
H437	H	0.965267555627	0.902784367350	0.642020458822
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H439	H	0.001048548262	0.882749002365	0.715227136771
H440	H	0.998951451738	0.382749002362	0.284772863229
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H442	H	0.128492354951	0.421660950108	0.316914176057
H443	H	0.890377051626	0.923911591023	0.727730760129
H444	H	0.109622948374	0.423911591020	0.272269239870
H445	H	0.920487308933	0.815958459022	0.750369857799
H446	H	0.079512691067	0.315958459018	0.249630142201
H447	H	0.906054895620	0.656146770550	0.723516441315
H448	H	0.093945104380	0.156146770547	0.276483558685
H449	H	0.967561062594	0.606073508170	0.766348359182
H450	H	0.032438937406	0.106073508167	0.233651640818
H451	H	0.948654517554	0.752034186644	0.809890648140
H452	H	0.051345482446	0.252034186641	0.190109351860
H453	H	0.912473913364	0.662313148782	0.817709924287
H454	H	0.087526086636	0.162313148779	0.182290075713
H455	H	0.068497192214	0.681963804041	0.768533190157
H456	H	0.931502807786	0.181963804037	0.231466809843
H457	H	0.027780680420	0.766262908281	0.757472738889
H458	H	0.972219319580	0.266262908278	0.242527261111
H459	H	0.034708908648	0.690037878405	0.726935683176
H460	H	0.965291091352	0.190037878402	0.273064316824
H461	H	0.021429849088	0.604100209385	0.829566206002
H462	H	0.978570150912	0.104100209382	0.170433793998
H463	H	0.998721255384	0.677968772071	0.858811865653
H464	H	0.001278744616	0.177968772067	0.141188134347
H465	H	0.055138123675	0.697245098492	0.825471723048
H466	H	0.944861876325	0.197245098489	0.174528276951
H467	H	0.842316028925	0.577934155939	0.764834153591
H468	H	0.157683971075	0.077934155935	0.235165846409
H469	H	0.779259287034	0.673572461777	0.816266273751
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H471	H	0.702811221599	0.534582980480	0.794310905322
H472	H	0.297188778401	0.034582980477	0.205689094678
H473	H	0.679603511663	0.693539197204	0.763275517739
H474	H	0.320396488337	0.193539197201	0.236724482261
H475	H	0.710637719191	0.614138401403	0.740721820407
H476	H	0.289362280809	0.114138401399	0.259278179593
H477	H	0.686861073602	0.601618772681	0.852237133683
H478	H	0.313138926398	0.101618772678	0.147762866317
H479	H	0.617695720343	0.596613272180	0.826718608443
H480	H	0.382304279657	0.096613272177	0.173281391556

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H482	H	0.340123561822	0.185050027454	0.170844436316
H483	H	0.611370312703	0.536807984241	0.754100572951
H484	H	0.388629687297	0.036807984238	0.245899427049
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H487	H	0.577919912748	0.617241534111	0.775882265369
H488	H	0.422080087252	0.117241534108	0.224117734631
H489	H	0.795954838722	0.623384683294	0.867215624516
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H491	H	0.829354203947	0.457599190378	0.869514029184
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H495	H	0.892884512977	0.648454799693	0.898211307995
H496	H	0.107115487024	0.148454799689	0.101788692005
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H498	H	0.163960736954	0.125569470177	0.069722276714
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H501	H	0.943456595480	0.533239826927	0.861404080088
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H506	H	0.079109818891	0.092149867907	0.027610356608
H507	H	0.934774169766	0.686172383865	0.954073058505
H508	H	0.065225830234	0.186172383861	0.045926941495
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H527	H	0.692633547332	0.562672593580	0.027487216636
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H535	H	0.719438982848	0.806419967760	0.025799559377
H536	H	0.280561017152	0.306419967757	0.974200440623
H537	H	0.779896238236	0.872335542247	0.038573643762
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H540	H	0.241898441835	0.295023553378	0.933414965822
H541	H	0.918608174493	0.695340465845	0.003660649748
H542	H	0.081391825507	0.195340465842	0.996339350252
H543	H	0.998624620510	0.789111196243	0.050622576968

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H545	H	0.029266969721	0.627764404421	0.022969580621
H546	H	0.970733030279	0.127764404417	0.977030419379
H547	H	0.948007271617	0.641722822026	0.069981775297
H548	H	0.051992728383	0.141722822022	0.930018224703
H549	H	0.126460181974	0.704800024399	0.035688346779
H550	H	0.873539818026	0.204800024396	0.964311653221
H551	H	0.115811339233	0.630152970269	0.067025315517
H552	H	0.884188660767	0.130152970266	0.932974684483
H553	H	0.095494449433	0.726021901897	0.078437296804
H554	H	0.904505550567	0.226021901893	0.921562703196
H555	H	0.015198647156	0.884404288320	0.009127869354
H556	H	0.984801352844	0.384404288316	0.990872130646
H557	H	0.059112604169	0.834889008864	0.939931274309
H558	H	0.940887395831	0.334889008861	0.060068725691
H559	H	0.039097899920	0.999192086883	0.967185228331
H560	H	0.960902100080	0.499192086879	0.032814771669
H561	H	0.066582299264	0.973476642290	0.924963725620
H562	H	0.933417700736	0.473476642287	0.075036274380
H563	H	0.251876872340	0.863837962216	0.988329200197
H564	H	0.748123127660	0.363837962213	0.011670799803
H565	H	0.311161233459	0.752425951167	0.942396347247
H566	H	0.688838766541	0.252425951164	0.057603652753
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H568	H	0.722287676126	0.231720313739	0.016060767822
H569	H	0.229571124333	0.680485522643	0.918189410242
H570	H	0.770428875667	0.180485522639	0.081810589758
H571	H	0.186820548124	0.676960818018	0.958804522053
H572	H	0.813179451876	0.176960818015	0.041195477947
H573	H	0.180394866151	0.800625730408	0.902587913692
H574	H	0.819605133849	0.300625730404	0.097412086308
H575	H	0.117802401523	0.759536167554	0.928591479150
H576	H	0.882197598477	0.259536167550	0.071408520850
H577	H	0.362387587630	0.894368529399	0.966528559506
H578	H	0.637612412370	0.394368529396	0.033471440494
H579	H	0.356936871541	0.022288383500	0.925105291661
H580	H	0.643063128459	0.522288383496	0.074894708339
H581	H	0.427085175119	0.969348915013	0.933593803213
H582	H	0.572914824881	0.469348915010	0.066406196787
H583	H	0.355677190841	0.836208238825	0.888831004957
H584	H	0.644322809159	0.336208238821	0.111168995043
H585	H	0.410209435992	0.885252276044	0.822330181444
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H587	H	0.367208765183	0.755335237634	0.803834432848
H588	H	0.632791234817	0.255335237631	0.196165567152
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H590	H	0.575665773392	0.250877523847	0.162873319510
H591	H	0.260573125613	0.828681857556	0.856058252036
H592	H	0.739426874387	0.328681857553	0.143941747963
H593	H	0.200091373597	0.929097378208	0.802241384408
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H595	H	0.140307538579	0.796307255734	0.843261368543
H596	H	0.859692461421	0.296307255730	0.156738631457
H597	H	0.100594288821	0.854638568135	0.812776063693
H598	H	0.899405711179	0.354638568131	0.187223936307
H599	H	0.227804602382	0.705384807549	0.823061364925
H600	H	0.772195397618	0.205384807546	0.176938635075
H601	H	0.125309665070	0.844206291433	0.749774446313
H602	H	0.874690334931	0.344206291430	0.250225553687
H603	H	0.276896049650	0.632921369330	0.775178391819
H604	H	0.723103950351	0.132921369327	0.224821608181
H605	H	0.168290339039	0.767346798367	0.701773154810
H606	H	0.831709660961	0.267346798363	0.298226845190

H607	H	0.232199085351	0.663494224310	0.687705831582
H608	H	0.767800914649	0.163494224306	0.312294168418
H609	H	0.241054912938	0.024819106732	0.835992202714
H610	H	0.758945087062	0.524819106729	0.164007797286
H611	H	0.210967567796	0.038120132417	0.906941098178
H612	H	0.789032432204	0.538120132413	0.093058901822
H613	H	0.307744982838	0.094108069767	0.876837891558
H614	H	0.692255017162	0.594108069763	0.123162108442
H615	H	0.266988018608	0.163921939374	0.902822628003
H616	H	0.733011981392	0.663921939371	0.097177371997
H617	H	0.258276675413	0.164966266547	0.856850819416
H618	H	0.741723324587	0.664966266544	0.143149180584
H619	H	0.121880110452	0.110654317165	0.836978492654
H620	H	0.878119889548	0.610654317162	0.163021507346
H621	H	0.068405133398	0.228270687678	0.885803176482
H622	H	0.931594866602	0.728270687674	0.114196823518
H623	H	0.091467816309	0.241934361313	0.806899972513
H624	H	0.908532183691	0.741934361309	0.193100027487
H625	H	0.064327069911	0.315502560316	0.835464267078
H626	H	0.935672930089	0.815502560313	0.164535732922
H627	H	0.146529204762	0.321156566287	0.891376326779
H628	H	0.853470795238	0.821156566283	0.108623673221
H629	H	0.223774570705	0.329941195644	0.875244317314
H630	H	0.776225429295	0.829941195641	0.124755682685
C1	C	0.669048416985	0.773316205126	0.903978490027
C2	C	0.330951583015	0.273316205122	0.096021509973
C3	C	0.720386258740	0.778612711599	0.875940724412
C4	C	0.279613741260	0.278612711596	0.124059275588
C5	C	0.691306001128	0.817407063196	0.937210171067
C6	C	0.308693998872	0.317407063193	0.062789828933
C7	C	0.683702918126	0.904059695902	0.933369417756
C8	C	0.316297081874	0.404059695899	0.066630582244
C9	C	0.764564485202	0.858324297621	0.830111288910
C10	C	0.235435514798	0.358324297617	0.169888711090
C11	C	0.819272347691	0.900964061514	0.847771878587
C12	C	0.180727652309	0.400964061510	0.152228121413
C13	C	0.737021509070	0.906261210017	0.799698665382
C14	C	0.262978490930	0.406261210013	0.200301334617
C15	C	0.702554906941	0.852394468981	0.774672751705
C16	C	0.297445093059	0.352394468978	0.225327248295
C17	C	0.936516285810	0.919823117015	0.840962497825
C18	C	0.063483714190	0.419823117012	0.159037502175
C19	C	0.969940676551	0.933448264646	0.805911498204
C20	C	0.030059323449	0.433448264642	0.194088501796
C21	C	0.980312197862	0.870911083841	0.863997692831
C22	C	0.019687802138	0.370911083838	0.136002307169
C23	C	0.031881060352	0.020733125233	0.770374776987
C24	C	0.968118939648	0.520733125230	0.229625223013
C25	C	0.104077147627	0.030915272805	0.770308783300
C26	C	0.895922852373	0.530915272802	0.229691216699
C27	C	0.999575088459	0.096568086191	0.759792006318
C28	C	0.000424911541	0.596568086187	0.240207993681
C29	C	0.205020081229	0.011636737783	0.738515086904
C30	C	0.794979918771	0.511636737780	0.261484913096
C31	C	0.233372976833	0.092282995653	0.739837880086
C32	C	0.766627023167	0.592282995650	0.260162119914
C33	C	0.218960022245	0.971435110007	0.703486395359
C34	C	0.781039977755	0.471435110003	0.296513604641
C35	C	0.158987800900	0.986724335042	0.682305339972
C36	C	0.841012199100	0.486724335039	0.317694660028
C37	C	0.105751436117	0.979555517173	0.708886103154
C38	C	0.894248563883	0.479555517169	0.291113896846
C39	C	0.218167746827	0.230649349752	0.736471752801

C40	C	0.781832253173	0.730649349748	0.263528247199
C41	C	0.161395191361	0.283484119851	0.742307245710
C42	C	0.838604808639	0.783484119847	0.257692754289
C43	C	0.253702381493	0.255805597103	0.703520856935
C44	C	0.746297618507	0.755805597100	0.296479143065
C45	C	0.127979849768	0.414643841451	0.756614097167
C46	C	0.872020150232	0.914643841448	0.243385902833
C47	C	0.091610055069	0.433979236646	0.723265380776
C48	C	0.908389944931	0.933979236642	0.276734619223
C49	C	0.157492556087	0.485698278014	0.774735854485
C50	C	0.842507443914	0.985698278011	0.225264145515
C51	C	0.175667180407	0.464279808977	0.812291145632
C52	C	0.824332819593	0.964279808973	0.187708854368
C53	C	0.111892995502	0.553585910199	0.773003932555
C54	C	0.888107004498	0.053585910195	0.226996067445
C55	C	0.205461897146	0.527889395071	0.834239877685
C56	C	0.794538102854	0.027889395068	0.165760122315
C57	C	0.093658725509	0.455288220204	0.660579990526
C58	C	0.906341274491	0.955288220200	0.339420009474
C59	C	0.057565948429	0.383247485487	0.648883427738
C60	C	0.942434051571	0.883247485483	0.351116572262
C61	C	0.139108872202	0.488103524748	0.632461102965
C62	C	0.860891127798	0.988103524744	0.367538897035
C63	C	0.110013361458	0.483410449502	0.596055819568
C64	C	0.889986638542	0.983410449499	0.403944180432
C65	C	0.156967663515	0.571097030707	0.642259863931
C66	C	0.843032336485	0.071097030704	0.357740136068
C67	C	0.043227847487	0.245486587315	0.648842711955
C68	C	0.956772152513	0.745486587312	0.351157288045
C69	C	0.979570630562	0.252250857443	0.668191303736
C70	C	0.020429369438	0.752250857439	0.331808696264
C71	C	0.077303930920	0.170856528717	0.657992249316
C72	C	0.922696069080	0.670856528713	0.342007750684
C73	C	0.922550606168	0.291783066580	0.720676896107
C74	C	0.077449393832	0.791783066577	0.279323103893
C75	C	0.881159962104	0.354080395942	0.703320245441
C76	C	0.118840037896	0.854080395938	0.296679754559
C77	C	0.936039479509	0.308985643988	0.759107227539
C78	C	0.063960520491	0.808985643985	0.240892772461
C79	C	0.875730110829	0.322215413123	0.780972591849
C80	C	0.124269889171	0.822215413119	0.219027408151
C81	C	0.831439556722	0.252937114990	0.786250109234
C82	C	0.168560443278	0.752937114987	0.213749890766
C83	C	0.825600795076	0.138466745775	0.824689483362
C84	C	0.174399204924	0.638466745771	0.175310516637
C85	C	0.871042938059	0.476413344105	0.672640529977
C86	C	0.128957061941	0.976413344102	0.327359470023
C87	C	0.835284722374	0.439790544510	0.641917461819
C88	C	0.164715277626	0.939790544506	0.358082538181
C89	C	0.912809979855	0.541696569324	0.658205112704
C90	C	0.087190020145	0.041696569320	0.341794887296
C91	C	0.848341704289	0.363164253864	0.588887841256
C92	C	0.151658295711	0.863164253860	0.411112158744
C93	C	0.797848478754	0.300444560274	0.596305418399
C94	C	0.202151521247	0.800444560271	0.403694581601
C95	C	0.905006128587	0.333550660599	0.567273119476
C96	C	0.094993871413	0.833550660596	0.432726880523
C97	C	0.950694122431	0.399281655579	0.556804748062
C98	C	0.049305877569	0.899281655576	0.443195251938
C99	C	0.767196690947	0.199548322013	0.638600828348
C100	C	0.232803309054	0.699548322009	0.361399171652
C101	C	0.704634412469	0.237839425728	0.649618884513
C102	C	0.295365587531	0.737839425724	0.350381115487

C103	C	0.800802253886	0.161543421980	0.669817396645
C104	C	0.199197746114	0.661543421977	0.330182603355
C105	C	0.758151688060	0.115764757067	0.693451098725
C106	C	0.241848311941	0.615764757063	0.306548901275
C107	C	0.722369678286	0.152442136657	0.719535858251
C108	C	0.277630321715	0.652442136653	0.280464141749
C109	C	0.753595259308	0.035851368443	0.689760087326
C110	C	0.246404740692	0.535851368440	0.310239912674
C111	C	0.681909814891	0.109559511727	0.740820031417
C112	C	0.318090185109	0.609559511724	0.259179968583
C113	C	0.713115101699	0.992952757411	0.711089047374
C114	C	0.286884898301	0.492952757407	0.288910952626
C115	C	0.676897539902	0.029910525247	0.736583261664
C116	C	0.323102460098	0.529910525244	0.263416738336
C117	C	0.654611605988	0.345867549420	0.679834461874
C118	C	0.345388394012	0.845867549416	0.320165538126
C119	C	0.611659110938	0.374249481082	0.650362528401
C120	C	0.388340889062	0.874249481078	0.349637471599
C121	C	0.675072724892	0.414139430949	0.702145747311
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C123	C	0.706155100720	0.391244802803	0.736403422362
C124	C	0.293844899281	0.891244802799	0.263596577638
C125	C	0.605615193983	0.419459449708	0.590389442052
C126	C	0.394384806017	0.919459449704	0.409610557948
C127	C	0.569989417612	0.348680236140	0.576877067838
C128	C	0.430010582388	0.848680236136	0.423122932161
C129	C	0.649117931079	0.456619187978	0.562560083168
C130	C	0.350882068921	0.956619187975	0.437439916832
C131	C	0.618869021309	0.453519957637	0.526583921443
C132	C	0.381130978691	0.953519957634	0.473416078557
C133	C	0.663985322510	0.539113766767	0.573573124437
C134	C	0.336014677490	0.039113766763	0.426426875563
C135	C	0.572819830231	0.210259491150	0.566864670315
C136	C	0.427180169769	0.710259491146	0.433135329685
C137	C	0.515684733230	0.192432954295	0.590914997880
C138	C	0.484315266770	0.692432954292	0.409085002120
C139	C	0.624377472452	0.147890547199	0.565981293483
C140	C	0.375622527548	0.647890547196	0.434018706516
C141	C	0.470103509773	0.182437148266	0.648722470540
C142	C	0.529896490227	0.682437148263	0.351277529460
C143	C	0.413783282914	0.237927883094	0.643976924917
C144	C	0.586216717086	0.737927883090	0.356023075083
C145	C	0.490630211764	0.183596831767	0.687073760271
C146	C	0.509369788236	0.683596831764	0.312926239728
C147	C	0.543888174175	0.127301102268	0.697273480280
C148	C	0.456111825825	0.627301102264	0.302726519720
C149	C	0.527456012329	0.041065002889	0.700388106962
C150	C	0.472543987671	0.541065002886	0.299611893038
C151	C	0.442516412685	0.016954672345	0.745110995336
C152	C	0.557483587315	0.516954672341	0.254889004664
C153	C	0.380978748689	0.373167157621	0.635465617822
C154	C	0.619021251311	0.873167157617	0.364534382178
C155	C	0.316213949430	0.351867454360	0.620263729994
C156	C	0.683786050570	0.851867454357	0.379736270006
C157	C	0.406514285750	0.446082502588	0.616712997811
C158	C	0.593485714250	0.946082502585	0.383287002189
C159	C	0.404665269644	0.520490502952	0.638331990057
C160	C	0.595334730356	0.020490502949	0.361668009943
C161	C	0.430898445837	0.586613954134	0.616061267223
C162	C	0.569101554163	0.086613954131	0.383938732777
C163	C	0.338221226928	0.540551816366	0.652348922995
C164	C	0.661778773072	0.040551816363	0.347651077005
C165	C	0.248989884212	0.308826310073	0.572757576497

C166	C	0.751010115788	0.808826310069	0.427242423503
C167	C	0.214859468763	0.236197988022	0.586098852249
C168	C	0.785140531237	0.736197988019	0.413901147751
C169	C	0.264639701068	0.300319271272	0.533989673920
C170	C	0.735360298933	0.800319271268	0.466010326080
C171	C	0.330672510494	0.263573900742	0.533726039802
C172	C	0.669327489507	0.763573900739	0.466273960198
C173	C	0.364494404088	0.305370705825	0.563229428891
C174	C	0.635505595912	0.805370705822	0.436770571109
C175	C	0.224273234959	0.115447620945	0.618449298602
C176	C	0.775726765041	0.615447620942	0.381550701398
C177	C	0.264319562004	0.043679307684	0.612926934845
C178	C	0.735680437996	0.543679307681	0.387073065155
C179	C	0.360510509220	0.985084666728	0.591630483995
C180	C	0.639489490780	0.485084666724	0.408369516005
C181	C	0.380905541646	0.952657199607	0.626899670828
C182	C	0.619094458354	0.452657199603	0.373100329172
C183	C	0.419946610758	0.006416345380	0.569977375319
C184	C	0.580053389242	0.506416345377	0.430022624681
C185	C	0.450887066438	0.933950775067	0.555750747223
C186	C	0.549112933562	0.433950775064	0.444249252777
C187	C	0.389106083150	0.847209410044	0.667707774206
C188	C	0.610893916850	0.347209410041	0.332292225794
C189	C	0.461593987607	0.841678461553	0.671003227916
C190	C	0.538406012393	0.341678461550	0.328996772084
C191	C	0.358532302293	0.766367905044	0.669414798501
C192	C	0.641467697707	0.266367905041	0.330585201499
C193	C	0.302005830969	0.772508606963	0.644717536184
C194	C	0.697994169032	0.272508606960	0.355282463816
C195	C	0.326531660225	0.825334165325	0.615754472084
C196	C	0.673468339775	0.325334165321	0.384245527916
C197	C	0.545228007399	0.826590698860	0.717182416486
C198	C	0.454771992601	0.326590698856	0.282817583514
C199	C	0.588221886223	0.781119562346	0.692050624318
C200	C	0.411778113777	0.281119562342	0.307949375682
C201	C	0.543078751191	0.785967477475	0.752841635087
C202	C	0.456921248809	0.285967477471	0.247158364913
C203	C	0.513730426001	0.831853716214	0.783315173511
C204	C	0.486269573999	0.331853716210	0.216684826489
C205	C	0.562175773074	0.880799110606	0.803449812011
C206	C	0.437824226926	0.380799110602	0.196550187989
C207	C	0.612825400625	0.657304491894	0.664215562470
C208	C	0.387174599375	0.157304491891	0.335784437530
C209	C	0.631799678964	0.686304756870	0.627976599850
C210	C	0.368200321036	0.186304756867	0.372023400150
C211	C	0.585293534335	0.576078140448	0.661358180888
C212	C	0.414706465665	0.076078140445	0.338641819111
C213	C	0.598436366261	0.743160006479	0.572998390268
C214	C	0.401563633739	0.243160006475	0.427001609732
C215	C	0.644274169245	0.811614100474	0.574481954171
C216	C	0.355725830755	0.311614100471	0.425518045829
C217	C	0.536373124325	0.765122618052	0.554794682741
C218	C	0.463626875675	0.265122618049	0.445205317259
C219	C	0.495706801039	0.696763987351	0.542476489417
C220	C	0.504293198961	0.196763987348	0.457523510582
C221	C	0.429266827645	0.724430264122	0.531890708147
C222	C	0.570733172355	0.224430264119	0.468109291852
C223	C	0.528275963126	0.652105427232	0.513157825617
C224	C	0.471724036874	0.152105427229	0.486842174383
C225	C	0.679345816281	0.924414563276	0.606361780808
C226	C	0.320654183720	0.424414563272	0.393638219192
C227	C	0.746096371170	0.902211568009	0.618958273157
C228	C	0.253903628830	0.402211568006	0.381041726843

C229	C	0.647179339648	0.985961770077	0.628534609346
C230	C	0.352820660353	0.485961770074	0.371465390654
C231	C	0.811739387328	0.797214833939	0.643423788557
C232	C	0.188260612672	0.297214833936	0.356576211443
C233	C	0.849179094535	0.777508999501	0.610070661546
C234	C	0.150820905465	0.277508999497	0.389929338454
C235	C	0.800810600273	0.727841354044	0.667214607406
C236	C	0.199189399727	0.227841354040	0.332785392594
C237	C	0.855802252468	0.714546725993	0.554076987376
C238	C	0.144197747532	0.214546725990	0.445923012624
C239	C	0.867555108416	0.787058145234	0.531802733857
C240	C	0.132444891585	0.287058145231	0.468197266143
C241	C	0.823770692374	0.650646246568	0.532941159799
C242	C	0.176229307626	0.150646246565	0.467058840201
C243	C	0.826754654280	0.572126909233	0.550430038422
C244	C	0.173245345720	0.072126909229	0.449569961578
C245	C	0.832195741174	0.916685504839	0.515569483661
C246	C	0.167804258826	0.416685504836	0.484430516339
C247	C	0.895103953206	0.958467114083	0.523185437539
C248	C	0.104896046794	0.458467114079	0.476814562461
C249	C	0.774688349393	0.969307776274	0.524347347492
C250	C	0.225311650607	0.469307776271	0.475652652508
C251	C	0.767360468365	0.041417294662	0.502819842037
C252	C	0.232639531635	0.541417294659	0.497180157963
C253	C	0.755636121030	0.037948363767	0.467129887952
C254	C	0.244363878970	0.537948363764	0.532870112047
C255	C	0.769327711244	0.114575350445	0.518168434799
C256	C	0.230672288756	0.614575350442	0.481831565201
C257	C	0.748083879195	0.104720798652	0.447497887562
C258	C	0.251916120805	0.604720798649	0.552502112438
C259	C	0.761938155534	0.182084039946	0.498991725031
C260	C	0.238061844466	0.682084039942	0.501008274969
C261	C	0.752468894662	0.177157408552	0.463252956126
C262	C	0.247531105339	0.677157408548	0.536747043874
C263	C	0.968819894284	0.997370481505	0.569674313491
C264	C	0.031180105716	0.497370481502	0.430325686509
C265	C	0.025931692598	0.956237066462	0.586074796405
C266	C	0.974068307402	0.456237066459	0.413925203595
C267	C	0.939858872201	0.049104050412	0.598455966964
C268	C	0.060141127799	0.549104050409	0.401544033036
C269	C	0.890986347772	0.106010362260	0.585042840348
C270	C	0.109013652228	0.606010362256	0.414957159651
C271	C	0.064399284641	0.839459704469	0.613716283962
C272	C	0.935600715359	0.339459704465	0.386283716038
C273	C	0.047398429663	0.844018366291	0.652487503578
C274	C	0.952601570337	0.344018366287	0.347512496422
C275	C	0.964818455285	0.874011409011	0.695241960071
C276	C	0.035181544715	0.374011409008	0.304758039928
C277	C	0.942884356491	0.788776446580	0.700475796128
C278	C	0.057115643509	0.288776446576	0.299524203872
C279	C	0.910097774353	0.931596143020	0.701571154309
C280	C	0.089902225647	0.431596143017	0.298428845691
C281	C	0.908556072169	0.696171592884	0.745406750364
C282	C	0.091443927831	0.196171592881	0.254593249636
C283	C	0.846786532347	0.695586664356	0.765864298495
C284	C	0.153213467653	0.195586664353	0.234135701505
C285	C	0.965586725742	0.669381315994	0.768960443484
C286	C	0.034413274258	0.169381315990	0.231039556516
C287	C	0.956231356917	0.689534590233	0.807710233166
C288	C	0.043768643083	0.189534590230	0.192289766834
C289	C	0.027381783385	0.703419898525	0.754517043893
C290	C	0.972618216615	0.203419898521	0.245482956107
C291	C	0.010920646808	0.666039876854	0.831502300767

C292	C	0.989079353192	0.166039876850	0.168497699233
C293	C	0.777095593447	0.618210060086	0.802659301661
C294	C	0.222904406553	0.118210060083	0.197340698339
C295	C	0.805728816555	0.554264125246	0.824822492051
C296	C	0.194271183445	0.054264125242	0.175177507949
C297	C	0.705789079168	0.597660765130	0.796375492205
C298	C	0.294210920832	0.097660765127	0.203624507795
C299	C	0.679023448102	0.630096332739	0.762476124796
C300	C	0.320976551898	0.130096332735	0.237523875204
C301	C	0.665552123079	0.621948634035	0.828010205856
C302	C	0.334447876921	0.121948634031	0.171989794144
C303	C	0.611941523307	0.600204665498	0.755489342837
C304	C	0.388058476694	0.100204665495	0.244510657163
C305	C	0.821907309745	0.510801876981	0.884410820818
C306	C	0.178092690255	0.010801876978	0.115589179182
C307	C	0.761184399708	0.502391581809	0.906088549445
C308	C	0.238815600292	0.002391581806	0.093911450555
C309	C	0.881758370968	0.525636425501	0.906975616780
C310	C	0.118241629032	0.025636425498	0.093024383220
C311	C	0.883439972291	0.609372810924	0.920222732119
C312	C	0.116560027709	0.109372810921	0.079777267881
C313	C	0.941247058361	0.502215249931	0.886280688475
C314	C	0.058752941639	0.002215249928	0.113719311525
C315	C	0.932548464659	0.624211076236	0.948411175317
C316	C	0.067451535341	0.124211076233	0.051588824683
C317	C	0.692124467337	0.423889618371	0.942384239669
C318	C	0.307875532663	0.923889618367	0.057615760331
C319	C	0.685256169595	0.476176644384	0.974563661949
C320	C	0.314743830405	0.976176644380	0.025436338051
C321	C	0.690651725094	0.336235911186	0.949472764649
C322	C	0.309348274906	0.836235911183	0.050527235351
C323	C	0.760029194653	0.309443291141	0.945639250588
C324	C	0.239970805347	0.809443291137	0.054360749412
C325	C	0.788058315858	0.362828706684	0.917936730816
C326	C	0.211941684142	0.862828706681	0.082063269184
C327	C	0.740737793829	0.559812100892	0.016172607306
C328	C	0.259262206171	0.059812100888	0.983827392694
C329	C	0.758072566442	0.641940281776	0.005035616329
C330	C	0.241927433558	0.141940281773	0.994964383671
C331	C	0.815242260196	0.760556551911	0.022170672230
C332	C	0.184757739804	0.260556551908	0.977829327770
C333	C	0.882335793825	0.775862723719	0.037144751231
C334	C	0.117664206175	0.275862723716	0.962855248769
C335	C	0.764987733867	0.811700571406	0.039335159279
C336	C	0.235012266133	0.311700571403	0.960664840721
C337	C	0.997026564024	0.744098110909	0.030595644990
C338	C	0.002973435976	0.244098110906	0.969404355010
C339	C	0.030982326716	0.770386527188	0.997122371348
C340	C	0.969017673284	0.270386527185	0.002877628652
C341	C	0.027968873954	0.669518699624	0.044717117574
C342	C	0.972031126046	0.169518699621	0.955282882426
C343	C	0.095779025926	0.684126751665	0.056935764624
C344	C	0.904220974074	0.184126751661	0.943064235376
C345	C	0.065048177221	0.877728421340	0.960407425148
C346	C	0.934951822779	0.377728421337	0.039592574852
C347	C	0.135643738686	0.886294987901	0.969894633729
C348	C	0.864356261314	0.386294987897	0.030105366271
C349	C	0.037971240295	0.953820456402	0.947227122531
C350	C	0.962028759705	0.453820456399	0.052772877469
C351	C	0.245986821349	0.841560215246	0.962063449837
C352	C	0.754013178651	0.341560215243	0.037936550163
C353	C	0.280956271170	0.896493956460	0.937208208751
C354	C	0.719043728830	0.396493956456	0.062791791249

C355	C	0.267845702724	0.756423019889	0.958266583070
C356	C	0.732154297276	0.256423019885	0.041733416930
C357	C	0.212213656559	0.714389929115	0.940306656950
C358	C	0.787786343441	0.214389929111	0.059693343050
C359	C	0.167323871935	0.778312041171	0.928316910188
C360	C	0.832676128065	0.278312041168	0.071683089812
C361	C	0.379009724018	0.964994646293	0.922805775503
C362	C	0.620990275982	0.464994646290	0.077194224497
C363	C	0.384971078241	0.949516387281	0.883707148754
C364	C	0.615028921759	0.449516387278	0.116292851245
C365	C	0.371310618042	0.857166027014	0.836457886262
C366	C	0.628689381958	0.357166027011	0.163542113738
C367	C	0.309935281844	0.892676880125	0.821387517925
C368	C	0.690064718156	0.392676880122	0.178612482074
C369	C	0.375403496207	0.769367942882	0.831287868153
C370	C	0.624596503793	0.269367942879	0.168712131847
C371	C	0.330502496709	0.717531625489	0.853613575112
C372	C	0.669497503291	0.217531625486	0.146386424888
C373	C	0.193199645854	0.896915329604	0.826425342861
C374	C	0.806800354146	0.396915329601	0.173574657139
C375	C	0.170185240053	0.954986707519	0.853851037994
C376	C	0.829814759947	0.454986707516	0.146148962006
C377	C	0.147230870853	0.830187207568	0.819394580286
C378	C	0.852769129147	0.330187207565	0.180605419714
C379	C	0.172736163075	0.780817871028	0.790160640985
C380	C	0.827263836925	0.280817871025	0.209839359015
C381	C	0.215517659371	0.720683318204	0.796567187532
C382	C	0.784482340629	0.220683318201	0.203432812468
C383	C	0.158390101016	0.797750137795	0.755623190258
C384	C	0.841609898985	0.297750137791	0.244376809742
C385	C	0.243133001270	0.678836370533	0.769534035249
C386	C	0.756866998730	0.178836370529	0.230465964751
C387	C	0.183773326415	0.755018235973	0.728203035633
C388	C	0.816226673586	0.255018235970	0.271796964367
C389	C	0.226335503645	0.695308937795	0.735340432748
C390	C	0.773664496355	0.195308937791	0.264659567252
C391	C	0.206543698096	0.072310791897	0.883160163523
C392	C	0.793456301904	0.572310791893	0.116839836477
C393	C	0.146054123026	0.119470213001	0.887708593298
C394	C	0.853945876974	0.619470212997	0.112291406702
C395	C	0.263434883135	0.127323042392	0.879653735219
C396	C	0.736565116865	0.627323042389	0.120346264781
C397	C	0.068705520345	0.203886789487	0.859569219591
C398	C	0.931294479655	0.703886789483	0.140430780409
C399	C	0.998505202330	0.185157064995	0.851928186983
C400	C	0.001494797670	0.685157064992	0.148071813017
C401	C	0.094458521620	0.263841649602	0.833566845443
C402	C	0.905541478380	0.763841649599	0.166433154557
C403	C	0.163735219819	0.284536736467	0.839814362724
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N2	N	0.339809699280	0.190765159748	0.086538729349
N3	N	0.714462147171	0.838142806474	0.854370408162
N4	N	0.285537852829	0.338142806471	0.145629591838
N5	N	0.876270312148	0.882617678980	0.833569609201
N6	N	0.123729687852	0.382617678976	0.166430390799
N7	N	0.008003342664	0.995258081245	0.803840669542
N8	N	0.991996657336	0.495258081242	0.196159330458
N9	N	0.135028380154	0.009625241029	0.740990425784
N10	N	0.864971619846	0.509625241026	0.259009574216
N11	N	0.194982277522	0.152487431653	0.733999655429
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N15	N	0.125874002526	0.442726419478	0.693613686624
N16	N	0.874125997474	0.942726419475	0.306386313376
N17	N	0.082157601179	0.313233541608	0.655786573741
N18	N	0.917842398821	0.813233541604	0.344213426259
N19	N	0.981046157966	0.277533096341	0.701315727318
N20	N	0.018953842034	0.777533096337	0.298684272682
N21	N	0.856766173099	0.200034440774	0.812274568898
N22	N	0.143233826901	0.700034440770	0.187725431102
N23	N	0.770341663816	0.115491907173	0.810738335542
N24	N	0.229658336184	0.615491907169	0.189261664458
N25	N	0.849412019420	0.102119616847	0.852428532500
N26	N	0.150587980580	0.602119616843	0.147571467500
N27	N	0.908240503795	0.419745720258	0.691959582872
N28	N	0.091759496205	0.919745720254	0.308040417128
N29	N	0.871370628791	0.395047843053	0.621396697377
N30	N	0.128629371209	0.895047843050	0.378603302623
N31	N	0.000038299285	0.380511616303	0.536077766951
N32	N	0.999961700715	0.880511616299	0.463922233049
N33	N	0.810912703344	0.255383566008	0.623674430262
N34	N	0.189087296656	0.755383566004	0.376325569738
N35	N	0.709825867179	0.304972889016	0.666586916237
N36	N	0.290174132821	0.804972889012	0.333413083763
N37	N	0.743751565377	0.447172274860	0.749807133183
N38	N	0.256248434623	0.947172274857	0.250192866817
N39	N	0.641318139884	0.400893814051	0.621633379729
N40	N	0.358681860116	0.900893814047	0.378366620271
N41	N	0.603581228897	0.282344042679	0.575904713648
N42	N	0.396418771103	0.782344042676	0.424095286352
N43	N	0.522548479414	0.201641235244	0.625247802055
N44	N	0.477451520586	0.701641235240	0.374752197945
N45	N	0.503539554433	0.017095308703	0.734598410960
N46	N	0.496460445567	0.517095308699	0.265401589040
N47	N	0.394373503707	0.019250649561	0.722585014892
N48	N	0.605626496294	0.519250649558	0.277414985108
N49	N	0.429093785050	0.012243569442	0.779058058675
N50	N	0.570906214950	0.512243569438	0.220941941325
N51	N	0.427785484233	0.311119081311	0.635232766129
N52	N	0.572214515767	0.811119081308	0.364767233871
N53	N	0.311978722420	0.322526742241	0.588124170642
N54	N	0.688021277580	0.822526742238	0.411875829358
N55	N	0.251186382843	0.185520792262	0.604313927543
N56	N	0.748813617157	0.685520792259	0.395686072457
N57	N	0.321501001932	0.052202861181	0.597515687336
N58	N	0.678498998068	0.552202861177	0.402484312664
N59	N	0.369536817660	0.877787410764	0.634227141478
N60	N	0.630463182340	0.377787410760	0.365772858522
N61	N	0.480315467387	0.835505554971	0.704525640285
N62	N	0.519684532613	0.335505554968	0.295474359715
N63	N	0.569010232049	0.709627831784	0.682108967352
N64	N	0.430989767951	0.209627831780	0.317891032648
N65	N	0.584428249470	0.713056317790	0.607663957323
N66	N	0.415571750530	0.213056317786	0.392336042677
N67	N	0.638011596555	0.858506661221	0.602299803916
N68	N	0.361988403446	0.358506661218	0.397700196084
N69	N	0.751384297432	0.834161658061	0.635129931170
N70	N	0.248615702568	0.334161658057	0.364870068830
N71	N	0.821827399812	0.730621619792	0.586471087292
N72	N	0.178172600188	0.230621619789	0.413528912708
N73	N	0.824923617151	0.845454823903	0.535163594748
N74	N	0.175076382849	0.345454823900	0.464836405251
N75	N	0.919314830094	0.948453523388	0.555434174036
N76	N	0.080685169906	0.448453523384	0.444565825964

N77	N	0.021957398157	0.878695897570	0.590317909166
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N79	N	0.993759906992	0.882956298030	0.661390123101
N80	N	0.006240093008	0.382956298026	0.338609876899
N81	N	0.917624312280	0.773698964083	0.731992823559
N82	N	0.082375687720	0.273698964080	0.268007176441
N83	N	0.818185154436	0.626366364309	0.771998374920
N84	N	0.181814845564	0.126366364305	0.228001625080
N85	N	0.811350145026	0.570633917091	0.858795875745
N86	N	0.188649854974	0.070633917088	0.141204124255
N87	N	0.751751689268	0.434935210892	0.922844892830
N88	N	0.248248310732	0.934935210889	0.077155107170
N89	N	0.739307946868	0.507104982694	0.987252594439
N90	N	0.260692053132	0.007104982690	0.012747405561
N91	N	0.799907405299	0.678433053309	0.025332566023
N92	N	0.200092594701	0.178433053306	0.974667433977
N93	N	0.929771085390	0.733858282322	0.022498507294
N94	N	0.070228914610	0.233858282318	0.977501492706
N95	N	0.031750308376	0.847328095368	0.990818696043
N96	N	0.968249691624	0.347328095365	0.009181303957
N97	N	0.178138272165	0.839948893113	0.954023358879
N98	N	0.821861727835	0.339948893109	0.045976641121
N99	N	0.344303550166	0.907513294306	0.942894994568
N100	N	0.655696449834	0.407513294303	0.057105005432
N101	N	0.377932731870	0.875827714499	0.873167711167
N102	N	0.622067268130	0.375827714496	0.126832288833
N103	N	0.255694421101	0.868976576733	0.836364213300
N104	N	0.744305578899	0.368976576730	0.163635786700
N105	N	0.206083949295	0.019745043740	0.854176199788
N106	N	0.793916050705	0.519745043736	0.145823800212
N107	N	0.111848822125	0.138044908418	0.860046091633
N108	N	0.888151177876	0.638044908415	0.139953908367
N109	N	0.177901721677	0.314460114502	0.871277055422
N110	N	0.822098278323	0.814460114498	0.128722944578
O1	O	0.765733995698	0.732621233346	0.876379380981
O2	O	0.234266004302	0.232621233343	0.123620619019
O3	O	0.655382974319	0.789833904918	0.965990636088
O4	O	0.344617025681	0.289833904914	0.034009363912
O5	O	0.811215073289	0.948610647706	0.871192558776
O6	O	0.188784926711	0.448610647703	0.128807441224
O7	O	0.699947219629	0.967848771697	0.813347985517
O8	O	0.300052780371	0.467848771693	0.186652014483
O9	O	0.962206960769	0.886879120325	0.781760047896
O10	O	0.037793039231	0.386879120322	0.218239952104
O11	O	0.132384688733	0.060020200372	0.795114481883
O12	O	0.867615311267	0.560020200368	0.204885518117
O13	O	0.291121499845	0.100913198686	0.744962293451
O14	O	0.708878500155	0.600913198682	0.255037706549
O15	O	0.105962123926	0.261749468265	0.737928814462
O16	O	0.894037876074	0.761749468262	0.262071185538
O17	O	0.209137102083	0.264476647548	0.676296214110
O18	O	0.790862897918	0.764476647544	0.323703785890
O19	O	0.033249070938	0.442014888039	0.724357772084
O20	O	0.966750929062	0.942014888035	0.275642227916
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O22	O	0.994162054018	0.890909748427	0.365842181435
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2) CRAMBIN CRYSTAL – optimized 84W

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H131	H	0.898271484113	0.369498874612	0.789319420786
H132	H	0.101728515887	0.869498874612	0.210680579214
H133	H	0.852199802743	0.384246497381	0.754107426280
H134	H	0.147800197257	0.884246497381	0.245892573720
H135	H	0.794075461485	0.305825778918	0.789900977779
H136	H	0.205924538515	0.805825778918	0.210099022221
H137	H	0.818182124519	0.246339229883	0.757210111578
H138	H	0.181817875481	0.746339229883	0.242789888422
H139	H	0.909347834386	0.240573913044	0.809210315045
H140	H	0.090652165614	0.740573913044	0.190789684955
H141	H	0.748012816383	0.194952858051	0.807774968551
H142	H	0.251987183617	0.694952858051	0.192225031449
H143	H	0.762343814424	0.101469349324	0.817724390639
H144	H	0.237656185576	0.601469349324	0.182275609361
H145	H	0.920091489136	0.134713673544	0.836800367591
H146	H	0.079908510864	0.634713673544	0.163199632408
H147	H	0.856023523051	0.085433232735	0.849389178213
H148	H	0.143976476949	0.585433232735	0.150610821787
H149	H	0.946018141272	0.410360313763	0.679562399515
H150	H	0.053981858728	0.910360313763	0.320437600485

H151	H	0.830013032238	0.480227929668	0.675226662508
H152	H	0.169986967763	0.980227929668	0.324773337491
H153	H	0.933111681167	0.494921120791	0.623077557714
H154	H	0.066888318833	0.994921120791	0.376922442286
H155	H	0.869864617624	0.557054036406	0.629569070797
H156	H	0.130135382376	0.057054036406	0.370430929203
H157	H	0.955107588646	0.600347062272	0.656900591444
H158	H	0.044892411354	0.100347062272	0.343099408556
H159	H	0.903585666711	0.365844960840	0.613599549869
H160	H	0.096414333289	0.865844960840	0.386400450131
H161	H	0.804712911967	0.373160906070	0.565959867243
H162	H	0.195287088033	0.873160906070	0.434040132757
H163	H	0.903598832656	0.251904197435	0.577024929861
H164	H	0.096401167344	0.751904197435	0.422975070139
H165	H	0.854605140311	0.258718959095	0.541790057435
H166	H	0.145394859689	0.758718959095	0.458209942565
H167	H	0.982014855395	0.260668490211	0.533942010256
H168	H	0.017985144605	0.760668490211	0.466057989744
H169	H	0.004637554999	0.350016448012	0.519858888589
H170	H	0.995362445001	0.850016448012	0.480141111410
H171	H	0.835256173138	0.246900746486	0.633618447592
H172	H	0.164743826862	0.746900746486	0.366381552408
H173	H	0.732629636465	0.149799077295	0.623567735844
H174	H	0.267370363535	0.649799077295	0.376432264156
H175	H	0.819284158184	0.121540937621	0.660694845483
H176	H	0.180715841816	0.621540937621	0.339305154517
H177	H	0.805161399604	0.202237761696	0.684864801723
H178	H	0.194838600396	0.702237761696	0.315135198277
H179	H	0.719643883371	0.208061699208	0.725608879566
H180	H	0.280356116630	0.708061699208	0.274391120434
H181	H	0.755824765758	0.008286164201	0.668371760080
H182	H	0.244175234242	0.508286164201	0.331628239920
H183	H	0.653128844756	0.135738201328	0.764149169617
H184	H	0.346871155244	0.635738201328	0.235850830383
H185	H	0.687631884571	0.935396592841	0.706516536742
H186	H	0.312368115430	0.435396592842	0.293483463258
H187	H	0.636234111315	0.000483381306	0.754878935871
H188	H	0.363765888685	0.500483381306	0.245121064129
H189	H	0.741729722189	0.319066234576	0.673797221584
H190	H	0.258270277811	0.819066234576	0.326202778416
H191	H	0.615154898878	0.301986994991	0.694401026655
H192	H	0.384845101123	0.801986994991	0.305598973345
H193	H	0.692580676532	0.446236828187	0.690391110687
H194	H	0.307419323468	0.946236828187	0.309608889313
H195	H	0.618713638533	0.436923642536	0.708555813985
H196	H	0.381286361467	0.936923642536	0.291444186015
H197	H	0.748068585506	0.472741332650	0.739372014685
H198	H	0.251931414494	0.972741332650	0.260627985315
H199	H	0.740907763013	0.416221662719	0.775291795026
H200	H	0.259092236987	0.916221662719	0.224708204974
H201	H	0.679084163474	0.383953472982	0.620688379838
H202	H	0.320915836526	0.883953472982	0.379311620162
H203	H	0.559333118600	0.440830292852	0.598510440848
H204	H	0.440666881400	0.940830292852	0.401489559152
H205	H	0.681713400684	0.408802013343	0.564238941640
H206	H	0.318286599316	0.908802013343	0.435761058360
H207	H	0.638501367326	0.465377004816	0.511967757219
H208	H	0.361498632675	0.965377004816	0.488032242781
H209	H	0.563256161028	0.462277788497	0.529431373464
H210	H	0.436743838972	0.962277788497	0.470568626535
H211	H	0.604056172470	0.377994992337	0.521446922094
H212	H	0.395943827530	0.877994992337	0.478553077906
H213	H	0.679192438706	0.550744640754	0.557852342032

H214	H	0.320807561294	0.050744640754	0.442147657968
H215	H	0.674270357846	0.522603788492	0.600063478508
H216	H	0.325729642154	0.022603788492	0.399936521492
H217	H	0.606788146482	0.551369726858	0.578637153938
H218	H	0.393211853518	0.051369726858	0.421362846062
H219	H	0.643178021107	0.270477267169	0.581231000084
H220	H	0.356821978893	0.770477267169	0.418768999916
H221	H	0.550282772744	0.202183087595	0.540665516594
H222	H	0.449717227256	0.702183087595	0.459334483406
H223	H	0.655259497245	0.152478889524	0.548563880485
H224	H	0.344740502755	0.652478889524	0.451436119515
H225	H	0.642402833130	0.140799591736	0.592263648479
H226	H	0.357597166870	0.640799591736	0.407736351520
H227	H	0.559294631779	0.215411161657	0.630002624275
H228	H	0.440705368221	0.715411161657	0.369997375725
H229	H	0.447690512102	0.129489593687	0.639744618548
H230	H	0.552309487898	0.629489593687	0.360255381452
H231	H	0.521049740886	0.238494670085	0.683580301952
H232	H	0.478950259114	0.738494670085	0.316419698048
H233	H	0.456323780954	0.190492896246	0.698713645596
H234	H	0.543676219046	0.690492896246	0.301286354404
H235	H	0.569579584952	0.109820394181	0.669469373305
H236	H	0.430420415048	0.609820394181	0.330530626695
H237	H	0.561640997955	0.132720384093	0.711935180717
H238	H	0.438359002045	0.632720384093	0.288064819283
H239	H	0.469995615697	0.035148086859	0.672753108000
H240	H	0.530004384303	0.535148086859	0.327246892000
H241	H	0.531774774758	0.999552081210	0.696267539592
H242	H	0.468225225242	0.499552081210	0.303732460408
H243	H	0.482073803181	0.077825454706	0.744955669440
H244	H	0.517926196819	0.577825454706	0.255044330560
H245	H	0.401755389315	0.962679752294	0.684682953960
H246	H	0.598244610685	0.462679752294	0.315317046040
H247	H	0.356096539019	0.923245814971	0.716352226422
H248	H	0.643903460981	0.423245814971	0.283647773578
H249	H	0.418469876059	0.024606082941	0.783701539497
H250	H	0.581530123941	0.524606082941	0.216298460503
H251	H	0.356943409406	0.969650504037	0.769936801688
H252	H	0.643056590594	0.469650504037	0.230063198312
H253	H	0.460619925910	0.315080430589	0.612428824817
H254	H	0.539380074091	0.815080430589	0.387571175183
H255	H	0.356470160870	0.369946099827	0.649637688410
H256	H	0.643529839131	0.869946099827	0.350362311590
H257	H	0.411602861996	0.415046345963	0.581884012902
H258	H	0.588397138004	0.915046345963	0.418115987097
H259	H	0.347808320941	0.460884589700	0.600021686882
H260	H	0.652191679059	0.960884589700	0.399978313118
H261	H	0.476128826413	0.449318385142	0.630965309696
H262	H	0.523871173587	0.949318385142	0.369034690304
H263	H	0.470677535033	0.526018228276	0.579292627073
H264	H	0.529322464967	0.026018228276	0.420707372927
H265	H	0.481727604534	0.585702857553	0.614307789476
H266	H	0.518272395466	0.085702857553	0.385692210523
H267	H	0.408026423770	0.578174968158	0.595668208594
H268	H	0.591973576230	0.078174968158	0.404331791406
H269	H	0.437020953394	0.546223664017	0.672063838098
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H271	H	0.400445404887	0.458799970200	0.676878681411
H272	H	0.599554595113	0.958799970200	0.323121318589
H273	H	0.361624624322	0.533425490484	0.656104438484
H274	H	0.638375375678	0.033425490484	0.343895561516
H275	H	0.217236247060	0.279643412531	0.574536815572
H276	H	0.782763752940	0.779643412531	0.425463184428

H277	H	0.241171373079	0.195953673788	0.519035598619
H278	H	0.758828626921	0.695953673788	0.480964401381
H279	H	0.256067669008	0.292798454802	0.519275152980
H280	H	0.743932330992	0.792798454802	0.480724847020
H281	H	0.349269577070	0.168567081586	0.533216993548
H282	H	0.650730422930	0.668567081586	0.466783006452
H283	H	0.355121364819	0.241314797434	0.503059238479
H284	H	0.644878635181	0.741314797434	0.496940761521
H285	H	0.407188314630	0.256528314927	0.565987147810
H286	H	0.592811685370	0.756528314927	0.434012852190
H287	H	0.372758997129	0.334929843090	0.545790204928
H288	H	0.627241002871	0.834929843090	0.454209795072
H289	H	0.306168127555	0.191135890639	0.623884845136
H290	H	0.693831872445	0.691135890639	0.376115154864
H291	H	0.275421211897	0.101527533411	0.660340572765
H292	H	0.724578788103	0.601527533411	0.339659427234
H293	H	0.210560921405	0.079687332157	0.634562094216
H294	H	0.789439078595	0.579687332157	0.365437905784
H295	H	0.345323221114	0.072258395885	0.590022083127
H296	H	0.654676778886	0.572258395885	0.409977916873
H297	H	0.338302795009	0.920671973104	0.573398662093
H298	H	0.661697204991	0.420671973104	0.426601337907
H299	H	0.455593950893	0.009954032995	0.585683643783
H300	H	0.544406049107	0.509954032995	0.414316356217
H301	H	0.429063079573	0.083609692107	0.549456612927
H302	H	0.570936920427	0.583609692107	0.450543387073
H303	H	0.476097055265	0.880700388383	0.569889348589
H304	H	0.523902944735	0.380700388383	0.430110651411
H305	H	0.493497125596	0.938673334635	0.534855319089
H306	H	0.506502874404	0.438673334635	0.465144680911
H307	H	0.424253315580	0.885463459291	0.535126303763
H308	H	0.575746684420	0.385463459291	0.464873696237
H309	H	0.383507360748	0.813332206160	0.673709834558
H310	H	0.616492639252	0.313332206160	0.326290165441
H311	H	0.443860347304	0.703537428152	0.625050750963
H312	H	0.556139652696	0.203537428152	0.374949249037
H313	H	0.402873637091	0.682661986915	0.663101112137
H314	H	0.597126362909	0.182661986915	0.336898887863
H315	H	0.340362232041	0.671150097943	0.604282370004
H316	H	0.659637767959	0.171150097943	0.395717629996
H317	H	0.305925015368	0.718673233602	0.638553484022
H318	H	0.694074984632	0.218673233602	0.361446515978
H319	H	0.363473756055	0.788457696679	0.576522302111
H320	H	0.636526243945	0.288457696679	0.423477697889
H321	H	0.298497787703	0.817976942267	0.600529925142
H322	H	0.701502212297	0.317976942267	0.399470074858
H323	H	0.460583199654	0.813366021460	0.708385040291
H324	H	0.539416800347	0.313366021460	0.291614959709
H325	H	0.575235796062	0.888269789338	0.690638345669
H326	H	0.424764203938	0.388269789338	0.309361654331
H327	H	0.546396755501	0.779053624712	0.747921307848
H328	H	0.453603244499	0.279053624712	0.252078692152
H329	H	0.614500666548	0.831036748089	0.743103526103
H330	H	0.385499333453	0.331036748089	0.256896473897
H331	H	0.544915686295	0.950907853642	0.743882476610
H332	H	0.455084313705	0.450907853642	0.256117523390
H333	H	0.484603501887	0.890780363028	0.756916260083
H334	H	0.515396498113	0.390780363028	0.243083739917
H335	H	0.537328645985	0.690214338687	0.693302926568
H336	H	0.462671354015	0.190214338687	0.306697073432
H337	H	0.657243693068	0.644284085512	0.678679072637
H338	H	0.342756306932	0.144284085512	0.321320927363
H339	H	0.570841095845	0.555390824958	0.691127507659

H340	H	0.429158904155	0.055390824958	0.308872492341
H341	H	0.612166022549	0.529486227072	0.654293222424
H342	H	0.387833977451	0.029486227072	0.345706777576
H343	H	0.538824808823	0.572992495145	0.651002048579
H344	H	0.461175191177	0.072992495145	0.348997951421
H345	H	0.550199285351	0.717374665136	0.619758687068
H346	H	0.449800714649	0.217374665136	0.380241312932
H347	H	0.629490958111	0.679883690137	0.561551659165
H348	H	0.370509041890	0.179883690137	0.438448340835
H349	H	0.512269595515	0.772228162838	0.572395208511
H350	H	0.487730404485	0.272228162838	0.427604791488
H351	H	0.552651591483	0.776186227794	0.534098924346
H352	H	0.447348408517	0.276186227794	0.465901075654
H353	H	0.506639369512	0.629393359038	0.564101079515
H354	H	0.493360630488	0.129393359038	0.435898920485
H355	H	0.415070934071	0.707104392844	0.556499414153
H356	H	0.584929065929	0.207104392844	0.443500585847
H357	H	0.416564114736	0.639410935605	0.524054126218
H358	H	0.583435885264	0.139410935605	0.475945873782
H359	H	0.438496383230	0.733641875856	0.515495645789
H360	H	0.561503616770	0.233641875856	0.484504354211
H361	H	0.516224129793	0.579419689698	0.506545705961
H362	H	0.483775870207	0.079419689698	0.493454294039
H363	H	0.587881008314	0.616052713146	0.519323854633
H364	H	0.412118991686	0.116052713146	0.480676145367
H365	H	0.540485275084	0.667955237011	0.491456333287
H366	H	0.459514724916	0.167955237011	0.508543666713
H367	H	0.595750155285	0.838333676624	0.614427246726
H368	H	0.404249844715	0.338333676624	0.385572753274
H369	H	0.679855185907	0.930791707783	0.575628565240
H370	H	0.320144814093	0.430791707783	0.424371434760
H371	H	0.633438122020	0.948238176913	0.648099215603
H372	H	0.366561877980	0.448238176913	0.351900784397
H373	H	0.676719830749	0.015891762270	0.625548774268
H374	H	0.323280169251	0.515891762270	0.374451225731
H375	H	0.706573940345	0.799662541700	0.639889300456
H376	H	0.293426059655	0.299662541700	0.360110699544
H377	H	0.835154553765	0.836685484830	0.648263982694
H378	H	0.164845446235	0.336685484830	0.351736017306
H379	H	0.782621032198	0.759521292063	0.690341092138
H380	H	0.217378967802	0.259521292063	0.309658907862
H381	H	0.837736247348	0.701051053252	0.670098976696
H382	H	0.162263752652	0.201051053252	0.329901023304
H383	H	0.758369487690	0.694388910603	0.659310547223
H384	H	0.241630512310	0.194388910603	0.340689452777
H385	H	0.763424343524	0.700165428324	0.591700421172
H386	H	0.236575656476	0.200165428324	0.408299578828
H387	H	0.887028264096	0.668664492555	0.564903366655
H388	H	0.112971735904	0.168664492555	0.435096633345
H389	H	0.834912343053	0.607625338668	0.518356825004
H390	H	0.165087656947	0.107625338668	0.481643174996
H391	H	0.732414042733	0.605841782331	0.516055810059
H392	H	0.267585957267	0.105841782331	0.483944189941
H393	H	0.858141842719	0.528541146934	0.567013969404
H394	H	0.141858157281	0.028541146934	0.432986030595
H395	H	0.786318257034	0.502584843524	0.550365561889
H396	H	0.213681742966	0.002584843524	0.449634438111
H397	H	0.788193886064	0.556929934765	0.587644782296
H398	H	0.211806113936	0.056929934765	0.412355217704
H399	H	0.772959212941	0.805537388227	0.545535564791
H400	H	0.227040787059	0.305537388227	0.454464435209
H401	H	0.834602392138	0.853561764481	0.485453391229
H402	H	0.165397607862	0.353561764481	0.514546608771

H403	H	0.726455264663	0.887762005884	0.507553674132
H404	H	0.273544735337	0.387762005884	0.492446325868
H405	H	0.761308466018	0.950061835018	0.535560150879
H406	H	0.238691533982	0.450061835018	0.464439849121
H407	H	0.746815127640	0.906747643272	0.443460453562
H408	H	0.253184872361	0.406747643272	0.556539546438
H409	H	0.788526030689	0.075572870036	0.516809811695
H410	H	0.211473969311	0.575572870036	0.483190188305
H411	H	0.747963017271	0.002418384071	0.398990555841
H412	H	0.252036982729	0.502418384071	0.601009444159
H413	H	0.789977148695	0.171994859500	0.471878183556
H414	H	0.210022851306	0.671994859500	0.528121816444
H415	H	0.761246643335	0.126115260454	0.386217723300
H416	H	0.238753356665	0.626115260454	0.613782276700
H417	H	0.846951011004	0.923477173540	0.569439803133
H418	H	0.153048988996	0.423477173540	0.430560196867
H419	H	0.939502068581	0.030510135101	0.545535046141
H420	H	0.060497931419	0.530510135101	0.454464953858
H421	H	0.930147948638	0.086756589863	0.601761529639
H422	H	0.069852051362	0.586756589863	0.398238470361
H423	H	0.844078610569	0.973848897610	0.619391689681
H424	H	0.155921389431	0.473848897610	0.380608310319
H425	H	0.852454055827	0.119395703959	0.558024400164
H426	H	0.147545944173	0.619395703959	0.441975599836
H427	H	0.826039245534	0.130666946753	0.599652741404
H428	H	0.173960754466	0.630666946753	0.400347258596
H429	H	0.800497913450	0.052312958195	0.575685324874
H430	H	0.199502086551	0.552312958195	0.424314675126
H431	H	0.946233517477	0.862223799675	0.589197153692
H432	H	0.053766482523	0.362223799675	0.410802846308
H433	H	0.038017849827	0.803898485987	0.608229179661
H434	H	0.961982150173	0.303898485987	0.391770820339
H435	H	0.075675580947	0.892311455507	0.609949554130
H436	H	0.924324419054	0.392311455507	0.390050445870
H437	H	0.942044772216	0.930959241731	0.645519785340
H438	H	0.057955227784	0.430959241731	0.354480214660
H439	H	0.984658118857	0.911591721264	0.714686611028
H440	H	0.015341881143	0.411591721264	0.285313388971
H441	H	0.855648610496	0.944252297465	0.686644029994
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H445	H	0.918042376907	0.844000868000	0.754959855418
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H447	H	0.880873958717	0.696055225439	0.726904089258
H448	H	0.119126041283	0.196055225439	0.273095910742
H449	H	0.941935085709	0.630854637928	0.767351235334
H450	H	0.058064914291	0.130854637928	0.232648764666
H451	H	0.995833495626	0.780987130296	0.790111488543
H452	H	0.004166504374	0.280987130296	0.209888511457
H453	H	0.943223982139	0.726620280280	0.813305671018
H454	H	0.056776017861	0.226620280280	0.186694328982
H455	H	0.047676015613	0.664473644298	0.743477947010
H456	H	0.952323984387	0.164473644298	0.256522052990
H457	H	0.014769446281	0.743233344660	0.724634228446
H458	H	0.985230553719	0.243233344660	0.275365771553
H459	H	0.989093614880	0.652430030709	0.713057444701
H460	H	0.010906385120	0.152430030709	0.286942555299
H461	H	0.021027394232	0.619924432864	0.814732096248
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H463	H	0.045810470588	0.702892729558	0.835570396408
H464	H	0.954189529412	0.202892729558	0.164429603592
H465	H	0.076031136532	0.680935233310	0.795571291243

H466	H	0.923968863468	0.180935233310	0.204428708757
H467	H	0.813017737131	0.629261408293	0.758476251709
H468	H	0.186982262869	0.129261408293	0.241523748291
H469	H	0.763780445609	0.706374108838	0.818921324833
H470	H	0.236219554391	0.206374108838	0.181078675167
H471	H	0.721816698897	0.562380800263	0.784430726881
H472	H	0.278183301103	0.062380800263	0.215569273118
H473	H	0.648570972577	0.707128916782	0.781599177401
H474	H	0.351429027423	0.207128916782	0.218400822599
H475	H	0.707444743639	0.689641352236	0.751950789754
H476	H	0.292555256361	0.189641352236	0.248049210246
H477	H	0.689143188863	0.563483956379	0.844745874876
H478	H	0.310856811137	0.063483956379	0.155254125124
H479	H	0.624140519936	0.580904445823	0.818901170102
H480	H	0.375859480064	0.080904445823	0.181098829898
H481	H	0.660559770999	0.655651345719	0.840214401983
H482	H	0.339440229001	0.155651345719	0.159785598017
H483	H	0.658340025020	0.573203601800	0.733151902033
H484	H	0.341659974980	0.073203601800	0.266848097967
H485	H	0.601919374727	0.645583432801	0.732971266144
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H487	H	0.601161163814	0.578656073738	0.765049612189
H488	H	0.398838836186	0.078656073738	0.234950387810
H489	H	0.780440135103	0.664252501593	0.869052503632
H490	H	0.219559864897	0.164252501593	0.130947496368
H491	H	0.827078360540	0.508985048901	0.875789579717
H492	H	0.172921639460	0.008985048901	0.124210420283
H493	H	0.882387098668	0.542609191743	0.927359268794
H494	H	0.117612901332	0.042609191743	0.072640731206
H495	H	0.866952022139	0.706742379478	0.906246968040
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H497	H	0.825452794571	0.663123988605	0.938933019360
H498	H	0.174547205429	0.163123988605	0.061066980640
H499	H	0.975169067703	0.594567669759	0.897794095979
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H501	H	0.928600246823	0.621202260774	0.863318411904
H502	H	0.071399753177	0.121202260774	0.136681588096
H503	H	0.937993265846	0.525039823637	0.873558204783
H504	H	0.062006734154	0.025039823637	0.126441795216
H505	H	0.924099940631	0.637352687835	0.970197054105
H506	H	0.075900059369	0.137352687835	0.029802945895
H507	H	0.912585483425	0.734442369292	0.962594142496
H508	H	0.087414516575	0.234442369292	0.037405857504
H509	H	0.966330911381	0.683597718266	0.938319160330
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H521	H	0.833974067299	0.420297085659	0.919008649458
H522	H	0.166025932701	0.920297085659	0.080991350542
H523	H	0.769484712939	0.398955825891	0.892605701229
H524	H	0.230515287061	0.898955825891	0.107394298771
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H531	H	0.836651919940	0.688682731406	0.057769013014
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H540	H	0.227494124299	0.311065675809	0.919608735602
H541	H	0.921444081580	0.722136396124	0.029516072908
H542	H	0.078555918420	0.222136396124	0.970483927092
H543	H	0.992209391110	0.859096515546	0.046635837006
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H545	H	0.019566446640	0.700103412139	0.070952169395
H546	H	0.980433553360	0.200103412139	0.929047830605
H547	H	0.941686602166	0.758351645378	0.098973007193
H548	H	0.058313397834	0.258351645378	0.901026992807
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H550	H	0.883631009741	0.268394839153	0.939409482846
H551	H	0.101314568532	0.759374748632	0.104226600078
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H554	H	0.911903792761	0.347289003046	0.916743613042
H555	H	0.014162731797	0.890611062414	0.996802624902
H556	H	0.985837268203	0.390611062414	0.003197375098
H557	H	0.045289561741	0.787849778469	0.943318481839
H558	H	0.954710438259	0.287849778469	0.056681518161
H559	H	0.060649144837	0.958051856503	0.952420523484
H560	H	0.939350855163	0.458051856503	0.047579476516
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H563	H	0.244160343362	0.770829816291	0.967946238791
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H565	H	0.291478146859	0.717154760051	0.907843222391
H566	H	0.708521853141	0.217154760051	0.092156777609
H567	H	0.239047047909	0.662770748588	0.931839101522
H568	H	0.760952952091	0.162770748588	0.068160898478
H569	H	0.209039116198	0.768657918067	0.873554591984
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H571	H	0.187786596978	0.672602829130	0.876920692582
H572	H	0.812213403022	0.172602829130	0.123079307418
H573	H	0.106880416108	0.782679883082	0.896079752591
H574	H	0.893119583893	0.282679883082	0.103920247409
H575	H	0.112174536253	0.697849328826	0.919518550386
H576	H	0.887825463747	0.197849328826	0.080481449614
H577	H	0.340316617457	0.820834014719	0.953089864084
H578	H	0.659683382544	0.320834014719	0.046910135916
H579	H	0.335807932551	0.978411769749	0.940121442235
H580	H	0.664192067450	0.478411769749	0.059878557765
H581	H	0.402257162975	0.922378083544	0.941328505004
H582	H	0.597742837025	0.422378083544	0.058671494996
H583	H	0.343812289184	0.831493898585	0.879999325095
H584	H	0.656187710816	0.331493898585	0.120000674905
H585	H	0.384918417955	0.940163685433	0.829195825098
H586	H	0.615081582045	0.440163685433	0.170804174902
H587	H	0.392910136770	0.829037828470	0.791246939191
H588	H	0.607089863230	0.329037828470	0.208753060809
H589	H	0.441574592719	0.826650784672	0.826099904846
H590	H	0.558425407281	0.326650784672	0.173900095154
H591	H	0.253139035471	0.899729038322	0.865047407538

H592	H	0.746860964529	0.399729038322	0.134952592462
H593	H	0.191231471071	0.961400916959	0.805657608114
H594	H	0.808768528929	0.461400916959	0.194342391886
H595	H	0.134838936527	0.837215216432	0.848577236145
H596	H	0.865161063473	0.337215216432	0.151422763855
H597	H	0.094328300829	0.894973302797	0.820332724121
H598	H	0.905671699171	0.394973302797	0.179667275879
H599	H	0.231700539233	0.761814490013	0.820174819051
H600	H	0.768299460767	0.261814490013	0.179825180949
H601	H	0.084829982875	0.864168243291	0.763894146023
H602	H	0.915170017125	0.364168243291	0.236105853977
H603	H	0.261950619422	0.690089073860	0.770591107195
H604	H	0.738049380579	0.190089073860	0.229408892805
H605	H	0.113893818925	0.789818125893	0.714326510041
H606	H	0.886106181075	0.289818125893	0.285673489959
H607	H	0.183022320536	0.699952798601	0.692705156918
H608	H	0.816977679464	0.199952798601	0.307294843082
H609	H	0.236543727398	0.056927660422	0.840824944707
H610	H	0.763456272602	0.556927660422	0.159175055293
H611	H	0.179871891568	0.073925400021	0.907600518422
H612	H	0.820128108432	0.573925400021	0.092399481578
H613	H	0.294145011253	0.092005493390	0.897384576973
H614	H	0.705854988747	0.592005493390	0.102615423027
H615	H	0.259570114062	0.175227203402	0.913807553083
H616	H	0.740429885938	0.675227203402	0.086192446917
H617	H	0.277716483126	0.168302634092	0.870313503802
H618	H	0.722283516874	0.668302634092	0.129686496198
H619	H	0.139421347784	0.130766928382	0.829634123597
H620	H	0.860578652216	0.630766928382	0.170365876403
H621	H	0.093402867125	0.275795891903	0.855726088187
H622	H	0.906597132875	0.775795891903	0.144273911813
H623	H	0.117138758885	0.231778246960	0.782695604116
H624	H	0.882861241115	0.731778246960	0.217304395884
H625	H	0.100300771735	0.322362235716	0.798644935148
H626	H	0.899699228265	0.822362235716	0.201355064851
H627	H	0.177985588113	0.360519554988	0.847327712300
H628	H	0.822014411887	0.860519554988	0.152672287700
H629	H	0.254306911562	0.337310676816	0.837020220869
H630	H	0.745693088438	0.837310676816	0.162979779131
H631	H	0.692217347540	0.034641708766	0.866572092650
H632	H	0.307782652460	0.534641708766	0.133427907350
H633	H	0.748286988652	0.026311274434	0.888666312534
H634	H	0.251713011348	0.526311274434	0.111333687466
H635	H	0.266283114802	0.149660292794	0.803484128728
H636	H	0.733716885198	0.649660292794	0.196515871272
H637	H	0.298055901929	0.083903726946	0.786453582932
H638	H	0.701944098071	0.583903726946	0.213546417068
H639	H	0.430958954321	0.034431089016	0.847348922418
H640	H	0.569041045679	0.534431089016	0.152651077582
H641	H	0.492444668717	0.007906142569	0.830186451821
H642	H	0.507555331283	0.507906142569	0.169813548179
H643	H	0.316675786093	0.345617682874	0.728774710097
H644	H	0.683324213907	0.845617682874	0.271225289903
H645	H	0.313407201490	0.434307039983	0.735672326944
H646	H	0.686592798510	0.934307039983	0.264327673056
H647	H	0.248911773417	0.409004261949	0.651338521626
H648	H	0.751088226584	0.909004261949	0.348661478374
H649	H	0.260639843844	0.426967784239	0.689140541910
H650	H	0.739360156156	0.926967784239	0.310859458090
H651	H	0.245366691711	0.540246891154	0.658792131545
H652	H	0.754633308289	0.040246891154	0.341207868455
H653	H	0.283884440375	0.610553940104	0.668674412875
H654	H	0.716115559625	0.110553940104	0.331325587125

H655	H	0.335039783154	0.602532491248	0.719040771234
H656	H	0.664960216846	0.102532491248	0.280959228766
H657	H	0.291139197010	0.668591107565	0.710335498684
H658	H	0.708860802990	0.168591107565	0.289664501316
H659	H	0.392620610655	0.510694770318	0.739682193354
H660	H	0.607379389345	0.010694770318	0.260317806646
H661	H	0.350460446097	0.528475124777	0.769735527461
H662	H	0.649539553903	0.028475124777	0.230264472539
H663	H	0.683946331011	0.290752058229	0.790891503926
H664	H	0.316053668989	0.790752058229	0.209108496074
H665	H	0.716174821269	0.312751585122	0.823615507189
H666	H	0.283825178732	0.812751585122	0.176384492811
H667	H	0.930829952479	0.502917266845	0.755414687305
H668	H	0.069170047521	0.002917266845	0.244585312695
H669	H	0.937189564756	0.520524994074	0.716594959758
H670	H	0.062810435244	0.020524994074	0.283405040242
H671	H	0.778832014088	0.563787050505	0.702434494842
H672	H	0.221167985912	0.063787050505	0.297565505158
H673	H	0.834746008061	0.539551602673	0.726424566805
H674	H	0.165253991939	0.039551602673	0.273575433195
H675	H	0.747799211735	0.507175062975	0.648661819111
H676	H	0.252200788266	0.007175062975	0.351338180889
H677	H	0.725981935652	0.590373320927	0.645772709663
H678	H	0.274018064348	0.090373320927	0.354227290337
H679	H	0.041509653345	0.190398702212	0.562328854586
H680	H	0.958490346655	0.690398702212	0.437671145414
H681	H	0.012895483381	0.112614956815	0.568473067223
H682	H	0.987104516619	0.612614956815	0.431526932777
H683	H	0.545535581964	0.212519126210	0.759985090916
H684	H	0.454464418036	0.712519126210	0.240014909084
H685	H	0.590491203992	0.277817795988	0.750345021125
H686	H	0.409508796008	0.777817795988	0.249654978875
H687	H	0.497990539845	0.326910438948	0.727898274303
H688	H	0.502009460155	0.826910438948	0.272101725697
H689	H	0.504502216024	0.367960903945	0.693478917206
H690	H	0.495497783976	0.867960903945	0.306521082794
H691	H	0.472395019598	0.491309452167	0.767564860329
H692	H	0.527604980402	0.991309452167	0.232435139671
H693	H	0.480558134686	0.449060970027	0.732865612511
H694	H	0.519441865314	0.949060970027	0.267134387489
H695	H	0.329747018135	0.206420074737	0.733736050445
H696	H	0.670252981865	0.706420074737	0.266263949555
H697	H	0.359567078633	0.242543637466	0.702875061463
H698	H	0.640432921367	0.742543637466	0.297124938537
H699	H	0.140874898298	0.190035934762	0.557389085319
H700	H	0.859125101702	0.690035934762	0.442610914681
H701	H	0.110098612758	0.243653090041	0.532016244570
H702	H	0.889901387242	0.743653090041	0.467983755430
H703	H	0.101675185689	0.009202058245	0.602631576275
H704	H	0.898324814311	0.509202058245	0.397368423725
H705	H	0.165466635804	0.035247603338	0.591165882807
H706	H	0.834533364196	0.535247603338	0.408834117193
H707	H	0.255874222131	0.869814933274	0.655764238760
H708	H	0.744125777869	0.369814933274	0.344235761240
H709	H	0.214776870786	0.797840150583	0.660902007322
H710	H	0.785223129214	0.297840150583	0.339097992678
H711	H	0.256791380171	0.059929299635	0.537358127283
H712	H	0.743208619829	0.559929299635	0.462641872717
H713	H	0.325042295543	0.044208088389	0.527740684484
H714	H	0.674957704458	0.544208088389	0.472259315516
H715	H	0.372924840663	0.787966774762	0.734532559744
H716	H	0.627075159337	0.287966774762	0.265467440256
H717	H	0.423901698920	0.724490310605	0.736887877057

H718	H	0.576098301080	0.224490310605	0.263112122943
H719	H	0.284795551710	0.852560509274	0.746557138877
H720	H	0.715204448290	0.352560509274	0.253442861123
H721	H	0.280553875634	0.830166530908	0.707401991561
H722	H	0.719446124366	0.330166530908	0.292598008439
H723	H	0.482552195123	0.598220267578	0.733349584459
H724	H	0.517447804878	0.098220267578	0.266650415541
H725	H	0.502887540506	0.666721143554	0.754321388700
H726	H	0.497112459494	0.166721143554	0.245678611300
H727	H	0.502991209764	0.112292644686	0.799818264227
H728	H	0.497008790236	0.612292644686	0.200181735773
H729	H	0.554305564578	0.064758242900	0.785220230266
H730	H	0.445694435422	0.564758242900	0.214779769734
H731	H	0.528673782179	0.751778432606	0.798139768956
H732	H	0.471326217821	0.251778432606	0.201860231044
H733	H	0.473990390163	0.696786499484	0.803697519798
H734	H	0.526009609837	0.196786499484	0.196302480202
H735	H	0.559672696836	0.714031917594	0.845424207642
H736	H	0.440327303165	0.214031917594	0.154575792358
H737	H	0.574408590176	0.797117664298	0.847939379153
H738	H	0.425591409824	0.297117664298	0.152060620847
H739	H	0.144916476312	0.704884562876	0.636588881870
H740	H	0.855083523688	0.204884562876	0.363411118130
H741	H	0.109147253348	0.765335808993	0.658449536198
H742	H	0.890852746652	0.265335808993	0.341550463802
H743	H	0.955519590103	0.702205375274	0.619687713634
H744	H	0.044480409897	0.202205375274	0.380312286365
H745	H	0.971030264823	0.717068247407	0.655865590060
H746	H	0.028969735177	0.217068247407	0.344134409940
H747	H	0.910510980641	0.516071369235	0.809149489383
H748	H	0.089489019359	0.016071369235	0.190850510617
H749	H	0.968034141978	0.468358200427	0.817714305959
H750	H	0.031965858022	0.968358200427	0.182285694041
H751	H	0.713280347888	0.450404872845	0.830716509390
H752	H	0.286719652112	0.950404872845	0.169283490610
H753	H	0.782829906750	0.456850100205	0.824258452885
H754	H	0.217170093250	0.956850100205	0.175741547115
H755	H	0.878366118365	0.422020722065	0.984045208411
H756	H	0.121633881635	0.922020722065	0.015954791589
H757	H	0.931960547485	0.472839456085	0.971101445866
H758	H	0.068039452515	0.972839456084	0.028898554134
H759	H	0.049552672516	0.485649539751	0.979649595522
H760	H	0.950447327484	0.985649539751	0.020350404478
H761	H	0.002911549320	0.528916506276	0.004106760705
H762	H	0.997088450680	0.028916506276	0.995893239295
H763	H	0.973887634241	0.598313999859	0.052638731766
H764	H	0.026112365759	0.098313999859	0.947361268234
H765	H	0.006392561036	0.640779947123	0.022387769486
H766	H	0.993607438964	0.140779947123	0.977612230514
H767	H	0.934496626085	0.546120445517	0.106978588412
H768	H	0.065503373915	0.046120445517	0.893021411588
H769	H	0.972882979868	0.614825566463	0.117751279893
H770	H	0.027117020132	0.114825566463	0.882248720107
H771	H	0.118479188112	0.550550201191	0.098322713435
H772	H	0.881520811889	0.050550201191	0.901677286565
H773	H	0.051354973059	0.575302593157	0.093794910429
H774	H	0.948645026941	0.075302593157	0.906205089571
H775	H	0.354388464314	0.686569211038	0.966555700938
H776	H	0.645611535686	0.186569211038	0.033444299062
H777	H	0.353277540915	0.724326010870	0.001150968688
H778	H	0.646722459085	0.224326010870	0.998849031312
H779	H	0.300663774069	0.636656101945	0.855862585639
H780	H	0.699336225932	0.136656101945	0.144137414361

H781	H	0.249167631361	0.576990959321	0.862042955119
H782	H	0.750832368639	0.076990959321	0.137957044881
H783	H	0.382809606879	0.598652420165	0.809988575473
H784	H	0.617190393121	0.098652420165	0.190011424527
H785	H	0.345163292690	0.540080548736	0.828409626758
H786	H	0.654836707310	0.040080548736	0.171590373242
H787	H	0.994093483457	0.366051628948	0.868521983114
H788	H	0.005906516543	0.866051628948	0.131478016886
H789	H	0.000921091875	0.349745812853	0.831440850918
H790	H	0.999078908125	0.849745812853	0.168559149082
H791	H	0.078223819813	0.409249621607	0.864468159414
H792	H	0.921776180187	0.909249621607	0.135531840586
H793	H	0.114887116814	0.403230446400	0.898387207972
H794	H	0.885112883186	0.903230446400	0.101612792028
H795	H	0.137602083213	0.572299305165	0.841267368901
H796	H	0.862397916787	0.072299305165	0.158732631099
H797	H	0.144872388171	0.509786933446	0.867691740591
H798	H	0.855127611829	0.009786933446	0.132308259409
C1	C	0.686001285101	0.810401429759	0.912889440538
C2	C	0.313998714899	0.310401429759	0.087110559462
C3	C	0.723229848918	0.815095288748	0.880638503843
C4	C	0.276770151082	0.315095288748	0.119361496157
C5	C	0.727606244869	0.817980302706	0.944324252072
C6	C	0.272393755131	0.317980302706	0.055675747928
C7	C	0.752899677476	0.897029341292	0.948733858068
C8	C	0.247100322524	0.397029341292	0.051266141932
C9	C	0.769903255926	0.895457944756	0.838905133836
C10	C	0.230096744074	0.395457944756	0.161094866164
C11	C	0.827424540276	0.938207648291	0.849648330972
C12	C	0.172575459724	0.438207648291	0.150351669028
C13	C	0.736734568752	0.932444845017	0.808602097307
C14	C	0.263265431248	0.432444845017	0.191397902693
C15	C	0.701934108444	0.872104647972	0.789517790255
C16	C	0.298065891556	0.372104647972	0.210482209745
C17	C	0.939635129854	0.943987583183	0.837965506548
C18	C	0.060364870146	0.443987583183	0.162034493452
C19	C	0.966072883651	0.961300512655	0.803053495957
C20	C	0.033927116349	0.461300512655	0.196946504043
C21	C	0.981915328352	0.884583336815	0.854009528190
C22	C	0.018084671648	0.384583336815	0.145990471810
C23	C	0.025831050398	0.041312959449	0.766645964287
C24	C	0.974168949602	0.541312959449	0.233354035712
C25	C	0.095887390839	0.047793124476	0.767507791008
C26	C	0.904112609161	0.547793124476	0.232492208992
C27	C	0.996334958230	0.113521867686	0.753280994472
C28	C	0.003665041770	0.613521867686	0.246719005528
C29	C	0.193923083150	0.024764904250	0.738804497461
C30	C	0.806076916851	0.524764904250	0.261195502539
C31	C	0.221139337905	0.102097209243	0.732190833572
C32	C	0.778860662095	0.602097209243	0.267809166428
C33	C	0.208223846377	0.969476546767	0.710396990919
C34	C	0.791776153623	0.469476546767	0.289603009081
C35	C	0.154065253511	0.978767578953	0.686400227698
C36	C	0.845934746489	0.478767578953	0.313599772302
C37	C	0.099112667163	0.987785304852	0.709905035575
C38	C	0.900887332837	0.487785304852	0.290094964425
C39	C	0.200909203519	0.232120735658	0.717101987437
C40	C	0.799090796481	0.732120735658	0.282898012563
C41	C	0.145251302387	0.282016993809	0.722933557112
C42	C	0.854748697613	0.782016993809	0.277066442887
C43	C	0.229800906834	0.248553805858	0.683053238035
C44	C	0.770199093166	0.748553805858	0.316946761965
C45	C	0.114053247212	0.411887187487	0.733294813646

C46	C	0.885946752788	0.911887187487	0.266705186354
C47	C	0.074539046725	0.421453871169	0.701717126225
C48	C	0.925460953275	0.921453871169	0.298282873775
C49	C	0.146143729633	0.485195504369	0.743748387542
C50	C	0.853856270367	0.985195504369	0.256251612458
C51	C	0.178128974250	0.476633290155	0.777990086333
C52	C	0.821871025750	0.976633290155	0.222009913667
C53	C	0.100898679140	0.550260587477	0.742964992663
C54	C	0.899101320860	0.050260587477	0.257035007337
C55	C	0.216167251099	0.545129083418	0.787448728014
C56	C	0.783832748901	0.045129083418	0.212551271986
C57	C	0.067083101925	0.432060113264	0.641290231217
C58	C	0.932916898075	0.932060113264	0.358709768783
C59	C	0.034599611132	0.359050977267	0.631692736328
C60	C	0.965400388868	0.859050977267	0.368307263672
C61	C	0.104657631131	0.470100404706	0.613061547328
C62	C	0.895342368869	0.970100404706	0.386938452672
C63	C	0.079630166470	0.454865928644	0.577823148312
C64	C	0.920369833530	0.954865928644	0.422176851688
C65	C	0.107440114947	0.554231416273	0.620908935408
C66	C	0.892559885053	0.054231416273	0.379091064592
C67	C	0.020964268804	0.225610142205	0.638450112702
C68	C	0.979035731196	0.725610142205	0.361549887298
C69	C	0.961776778276	0.235027174048	0.659347541807
C70	C	0.038223221724	0.735027174048	0.340652458192
C71	C	0.056905944930	0.154799219445	0.647210497594
C72	C	0.943094055070	0.654799219445	0.352789502406
C73	C	0.913329043030	0.287206744852	0.709970577815
C74	C	0.086670956970	0.787206744852	0.290029422185
C75	C	0.872537928012	0.344287891009	0.691757068116
C76	C	0.127462071988	0.844287891009	0.308242931884
C77	C	0.932759179639	0.316240804113	0.744729207951
C78	C	0.067240820361	0.816240804113	0.255270792049
C79	C	0.879138148932	0.341136669156	0.767136921760
C80	C	0.120861851068	0.841136669156	0.232863078240
C81	C	0.834758168197	0.279957760413	0.778544648271
C82	C	0.165241831803	0.779957760413	0.221455351729
C83	C	0.839132463785	0.167517113706	0.815298461984
C84	C	0.160867536215	0.667517113706	0.184701538016
C85	C	0.863238351379	0.455904149905	0.657698816614
C86	C	0.136761648621	0.955904149905	0.342301183386
C87	C	0.825526206716	0.417761530638	0.629895894543
C88	C	0.174473793284	0.917761530638	0.370104105457
C89	C	0.902062359413	0.518664135749	0.642267889423
C90	C	0.097937640587	0.018664135749	0.357732110577
C91	C	0.828353676217	0.332486950925	0.582068639631
C92	C	0.171646323783	0.832486950925	0.417931360369
C93	C	0.778113002215	0.279402179297	0.595272534743
C94	C	0.221886997785	0.779402179297	0.404727465257
C95	C	0.877623111753	0.291765112364	0.561459062937
C96	C	0.122376888247	0.791765112364	0.438540937063
C97	C	0.921961529740	0.347412932326	0.544313007043
C98	C	0.078038470260	0.847412932326	0.455686992957
C99	C	0.748910876201	0.193414179828	0.640924948664
C100	C	0.251089123800	0.693414179828	0.359075051336
C101	C	0.690698364097	0.234956286871	0.651803901507
C102	C	0.309301635903	0.734956286871	0.348196098493
C103	C	0.782630212756	0.157183786758	0.670827214762
C104	C	0.217369787244	0.657183786758	0.329172785238
C105	C	0.741973549580	0.112988739186	0.694136817334
C106	C	0.258026450420	0.612988739186	0.305863182666
C107	C	0.712950574196	0.148265768377	0.721337794494
C108	C	0.287049425804	0.648265768377	0.278662205506

C109	C	0.732582623377	0.036140890611	0.689256289129
C110	C	0.267417376623	0.536140890611	0.310743710871
C111	C	0.675271882332	0.107704000719	0.743019271243
C112	C	0.324728117668	0.607704000719	0.256980728757
C113	C	0.694369819902	0.995364464838	0.710743588347
C114	C	0.305630180098	0.495364464838	0.289256411652
C115	C	0.665572974720	0.031359251275	0.737646841952
C116	C	0.334427025280	0.531359251275	0.262353158048
C117	C	0.644584123521	0.340635424321	0.680160606449
C118	C	0.355415876479	0.840635424321	0.319839393550
C119	C	0.604070888660	0.366993728350	0.650941026209
C120	C	0.395929111340	0.866993728350	0.349058973791
C121	C	0.661632506043	0.406464643800	0.702922470406
C122	C	0.338367493957	0.906464643800	0.297077529594
C123	C	0.686734913573	0.382461539315	0.736853777446
C124	C	0.313265086427	0.882461539315	0.263146222554
C125	C	0.596819454253	0.402423485640	0.591841172814
C126	C	0.403180545748	0.902423485640	0.408158827186
C127	C	0.563508440292	0.332698039138	0.578733713148
C128	C	0.436491559708	0.832698039138	0.421266286851
C129	C	0.637892318580	0.440011479240	0.565048962067
C130	C	0.362107681420	0.940011479240	0.434951037933
C131	C	0.609104599645	0.436179945177	0.530098162765
C132	C	0.390895400355	0.936179945177	0.469901837235
C133	C	0.650424684964	0.520556076801	0.575906403483
C134	C	0.349575315036	0.020556076801	0.424093596517
C135	C	0.569005434074	0.198712694148	0.566208322588
C136	C	0.430994565927	0.698712694148	0.433791677412
C137	C	0.512734753366	0.180248443482	0.588440669113
C138	C	0.487265246634	0.680248443482	0.411559330887
C139	C	0.620106440754	0.139298392207	0.567585990735
C140	C	0.379893559246	0.639298392207	0.432414009265
C141	C	0.468492673033	0.184531882703	0.644960314912
C142	C	0.531507326967	0.684531882703	0.355039685087
C143	C	0.414694652441	0.239123194578	0.642044850561
C144	C	0.585305347559	0.739123194578	0.357955149439
C145	C	0.494622598096	0.186669010726	0.680782029896
C146	C	0.505377401904	0.686669010726	0.319217970104
C147	C	0.535227698633	0.119339814436	0.689266067374
C148	C	0.464772301367	0.619339814436	0.310733932626
C149	C	0.499309256590	0.046929147061	0.694470167905
C150	C	0.500690743410	0.546929147061	0.305529832095
C151	C	0.414488296547	0.005606493239	0.732388608714
C152	C	0.585511703453	0.505606493239	0.267611391285
C153	C	0.370613494188	0.357285074793	0.623785101737
C154	C	0.629386505812	0.857285074793	0.376214898263
C155	C	0.311869773624	0.325576001606	0.608164740300
C156	C	0.688130226376	0.825576001606	0.391835259700
C157	C	0.389884913077	0.429417032142	0.605967484709
C158	C	0.610115086923	0.929417032142	0.394032515291
C159	C	0.433568350939	0.480615347397	0.625757804312
C160	C	0.566431649061	0.980615347397	0.374242195688
C161	C	0.449425436799	0.546298083105	0.602679326407
C162	C	0.550574563201	0.046298083105	0.397320673593
C163	C	0.406468309534	0.506039661962	0.659434605116
C164	C	0.593531690466	0.006039661962	0.340565394884
C165	C	0.257850592556	0.245516407494	0.568575422497
C166	C	0.742149407444	0.745516407494	0.431424577503
C167	C	0.246010046708	0.169327861276	0.585134127930
C168	C	0.753989953292	0.669327861276	0.414865872070
C169	C	0.268571595618	0.239600302779	0.530908084704
C170	C	0.731428404382	0.739600302779	0.469091915296
C171	C	0.337808530981	0.227348976721	0.528103589226

C172	C	0.662191469019	0.727348976721	0.471896410774
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C174	C	0.635485654416	0.778023473477	0.444635070861
C175	C	0.260312856066	0.089871671215	0.634612204672
C176	C	0.739687143934	0.589871671215	0.365387795328
C177	C	0.290732929433	0.017264662862	0.623987200863
C178	C	0.709267070567	0.517264662862	0.376012799137
C179	C	0.367945777856	0.956839187814	0.588760425241
C180	C	0.632054222144	0.456839187814	0.411239574759
C181	C	0.392221913305	0.916247243766	0.619938236195
C182	C	0.607778086695	0.416247243766	0.380061763805
C183	C	0.423897623527	0.983086927420	0.567986604108
C184	C	0.576102376473	0.483086927420	0.432013395892
C185	C	0.456067800030	0.917860990003	0.550868045739
C186	C	0.543932199970	0.417860990003	0.449131954261
C187	C	0.411236785620	0.801900771528	0.651231792366
C188	C	0.588763214380	0.301900771528	0.348768207634
C189	C	0.478079487973	0.822371291837	0.657574976298
C190	C	0.521920512027	0.322371291837	0.342425023702
C191	C	0.404736413786	0.719417296929	0.641110045221
C192	C	0.595263586214	0.219417296929	0.358889954779
C193	C	0.344850493743	0.719218588246	0.621128281397
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C195	C	0.344796783767	0.793756316260	0.602060931577
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C197	C	0.556976885921	0.834716020389	0.700085274928
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C199	C	0.598168485250	0.775815839048	0.683571349939
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C201	C	0.564755600256	0.832093615663	0.738349622135
C202	C	0.435244399744	0.332093615663	0.261650377865
C203	C	0.534809978452	0.898253147426	0.756824504064
C204	C	0.465190021548	0.398253147426	0.243175495936
C205	C	0.555225213840	0.905185072980	0.793388110251
C206	C	0.444774786160	0.405185072980	0.206611889749
C207	C	0.613968724432	0.648027564078	0.664666257582
C208	C	0.386031275568	0.148027564078	0.335333742418
C209	C	0.632965701182	0.669125500291	0.628656412024
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C211	C	0.581815049911	0.571927144929	0.665286874400
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C215	C	0.643625180591	0.791933033476	0.574545241148
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C219	C	0.507667594605	0.669354914916	0.543164078439
C220	C	0.492332405395	0.169354914916	0.456835921560
C221	C	0.440880433133	0.688399274304	0.534333558327
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C223	C	0.540043207250	0.631334300102	0.513684467481
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C226	C	0.327308373884	0.407805692702	0.399051585459
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C228	C	0.261890925829	0.386434328448	0.388029015725
C229	C	0.644506268775	0.969023291314	0.622806884074
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C235	C	0.795204744302	0.732769261833	0.666455297757
C236	C	0.204795255698	0.232769261833	0.333544702243
C237	C	0.840350613743	0.686152311814	0.557920353677
C238	C	0.159649386258	0.186152311814	0.442079646323
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C241	C	0.808573139764	0.618431013519	0.541609226137
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C243	C	0.810725376382	0.548062416282	0.563284662328
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C271	C	0.031710167750	0.863387126362	0.614359790381
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C273	C	0.018299849586	0.865505406901	0.652041963274
C274	C	0.981700150414	0.365505406901	0.347958036726
C275	C	0.946882931163	0.900040510747	0.697216172225
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C277	C	0.924862770893	0.819004869368	0.704884583727
C278	C	0.075137229107	0.319004869368	0.295115416273
C279	C	0.894626750229	0.956076855919	0.703388716375
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C281	C	0.896997831678	0.728554669065	0.748517702029
C282	C	0.103002168322	0.228554669065	0.251482297971
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C284	C	0.152634267211	0.230076031834	0.224505165467
C285	C	0.956121582312	0.688784853398	0.762056556732
C286	C	0.043878417688	0.188784853398	0.237943443268
C287	C	0.980999226449	0.722894546929	0.794908216757
C288	C	0.019000773551	0.222894546929	0.205091783243
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C293	C	0.772126350789	0.653332242257	0.805907606296
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C295	C	0.804354674215	0.598536066809	0.829573804392
C296	C	0.195645325785	0.098536066809	0.170426195608
C297	C	0.710115373663	0.616840762713	0.795756210169

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C307	C	0.761514311710	0.553400116941	0.911579263106
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C313	C	0.932416279344	0.581382223619	0.884323944935
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C320	C	0.278246257783	0.015559451276	0.013335158761
C321	C	0.697589876135	0.392611677596	0.955450459064
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C323	C	0.760224246299	0.360518491319	0.944854714434
C324	C	0.239775753701	0.860518491319	0.055145285566
C325	C	0.783895603140	0.415082555393	0.918102717583
C326	C	0.216104396860	0.915082555393	0.081897282417
C327	C	0.799969192222	0.576469154867	0.020622427251
C328	C	0.200030807778	0.076469154867	0.979377572749
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C331	C	0.817657503657	0.789040056325	0.032690618590
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C333	C	0.881070197794	0.822310720299	0.041389718404
C334	C	0.118929802206	0.322310720299	0.958610281596
C335	C	0.766467253787	0.824532095464	0.053684808626
C336	C	0.233532746213	0.324532095464	0.946315191374
C337	C	0.992952492915	0.798487568229	0.042241623012
C338	C	0.007047507085	0.298487568229	0.957758376988
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C355	C	0.244747979398	0.716004827930	0.918188216172
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C357	C	0.195482484079	0.724170565351	0.891051485501
C358	C	0.804517515921	0.224170565351	0.108948514498
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C360	C	0.861855685466	0.247162548800	0.089265447806

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C364	C	0.633530806941	0.440958531243	0.107901047276
C365	C	0.358603041261	0.889311371696	0.834835688376
C366	C	0.641396958739	0.389311371696	0.165164311624
C367	C	0.295162547165	0.904589462925	0.819172447863
C368	C	0.704837452835	0.404589462925	0.180827552137
C369	C	0.392877153085	0.823529888702	0.818683152512
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C371	C	0.369258915492	0.744651280940	0.826879893133
C372	C	0.630741084508	0.244651280940	0.173120106867
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C374	C	0.814466362347	0.432454073514	0.170285492521
C375	C	0.163804284886	0.990795244846	0.855348580076
C376	C	0.836195715114	0.490795244847	0.144651419924
C377	C	0.139095282753	0.868704508647	0.824996566280
C378	C	0.860904717247	0.368704508647	0.175003433720
C379	C	0.155466932977	0.818910174688	0.795872421252
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C381	C	0.204907473667	0.768520623331	0.797326840276
C382	C	0.795092526333	0.268520623331	0.202673159724
C383	C	0.123739124146	0.825619069762	0.765582751794
C384	C	0.876260875854	0.325619069762	0.234417248206
C385	C	0.222236498304	0.727180307548	0.769361054805
C386	C	0.777763501696	0.227180307548	0.230638945195
C387	C	0.139843394877	0.783555545332	0.737418900907
C388	C	0.860156605123	0.283555545332	0.262581099093
C389	C	0.189141828705	0.733492016209	0.739370036353
C390	C	0.810858171295	0.233492016209	0.260629963647
C391	C	0.197236943956	0.103551054450	0.885313901892
C392	C	0.802763056044	0.603551054450	0.114686098108
C393	C	0.150740711852	0.165839261192	0.878124557013
C394	C	0.849259288148	0.665839261192	0.121875442987
C395	C	0.261017118520	0.137051878869	0.892298119470
C396	C	0.738982881480	0.637051878869	0.107701880530
C397	C	0.092827455112	0.233957859579	0.835642960395
C398	C	0.907172544888	0.733957859579	0.164357039604
C399	C	0.024691853496	0.212748750420	0.830670665550
C400	C	0.975308146504	0.712748750420	0.169329334450
C401	C	0.122810933772	0.268811140786	0.804322889002
C402	C	0.877189066228	0.768811140786	0.195677110997
C403	C	0.191699966870	0.279579083287	0.809815726470
C404	C	0.808300033130	0.779579083287	0.190184273530
N1	N	0.655528592047	0.735920891943	0.913616118429
N2	N	0.344471407954	0.235920891943	0.086383881571
N3	N	0.728583467397	0.882997056067	0.866841802912
N4	N	0.271416532603	0.382997056067	0.133158197087
N5	N	0.877813944435	0.915557136454	0.833179513374
N6	N	0.122186055565	0.415557136454	0.166820486626
N7	N	0.002248365501	0.021594412760	0.799584777492
N8	N	0.997751634499	0.521594412760	0.200415222508
N9	N	0.126189885208	0.024201017104	0.739948156215
N10	N	0.873810114792	0.524201017104	0.260051843785
N11	N	0.182397189073	0.154968103685	0.721050451058
N12	N	0.817602810928	0.654968103685	0.278949548942
N13	N	0.159812706914	0.353405683486	0.729249725470
N14	N	0.840187293086	0.853405683486	0.270750274529
N15	N	0.103260831005	0.424174977746	0.671896161995
N16	N	0.896739168995	0.924174977746	0.328103838005
N17	N	0.058630137097	0.293043013356	0.641376489430
N18	N	0.941369862903	0.793043013356	0.358623510570
N19	N	0.967087233686	0.265804352289	0.690200656741

N20	N	0.032912766314	0.765804352289	0.309799343258
N21	N	0.863973431339	0.230384579330	0.803127699337
N22	N	0.136026568661	0.730384579330	0.196872300663
N23	N	0.779595908864	0.151714644602	0.810209675189
N24	N	0.220404091136	0.651714644602	0.189790324811
N25	N	0.875637547278	0.118719852079	0.831566888636
N26	N	0.124362452722	0.618719852079	0.168433111364
N27	N	0.900149742767	0.400684277218	0.675400492922
N28	N	0.099850257233	0.900684277218	0.324599507078
N29	N	0.856984980832	0.371939357721	0.609911491191
N30	N	0.143015019168	0.871939357721	0.390088508809
N31	N	0.972421662924	0.315911962980	0.530484867401
N32	N	0.027578337076	0.815911962980	0.469515132599
N33	N	0.791734947030	0.242926714388	0.623812884578
N34	N	0.208265052971	0.742926714388	0.376187115422
N35	N	0.698230124094	0.300106904891	0.668288929853
N36	N	0.301769875906	0.800106904891	0.331711070147
N37	N	0.727923386192	0.427380901862	0.751195931861
N38	N	0.272076613809	0.927380901862	0.248804068139
N39	N	0.632129265336	0.386072961952	0.622124493481
N40	N	0.367870734664	0.886072961952	0.377875506519
N41	N	0.596989025532	0.269676241845	0.575819886357
N42	N	0.403010974468	0.769676241845	0.424180113643
N43	N	0.517491162854	0.198156599079	0.620961351580
N44	N	0.482508837146	0.698156599079	0.379038648419
N45	N	0.461732151455	0.051265923514	0.724906282175
N46	N	0.538267848545	0.551265923514	0.275093717824
N47	N	0.387279774285	0.963580014093	0.709164489146
N48	N	0.612720225715	0.463580014093	0.290835510854
N49	N	0.393891737418	0.002921886090	0.764097084205
N50	N	0.606108262583	0.502921886090	0.235902915795
N51	N	0.420937640423	0.303338422265	0.625226157217
N52	N	0.579062359577	0.803338422265	0.374773842783
N53	N	0.314320324024	0.281488178982	0.580902291397
N54	N	0.685679675976	0.781488178982	0.419097708603
N55	N	0.275351681189	0.154087080217	0.613880974187
N56	N	0.724648318811	0.654087080217	0.386119025813
N57	N	0.333209699717	0.021681300940	0.599542182959
N58	N	0.666790300283	0.521681300940	0.400457817040
N59	N	0.385326212530	0.841970035085	0.622441506251
N60	N	0.614673787470	0.341970035085	0.377558493749
N61	N	0.493342453349	0.826957752231	0.690029625175
N62	N	0.506657546652	0.326957752231	0.309970374825
N63	N	0.575232308047	0.706067614724	0.679464200450
N64	N	0.424767691954	0.206067614724	0.320535799550
N65	N	0.588747859938	0.696614282888	0.608450566003
N66	N	0.411252140062	0.196614282888	0.391549433997
N67	N	0.632858304425	0.843263537594	0.598657478118
N68	N	0.367141695575	0.343263537594	0.401342521882
N69	N	0.745108064053	0.824222101365	0.629992192832
N70	N	0.254891935948	0.324222101365	0.370007807168
N71	N	0.808886337642	0.712677693829	0.588073412062
N72	N	0.191113662359	0.212677693829	0.411926587937
N73	N	0.814045991815	0.809370172822	0.533096482621
N74	N	0.185954008185	0.309370172822	0.466903517379
N75	N	0.882878519508	0.939083037877	0.554508885505
N76	N	0.117121480492	0.439083037877	0.445491114495
N77	N	0.984329159071	0.894620615764	0.593220882368
N78	N	0.015670840929	0.394620615764	0.406779117632
N79	N	0.969447675726	0.904964504757	0.662903961424
N80	N	0.030552324274	0.404964504757	0.337096038576
N81	N	0.909229938955	0.804595955981	0.736938431092
N82	N	0.090770061045	0.304595955981	0.263061568907

N83	N	0.811768086412	0.668620378355	0.777317785577
N84	N	0.188231913588	0.168620378355	0.222682214423
N85	N	0.801357583170	0.615142160778	0.862129338035
N86	N	0.198642416830	0.115142160778	0.137870661965
N87	N	0.754251027016	0.486942745901	0.927291931428
N88	N	0.245748972985	0.986942745901	0.072708068572
N89	N	0.781586811807	0.531458112630	0.992525232086
N90	N	0.218413188193	0.031458112630	0.007474767914
N91	N	0.819562372994	0.707522965579	0.035207243753
N92	N	0.180437627006	0.207522965579	0.964792756247
N93	N	0.929443008830	0.776209678817	0.036463094456
N94	N	0.070556991170	0.276209678817	0.963536905544
N95	N	0.032544357228	0.840249239309	0.989361791568
N96	N	0.967455642772	0.340249239309	0.010638208432
N97	N	0.163466603854	0.788302967861	0.939769093117
N98	N	0.836533396146	0.288302967861	0.060230906883
N99	N	0.321082854883	0.861592011329	0.938410265102
N100	N	0.678917145117	0.361592011329	0.061589734898
N101	N	0.356608711443	0.882749293929	0.871150900674
N102	N	0.643391288557	0.382749293929	0.128849099326
N103	N	0.246603205770	0.907526811050	0.839894512201
N104	N	0.753396794230	0.407526811050	0.160105487799
N105	N	0.202137060563	0.049203027521	0.858510012451
N106	N	0.797862939437	0.549203027521	0.141489987549
N107	N	0.129774659126	0.171448858718	0.846961924666
N108	N	0.870225340874	0.671448858718	0.153038075334
N109	N	0.208544045251	0.329360849467	0.833487264397
N110	N	0.791455954749	0.829360849467	0.166512735603
O1	O	0.747949308550	0.757735045431	0.869506857597
O2	O	0.252050691450	0.257735045431	0.130493142403
O3	O	0.691615746532	0.795629061569	0.972300495803
O4	O	0.308384253468	0.295629061569	0.027699504197
O5	O	0.826390069803	0.989607342012	0.870950945112
O6	O	0.173609930198	0.489607342012	0.129049054888
O7	O	0.699039299891	0.993749691967	0.819199957305
O8	O	0.300960700109	0.493749691967	0.180800042695
O9	O	0.955607982911	0.917162376759	0.779720105512
O10	O	0.044392017089	0.417162376759	0.220279894488
O11	O	0.122920510577	0.075029140035	0.791977674852
O12	O	0.877079489423	0.575029140035	0.208022325148
O13	O	0.277197174639	0.112437986904	0.736091906720
O14	O	0.722802825361	0.612437986904	0.263908093280
O15	O	0.091761559832	0.257650599089	0.721232082033
O16	O	0.908238440168	0.757650599089	0.278767917966
O17	O	0.184547555882	0.248066292969	0.657319899247
O18	O	0.815452444118	0.748066292969	0.342680100753
O19	O	0.017864556332	0.426907074735	0.704652970979
O20	O	0.982135443668	0.926907074735	0.295347029021
O21	O	0.984747027214	0.362886907620	0.616748798828
O22	O	0.015252972786	0.862886907620	0.383251201172
O23	O	0.911553394608	0.215718483540	0.647496453324
O24	O	0.088446605392	0.715718483540	0.352503546675
O25	O	0.815604855777	0.336972763467	0.692825096002
O26	O	0.184395144223	0.836972763467	0.307174903998
O27	O	0.769188323997	0.430328373041	0.626411894524
O28	O	0.230811676003	0.930328373041	0.373588105476
O29	O	0.935345532026	0.556441944035	0.667630014501
O30	O	0.064654467974	0.056441944035	0.332369985499
O31	O	0.728416822200	0.272344302443	0.580318955742
O32	O	0.271583177800	0.772344302443	0.419681044258
O33	O	0.910259697814	0.414780488802	0.543027734231
O34	O	0.089740302186	0.914780488802	0.456972265769
O35	O	0.639381233874	0.207948115298	0.645725104708

O36	O	0.360618766126	0.707948115298	0.354274895292
O37	O	0.547295528908	0.369744811387	0.654421663951
O38	O	0.452704471092	0.869744811387	0.345578336049
O39	O	0.666357138597	0.324883767956	0.750979617150
O40	O	0.333642861403	0.824883767956	0.249020382850
O41	O	0.508090313730	0.335321359850	0.571481323594
O42	O	0.491909686270	0.835321359850	0.428518676406
O43	O	0.465505989384	0.151859700503	0.576341321172
O44	O	0.534494010617	0.651859700503	0.423658678828
O45	O	0.364972581277	0.222124989399	0.656022367844
O46	O	0.635027418723	0.722124989399	0.343977632156
O47	O	0.261273898606	0.341129822746	0.621546290259
O48	O	0.738726101394	0.841129822746	0.378453709741
O49	O	0.208829654530	0.124954033746	0.571895832921
O50	O	0.791170345470	0.624954033746	0.428104167078
O51	O	0.277328271635	0.957654093758	0.637882630482
O52	O	0.722671728365	0.457654093758	0.362117369518
O53	O	0.420805297837	0.953470534007	0.641159122064
O54	O	0.579194702163	0.453470534007	0.358840877936
O55	O	0.404303281533	0.038841714795	0.544564555828
O56	O	0.595696718467	0.538841714795	0.455435444172
O57	O	0.515829663403	0.827381838304	0.634073805464
O58	O	0.484170336597	0.327381838304	0.365926194536
O59	O	0.650690670858	0.793546560370	0.674437606295
O60	O	0.349309329142	0.293546560370	0.325562393705
O61	O	0.553443979761	0.846612729828	0.811052897974
O62	O	0.446556020239	0.346612729828	0.188947102026
O63	O	0.572997286946	0.969121880993	0.803981373028
O64	O	0.427002713054	0.469121880993	0.196018626972
O65	O	0.686415684346	0.657996732547	0.618725293800
O66	O	0.313584315654	0.157996732547	0.381274706200
O67	O	0.684702700416	0.799598890296	0.553318240386
O68	O	0.315297299584	0.299598890296	0.446681759613
O69	O	0.781664884242	0.927009493450	0.602663054236
O70	O	0.218335115758	0.427009493451	0.397336945764
O71	O	0.893760991702	0.776593519864	0.603918428794
O72	O	0.106239008298	0.276593519864	0.396081571206
O73	O	0.895395871145	0.743315411015	0.512618491902
O74	O	0.104604128855	0.243315411015	0.487381508098
O75	O	0.747363950347	0.640275276405	0.533623515596
O76	O	0.252636049653	0.140275276405	0.466376484404
O77	O	0.923320560735	0.933904019409	0.501766905380
O78	O	0.076679439265	0.433904019409	0.498233094620
O79	O	0.771375806498	0.147849139019	0.408644057027
O80	O	0.228624193502	0.647849139019	0.591355942973
O81	O	0.026833239518	0.011028993259	0.586950812045
O82	O	0.973166760482	0.511028993259	0.413049187955
O83	O	0.881592409012	0.003193186005	0.623636903828
O84	O	0.118407590988	0.503193186005	0.376363096172
O85	O	0.052941466837	0.830648125756	0.671358430378
O86	O	0.947058533163	0.330648125756	0.328641569622
O87	O	0.922009679025	0.771917060148	0.682311781172
O88	O	0.077990320975	0.271917060148	0.317688218827
O89	O	0.843486491322	0.783216671829	0.795601960804
O90	O	0.156513508678	0.283216671829	0.204398039196
O91	O	0.827506097798	0.539091614714	0.818438437103
O92	O	0.172493902203	0.039091614714	0.181561562897
O93	O	0.725455867229	0.606177482503	0.916648835468
O94	O	0.274544132771	0.106177482503	0.083351164532
O95	O	0.679924505474	0.528665329943	0.006684938657
O96	O	0.320075494527	0.028665329943	0.993315061343
O97	O	0.764311782990	0.682074358857	0.988075007040
O98	O	0.235688217010	0.182074358857	0.011924992960

O99	O	0.886267904321	0.887921698012	0.051218271804
O100	O	0.113732095679	0.387921698012	0.948781728196
O101	O	0.047922249915	0.717849234874	0.003153529726
O102	O	0.952077750085	0.217849234874	0.996846470274
O103	O	0.982337527320	0.781968751912	0.101575314672
O104	O	0.017662472680	0.281968751912	0.898424685328
O105	O	0.158367745065	0.865382711707	0.984724229790
O106	O	0.841632254935	0.365382711707	0.015275770210
O107	O	0.233491587352	0.902172252342	0.913062888100
O108	O	0.766508412648	0.402172252342	0.086937111900
O109	O	0.383317506449	0.003839101315	0.882695207192
O110	O	0.616682493551	0.503839101315	0.117304792808
O111	O	0.291168802909	0.916860328788	0.788460170351
O112	O	0.708831197091	0.416860328788	0.211539829649
O113	O	0.324158892286	0.737268749047	0.846703135437
O114	O	0.675841107714	0.237268749047	0.153296864563
O115	O	0.398072692041	0.691812493113	0.812591923216
O116	O	0.601927307959	0.191812493113	0.187408076784
O117	O	0.115790690340	0.982724613400	0.871991185552
O118	O	0.884209309661	0.482724613400	0.128008814448
O119	O	0.206858471162	0.689113538025	0.713308209895
O120	O	0.793141528838	0.189113538025	0.286691790104
O121	O	0.135670636194	0.210315306232	0.901010298590
O122	O	0.864329363806	0.710315306232	0.098989701410
O123	O	0.005791804658	0.150562602653	0.841960086277
O124	O	0.994208195342	0.650562602653	0.158039913723
O125	O	0.229849273812	0.242284810464	0.793830001769
O126	O	0.770150726188	0.742284810464	0.206169998231
O127	O	0.991554330988	0.259972708917	0.815613472096
O128	O	0.008445669012	0.759972708917	0.184386527904
O129	O	0.703260959321	0.027536933647	0.890128618373
O130	O	0.296739040679	0.527536933647	0.109871381627
O131	O	0.283816578692	0.100194092812	0.808496851019
O132	O	0.716183421308	0.600194092812	0.191503148981
O133	O	0.456590929383	0.040218166605	0.827057976451
O134	O	0.543409070618	0.540218166605	0.172942023549
O135	O	0.290477680124	0.390675059370	0.726363649190
O136	O	0.709522319876	0.890675059370	0.273636350810
O137	O	0.236676525789	0.444035046420	0.669369284041
O138	O	0.763323474211	0.944035046420	0.330630715958
O139	O	0.253349424860	0.592611877085	0.652201866166
O140	O	0.746650575140	0.092611877085	0.347798133834
O141	O	0.330010477372	0.645322765857	0.703582827930
O142	O	0.669989522628	0.145322765857	0.296417172070
O143	O	0.348686340509	0.518534641481	0.744853018091
O144	O	0.651313659491	0.018534641480	0.255146981909
O145	O	0.695338299289	0.270462564532	0.813116193625
O146	O	0.304661700711	0.770462564532	0.186883806375
O147	O	0.907865044350	0.515399496610	0.734995895897
O148	O	0.092134955650	0.015399496610	0.265004104103
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3) CRAMBIN CRYSTAL – optimized 172W

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H5   H     0.659391833414   0.766290797433   0.971352084626
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H174	H	0.293039284367	0.639359394648	0.391624744701
H175	H	0.802049605268	0.130321833842	0.697285945902
H176	H	0.203800820137	0.624012566391	0.351466180756
H177	H	0.768988629651	0.198962269120	0.722600335868
H178	H	0.235602376933	0.691238475515	0.324943522491
H179	H	0.672925758034	0.168886323802	0.754595809227
H180	H	0.331859923655	0.662375587558	0.293630268937
H181	H	0.760956391763	0.007362050797	0.692569319510
H182	H	0.247435367814	0.501332397528	0.357505958128
H183	H	0.610498439414	0.070551878362	0.779817517646
H184	H	0.395712742101	0.564210961692	0.269449146252
H185	H	0.697587899979	0.907677846018	0.717962634814
H186	H	0.314272442808	0.403192411879	0.333930713873
H187	H	0.622588308866	0.939812436174	0.761259042883
H188	H	0.388718893379	0.435655224328	0.290051964342
H189	H	0.718171013611	0.312060496721	0.702954798217
H190	H	0.286382940556	0.807023929044	0.342974785853
H191	H	0.593353291904	0.294434899178	0.722454970107
H192	H	0.411757028960	0.797055473295	0.323782546160
H193	H	0.666414974658	0.438854313489	0.716820965385
H194	H	0.327532682388	0.931387066620	0.329452605318
H195	H	0.594801601436	0.427254939376	0.735641575761
H196	H	0.401956268856	0.934038348995	0.313772393102
H197	H	0.718123830554	0.475822339217	0.764721920235
H198	H	0.293853761767	0.974157359096	0.277475808172

H199	H	0.717457432925	0.422647860237	0.802115484290
H200	H	0.303939597045	0.923946385466	0.239583918249
H201	H	0.657407167391	0.375613941337	0.648956643850
H202	H	0.342991019402	0.878294917283	0.397117444917
H203	H	0.540010261644	0.429272262515	0.624574748521
H204	H	0.458455902265	0.932250893796	0.422972000161
H205	H	0.660172018080	0.394415915034	0.591442321770
H206	H	0.339743295591	0.890111552001	0.456247033749
H207	H	0.617562639046	0.454305002725	0.539010900019
H208	H	0.381014530527	0.951584015995	0.508577294163
H209	H	0.544141679343	0.451149000679	0.556509281281
H210	H	0.454242012869	0.951570959737	0.490897671882
H211	H	0.583211142343	0.367958847968	0.547835013114
H212	H	0.417447006203	0.866699092821	0.499432811025
H213	H	0.664169013252	0.532746165313	0.585157078046
H214	H	0.331018567764	0.027570859817	0.463852436457
H215	H	0.655352420308	0.507779222619	0.627624413839
H216	H	0.338928896617	0.005554226039	0.420993074778
H217	H	0.591937091267	0.539765422947	0.604034911918
H218	H	0.402083692654	0.039861619525	0.444250237995
H219	H	0.622022243134	0.260209183408	0.611017985991
H220	H	0.380871470533	0.759357257969	0.436259424885
H221	H	0.534233639294	0.193579122532	0.567175337314
H222	H	0.472803422731	0.697999228117	0.479501557439
H223	H	0.637489632457	0.146051414384	0.577432338081
H224	H	0.370025466706	0.646935906913	0.472623560265
H225	H	0.622471203809	0.131887182144	0.620699543650
H226	H	0.381193792629	0.631311039119	0.429111082457
H227	H	0.536165905695	0.205752686787	0.656672903498
H228	H	0.464836072669	0.708637110250	0.390108323511
H229	H	0.427788302201	0.115625283134	0.662066749078
H230	H	0.575525361779	0.623479902612	0.383621155949
H231	H	0.490779220971	0.223437360545	0.710813465606
H232	H	0.501977025523	0.720952230559	0.335230489897
H233	H	0.429537350466	0.167558753279	0.721998299429
H234	H	0.567912812235	0.674164042909	0.323032743837
H235	H	0.548236062837	0.102960605071	0.694868091075
H236	H	0.458158698571	0.595173042861	0.353884484468
H237	H	0.536773931306	0.122089520862	0.737441687678
H238	H	0.465056984181	0.610830150284	0.310827430410
H239	H	0.453589767140	0.019224240878	0.695879566463
H240	H	0.558113136773	0.524041845195	0.353460124267
H241	H	0.517605664901	0.988537400682	0.718717612501
H242	H	0.497561006933	0.483691751400	0.330825296636
H243	H	0.468094669836	0.050484816053	0.769965027622
H244	H	0.544576999995	0.552856096337	0.279469386564
H245	H	0.382315353942	0.949798697969	0.706897338250
H246	H	0.623685412873	0.445937517796	0.342823355170
H247	H	0.331993690529	0.920497610321	0.737823300914
H248	H	0.674280892775	0.414532222901	0.312383146028
H249	H	0.402104490108	0.020486031416	0.803958202836
H250	H	0.611655168690	0.515195258682	0.245273407147
H251	H	0.338615610338	0.964311109612	0.792959699311
H252	H	0.669781481683	0.454617138362	0.256933230088
H253	H	0.440885450419	0.299613528174	0.636859434152
H254	H	0.557896330513	0.806700795780	0.407234629245
H255	H	0.334991102685	0.352451695090	0.670143337259
H256	H	0.662574586382	0.863172866284	0.374972992227
H257	H	0.393590524073	0.397729627218	0.603818662758
H258	H	0.598209299518	0.899782187279	0.440416297864
H259	H	0.330219901558	0.442678068482	0.620937229067
H260	H	0.666451300273	0.944651153401	0.430173411924
H261	H	0.454846898015	0.431614675098	0.654822119771

H262	H	0.553185016129	0.945659372093	0.385231496389
H263	H	0.451888970942	0.509799459137	0.603200698283
H264	H	0.535896092688	0.007331861180	0.440207836555
H265	H	0.460971242237	0.566190304741	0.639495661702
H266	H	0.539875189606	0.074653994564	0.407737174952
H267	H	0.389463120155	0.560143578638	0.618887229450
H268	H	0.602368828472	0.061044752105	0.435492969698
H269	H	0.413455275954	0.526450056161	0.695132037118
H270	H	0.607267500804	0.050966051325	0.356569360676
H271	H	0.377856695202	0.439827758351	0.699063049695
H272	H	0.647266750267	0.967573308490	0.352508695364
H273	H	0.340205280244	0.512932143732	0.677401193941
H274	H	0.671823049745	0.034272613928	0.382412908523
H275	H	0.204790195943	0.267911537552	0.587081028601
H276	H	0.793036767901	0.768877482199	0.455657132609
H277	H	0.236649897652	0.156834697373	0.542591460047
H278	H	0.761209366477	0.675776217414	0.506052868943
H279	H	0.246754241259	0.251273839844	0.533065714306
H280	H	0.748069447578	0.771248909587	0.509511543030
H281	H	0.341793713084	0.144500813112	0.560699589062
H282	H	0.655406528389	0.656276567821	0.486481850459
H283	H	0.348156442290	0.207692951211	0.526698100832
H284	H	0.647891411713	0.722979033512	0.518955911900
H285	H	0.391653872943	0.244279466020	0.589525486601
H286	H	0.605077709093	0.752996403746	0.455267859466
H287	H	0.355292345248	0.312383884205	0.564167278303
H288	H	0.641798709352	0.823530061019	0.478903612957
H289	H	0.292061178946	0.168734975489	0.640528207486
H290	H	0.709011344764	0.678725136921	0.401570746125
H291	H	0.251473698117	0.086843993290	0.678745981460
H292	H	0.737390268636	0.585857949561	0.367377468589
H293	H	0.192528304966	0.062226758893	0.649496935176
H294	H	0.804550541597	0.571798891204	0.392229084049
H295	H	0.322340337355	0.051444404868	0.606847254391
H296	H	0.667809346992	0.561895706653	0.434582648580
H297	H	0.324316577542	0.903753654298	0.594864425456
H298	H	0.680012018104	0.414606389699	0.457122113975
H299	H	0.436595145937	0.996557331311	0.610093921869
H300	H	0.563710357641	0.494455421694	0.437053910531
H301	H	0.413135287896	0.064150606924	0.570708268127
H302	H	0.581898732756	0.570933874898	0.473808465795
H303	H	0.462115758738	0.869082386259	0.597027821908
H304	H	0.542826409021	0.368258977715	0.452454476532
H305	H	0.479939476981	0.924056312087	0.561420874370
H306	H	0.521659558948	0.424055206824	0.487210153082
H307	H	0.413560473424	0.868408789905	0.560583396039
H308	H	0.590292748172	0.373114646646	0.489244010711
H309	H	0.365944284307	0.800514985405	0.696957939170
H310	H	0.644672919211	0.294836210776	0.357591291479
H311	H	0.427370458589	0.691171115078	0.649879214652
H312	H	0.583042424257	0.190063046574	0.406432379838
H313	H	0.385833491516	0.671807196708	0.687454295474
H314	H	0.626370897281	0.167138556497	0.370304366483
H315	H	0.326057742578	0.657756728623	0.627613299196
H316	H	0.682659664600	0.162002058981	0.431824576183
H317	H	0.291257302173	0.707454912579	0.660624918031
H318	H	0.719823763168	0.206948717053	0.398249184746
H319	H	0.353835723749	0.771316179984	0.599264393516
H320	H	0.652810805753	0.278767478260	0.456153874871
H321	H	0.286640625942	0.801390769218	0.619683179428
H322	H	0.720733012555	0.307479310269	0.436070055459
H323	H	0.441723718127	0.797001805341	0.733024527021
H324	H	0.570814250174	0.286985361237	0.321480385946

H325	H	0.553071594068	0.873989813506	0.718952274853
H326	H	0.462009022713	0.373046142568	0.334282208658
H327	H	0.528393987430	0.755142783245	0.772025089028
H328	H	0.484921100209	0.254981734952	0.280885480072
H329	H	0.593568423049	0.810157627753	0.770050689768
H330	H	0.424184914778	0.317438749260	0.280925771801
H331	H	0.526501805350	0.924975316132	0.778091012502
H332	H	0.495720034878	0.424087896708	0.273450852065
H333	H	0.464195391833	0.865459203215	0.782539981100
H334	H	0.557781175373	0.363540676473	0.276418355656
H335	H	0.520743288527	0.677161329696	0.716280520392
H336	H	0.486562955909	0.173716865703	0.336173969828
H337	H	0.640626376640	0.638973745360	0.702906258341
H338	H	0.361895230258	0.144844889362	0.345987634628
H339	H	0.560272774164	0.548283633230	0.716058940156
H340	H	0.438076990755	0.048755309238	0.332573175099
H341	H	0.598015139265	0.523060885263	0.678447029947
H342	H	0.395365085387	0.024484600126	0.368623917139
H343	H	0.524578964118	0.563423145074	0.676348541740
H344	H	0.471113940545	0.056954290738	0.373473008022
H345	H	0.532750261757	0.707456174454	0.643337224002
H346	H	0.469066910007	0.207222316747	0.406948443709
H347	H	0.613766484475	0.673573958083	0.586431771978
H348	H	0.384958377977	0.175275245773	0.462637178932
H349	H	0.493972801074	0.756647377171	0.593850633913
H350	H	0.505782696471	0.257825089596	0.457208199101
H351	H	0.535915661339	0.763081938006	0.556540980160
H352	H	0.462856966319	0.260319226310	0.494281477714
H353	H	0.495139951788	0.615540011853	0.586042587071
H354	H	0.504222720991	0.115672433314	0.462367407084
H355	H	0.403164304905	0.687297903810	0.573457484944
H356	H	0.596204779480	0.186830367526	0.475056890076
H357	H	0.410873304722	0.617518114971	0.542605354270
H358	H	0.589645479773	0.115432076214	0.505294386987
H359	H	0.429705459187	0.710662621253	0.532813802553
H360	H	0.570911335895	0.208003605877	0.516133197424
H361	H	0.514312767201	0.567213254670	0.528066211005
H362	H	0.486921018181	0.063519202152	0.519949797982
H363	H	0.580997524561	0.605119946434	0.545820860356
H364	H	0.419628736499	0.101137389391	0.502705560163
H365	H	0.539230981769	0.655760063712	0.515281676279
H366	H	0.461128167212	0.150797281360	0.533862622752
H367	H	0.577288348530	0.827335185885	0.639599890244
H368	H	0.428683268364	0.329465913974	0.411176402382
H369	H	0.658921010665	0.921283428206	0.601819240817
H370	H	0.347331740178	0.426567880317	0.447494238724
H371	H	0.610923965903	0.935108536540	0.673731377748
H372	H	0.397522253836	0.437382470340	0.375892578784
H373	H	0.655824924140	0.002451419502	0.653430967060
H374	H	0.353059897498	0.506031017842	0.395398168972
H375	H	0.686304650262	0.793400949424	0.668081223693
H376	H	0.322329721426	0.300701054770	0.380371169119
H377	H	0.811753726995	0.833160716350	0.677295473569
H378	H	0.199353400880	0.347121005678	0.367149896069
H379	H	0.760537990045	0.752441300362	0.718146853933
H380	H	0.256564354427	0.268050973396	0.327531274684
H381	H	0.820194335863	0.701814487352	0.699116800320
H382	H	0.189402987985	0.222438230415	0.341034032134
H383	H	0.743807829146	0.686043135541	0.686317623520
H384	H	0.260974552880	0.195863970048	0.357911509744
H385	H	0.745292473654	0.695367248893	0.619586888540
H386	H	0.256140672214	0.199788677162	0.423359522571
H387	H	0.867525572026	0.671805606834	0.593290713022

H388	H	0.132477900911	0.178834251632	0.445532147958
H389	H	0.817274995804	0.614585080757	0.544746250300
H390	H	0.176968936870	0.119199934292	0.495879164116
H391	H	0.718060487309	0.601585610117	0.544086496653
H392	H	0.277044843457	0.100424839897	0.496972914551
H393	H	0.847364958016	0.534537632761	0.592693510402
H394	H	0.146775989593	0.044657978270	0.448114353869
H395	H	0.780599143515	0.502504877601	0.573085473794
H396	H	0.214115515164	0.008014770689	0.465498369060
H397	H	0.775536398388	0.550308539955	0.612143296192
H398	H	0.217828032860	0.060099352570	0.427566610103
H399	H	0.749647420165	0.802193163501	0.572532626646
H400	H	0.251022122121	0.301244245531	0.474907552944
H401	H	0.812341763128	0.847404994321	0.513541362782
H402	H	0.184878461698	0.347194174815	0.532506552463
H403	H	0.703802961591	0.879259874763	0.527385825392
H404	H	0.294056650300	0.377599764352	0.520121641865
H405	H	0.729988996558	0.941871670157	0.558172015358
H406	H	0.270297576869	0.438087855485	0.487975867745
H407	H	0.757039243643	0.896327910992	0.466825709568
H408	H	0.248389820774	0.401144269477	0.580050350375
H409	H	0.746979180504	0.068771156131	0.540846306155
H410	H	0.247034028577	0.566306025786	0.502360653810
H411	H	0.780876415120	0.987533157085	0.423349136610
H412	H	0.230457958392	0.496894507273	0.622685126212
H413	H	0.772747393342	0.161248195780	0.496935273538
H414	H	0.228313695704	0.663144974389	0.545461727945
H415	H	0.789841702876	0.112264252279	0.411309532478
H416	H	0.219325300426	0.619626016634	0.632810879832
H417	H	0.828044597108	0.913264345718	0.596802854390
H418	H	0.182966736217	0.424377573757	0.449733506012
H419	H	0.910990027340	0.029764699779	0.572681520829
H420	H	0.097682632081	0.537994251369	0.471611274729
H421	H	0.900641241878	0.080480214453	0.630248017615
H422	H	0.097715587043	0.577447153869	0.412237836393
H423	H	0.821278340983	0.961994028273	0.645295758834
H424	H	0.181614663076	0.462131131697	0.399627141141
H425	H	0.821061753491	0.110740676671	0.586553439463
H426	H	0.177192879849	0.622611424784	0.452586451980
H427	H	0.795358561124	0.115671794842	0.628566789139
H428	H	0.201158371145	0.619640336976	0.410387227859
H429	H	0.774579182353	0.038786463665	0.602854383940
H430	H	0.226731876508	0.550625998281	0.439237575606
H431	H	0.925831607137	0.859688982753	0.609519913998
H432	H	0.083536574409	0.367154917214	0.430271688602
H433	H	0.014417009473	0.800780765740	0.627359437063
H434	H	0.987870462517	0.306361078940	0.420884074452
H435	H	0.054034321626	0.885988175470	0.628549031523
H436	H	0.951779539293	0.393936275815	0.418745693621
H437	H	0.925449131545	0.923616500988	0.667518892035
H438	H	0.076838001794	0.425454088626	0.377681186427
H439	H	0.976029670541	0.910094456290	0.735907512187
H440	H	0.025565416669	0.406241444110	0.309811779405
H441	H	0.845486127457	0.939090409398	0.711741468703
H442	H	0.157163318469	0.432497874880	0.332808885365
H443	H	0.874122294846	0.949837101708	0.753263412183
H444	H	0.128021416052	0.439162393478	0.291263119140
H445	H	0.918248780015	0.845376330925	0.777814204223
H446	H	0.071944673267	0.334032743831	0.269491658303
H447	H	0.874707818873	0.700785694411	0.751291383018
H448	H	0.117438647988	0.192029905694	0.297530526579
H449	H	0.936201021966	0.636477093691	0.792226643562
H450	H	0.052130831823	0.123516582463	0.261085683018

H451	H	0.992987656060	0.783645617053	0.812993188784
H452	H	0.996047723263	0.266927895614	0.234920349281
H453	H	0.939964850600	0.733641558846	0.836727657788
H454	H	0.049423749796	0.213822658798	0.212979642084
H455	H	0.038914204742	0.667024755100	0.766838381490
H456	H	0.950854968020	0.163667211998	0.286968859047
H457	H	0.005605286762	0.743039102299	0.746698123983
H458	H	0.987596606339	0.242426389344	0.302414182040
H459	H	0.979684852980	0.652382801849	0.737159910759
H460	H	0.011644146926	0.154384650972	0.316287125508
H461	H	0.012836357901	0.624975067664	0.838899882847
H462	H	0.977538453880	0.104888257113	0.212464476019
H463	H	0.041143281398	0.706194794082	0.859146069776
H464	H	0.946717111368	0.182888217450	0.191735070170
H465	H	0.068201187650	0.681326202649	0.819067845974
H466	H	0.922335520961	0.160409330263	0.232493871120
H467	H	0.821390281368	0.630637272400	0.788783840959
H468	H	0.164951339964	0.117371147563	0.258589993304
H469	H	0.767981155008	0.718731833892	0.844386599601
H470	H	0.217820158254	0.207052716297	0.203298524057
H471	H	0.711340677506	0.578699806257	0.814677831324
H472	H	0.283922637291	0.079839786645	0.238605494027
H473	H	0.662407580878	0.733481484897	0.801566589906
H474	H	0.293941556215	0.245809041782	0.251711558641
H475	H	0.709718243540	0.685715095863	0.773082090810
H476	H	0.266683894625	0.178037602073	0.278585577669
H477	H	0.683646027223	0.603858884443	0.874689008979
H478	H	0.314667553763	0.104738082494	0.178797531354
H479	H	0.620661118777	0.621020810981	0.848331826520
H480	H	0.373550956633	0.129209511960	0.206980555860
H481	H	0.664212582818	0.696078651186	0.864104114530
H482	H	0.327075648722	0.198512284667	0.188536890499
H483	H	0.636749150923	0.581270772581	0.769318195484
H484	H	0.366587850273	0.114108814364	0.281630497599
H485	H	0.601251228951	0.665289238141	0.757712593564
H486	H	0.369218605530	0.206712010587	0.296364754412
H487	H	0.586882275123	0.626470732645	0.797314616257
H488	H	0.399644468483	0.183570530097	0.256523901525
H489	H	0.789377222624	0.678093274777	0.895303751492
H490	H	0.195126431643	0.169602570495	0.154487376908
H491	H	0.831973868448	0.522780737592	0.899131243834
H492	H	0.167869680152	0.009983663666	0.146344694129
H493	H	0.894432600498	0.550339784281	0.948545428940
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H495	H	0.868003217955	0.713847336758	0.935045598307
H496	H	0.121864766176	0.198897129322	0.110569204142
H497	H	0.838464721010	0.661781912671	0.968514775146
H498	H	0.147687153971	0.145384170044	0.076795517603
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H500	H	0.013611431660	0.081951782650	0.132314654355
H501	H	0.928964848162	0.647725594501	0.888153306766
H502	H	0.062317977731	0.133644615987	0.159123828729
H503	H	0.935609403373	0.550312811765	0.889030166021
H504	H	0.062654943880	0.036357196285	0.161267014902
H505	H	0.943295302992	0.640648475044	0.992021496864
H506	H	0.038866211775	0.119754164255	0.058720013069
H507	H	0.925259145948	0.735733610061	0.988668992137
H508	H	0.057836115194	0.214844821938	0.058622839278
H509	H	0.973876138968	0.694305447433	0.959015831608
H510	H	0.013884442396	0.177791180398	0.091579471718
H511	H	0.678870451700	0.492989460197	0.970177411882
H512	H	0.318920320708	0.036715184061	0.073996386782
H513	H	0.731230278216	0.385944254885	0.013401271435

H514	H	0.312447253649	0.905964678706	0.037672554593
H515	H	0.688478391968	0.370068981669	0.975964389489
H516	H	0.336815194300	0.908514011487	0.080285876356
H517	H	0.825050557210	0.371185447788	0.986353409627
H518	H	0.210017158998	0.872821310848	0.052194130569
H519	H	0.782189166940	0.313545441204	0.959007334135
H520	H	0.251027430964	0.822357217696	0.083197841610
H521	H	0.845576238992	0.434536375344	0.936123213020
H522	H	0.164751177841	0.923721939015	0.101271345829
H523	H	0.775467018856	0.408980285274	0.916246994778
H524	H	0.232591995933	0.913234036259	0.126311085154
H525	H	0.827328092107	0.534496182985	0.003689120224
H526	H	0.168593038720	0.018781371914	0.043670126420
H527	H	0.781421749969	0.575266413741	0.068906831044
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H529	H	0.854858436876	0.589956995495	0.051937054432
H530	H	0.126312043294	0.076273798198	0.998465297802
H531	H	0.835341361075	0.696242393763	0.088325755349
H532	H	0.156847445912	0.193649308674	0.959088292508
H533	H	0.776048628352	0.820282710132	0.052162782137
H534	H	0.206992770818	0.305623355808	0.006519041925
H535	H	0.743469323822	0.805796564051	0.111250008234
H536	H	0.264651024263	0.294413234120	0.954512257783
H537	H	0.785259846984	0.888642628732	0.105341414685
H538	H	0.224486013929	0.380244170693	0.954828189803
H539	H	0.820167171424	0.811218791100	0.125470244019
H540	H	0.198152609452	0.305570868469	0.929201124665
H541	H	0.913609337918	0.738415758551	0.064568450815
H542	H	0.077788586023	0.232520940610	0.984395909084
H543	H	0.977357983575	0.882323155793	0.068864068642
H544	H	0.014050398483	0.375091785893	0.974581269516
H545	H	0.018082250309	0.730366116336	0.094488644363
H546	H	0.986860516308	0.223394017586	0.944072901116
H547	H	0.939364906800	0.761995650023	0.124867194431
H548	H	0.064086289771	0.272108919939	0.918912514537
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H551	H	0.090631255095	0.801371097744	0.129503121073
H552	H	0.913402262322	0.292389096420	0.908023538025
H553	H	0.065549847560	0.886030835981	0.110238195889
H554	H	0.923410551328	0.372090955047	0.934584349693
H555	H	0.998273140836	0.907073846764	0.017540472807
H556	H	0.992450919465	0.398962968472	0.025601274545
H557	H	0.026196373660	0.800690775626	0.966474701489
H558	H	0.957282635404	0.288056358247	0.073384802493
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H560	H	0.954271395231	0.457753739033	0.072989765511
H561	H	0.067236838839	0.915666070840	0.936538400048
H562	H	0.933143515755	0.405313070654	0.108410513884
H563	H	0.221833950802	0.769141999018	0.991001405675
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H565	H	0.261931375572	0.716130283072	0.930686816448
H566	H	0.716601422716	0.211905767019	0.101990698021
H567	H	0.211014158583	0.664202757107	0.955182781018
H568	H	0.761127241331	0.169605038485	0.070692210993
H569	H	0.179294189302	0.767698703471	0.896509592675
H570	H	0.804136594067	0.232272539195	0.138795932836
H571	H	0.157042864790	0.673341694234	0.901036834012
H572	H	0.820565029353	0.143135060186	0.122947232064
H573	H	0.081629395425	0.786277800362	0.920836802582
H574	H	0.901399339309	0.256160857293	0.115927403970
H575	H	0.086579603289	0.702757346918	0.944547187562
H576	H	0.891880891952	0.190058910614	0.083004546276

H577	H	0.312756492280	0.825203113100	0.980695324212
H578	H	0.671281152795	0.338747822366	0.067675788038
H579	H	0.306216763496	0.976583876271	0.964363587649
H580	H	0.681293487871	0.484519056851	0.092825204004
H581	H	0.372898523516	0.925575236145	0.970585885660
H582	H	0.614777247105	0.430354258824	0.089614674626
H583	H	0.319713555192	0.837755631068	0.904801775274
H584	H	0.669930393240	0.319991096778	0.142373135298
H585	H	0.362151303640	0.949140039533	0.856786625983
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H590	H	0.589264484985	0.287790464946	0.197813506928
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H592	H	0.763879636501	0.386218209725	0.160812345066
H593	H	0.174364152474	0.954531038380	0.824181681480
H594	H	0.821402783508	0.449342725764	0.221953095644
H595	H	0.119205655432	0.834014930116	0.868028464466
H596	H	0.875962581686	0.329359339515	0.177605139181
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H598	H	0.917392703284	0.384672522818	0.206544981914
H599	H	0.207448195421	0.748841853965	0.843785546579
H600	H	0.792059148029	0.242837121507	0.203138371010
H601	H	0.079960247769	0.865898860472	0.780734923198
H602	H	0.917548880348	0.366617271765	0.264667838206
H603	H	0.235688176480	0.671330585562	0.795451452018
H604	H	0.763362653310	0.169283665047	0.252640508599
H605	H	0.108317904145	0.789267563231	0.732373319644
H606	H	0.890391831249	0.291862717559	0.314099713623
H607	H	0.166608470911	0.689381938124	0.714566173412
H608	H	0.835163569352	0.190379459704	0.332886436654
H609	H	0.215767390555	0.053077553440	0.859621246188
H610	H	0.778164156017	0.547949639496	0.188974956458
H611	H	0.156327480814	0.068676200125	0.924963983733
H612	H	0.825668121722	0.570097649206	0.122003722412
H613	H	0.271477022855	0.081195388330	0.915379507928
H614	H	0.719590445631	0.599125436900	0.141458505246
H615	H	0.239831966583	0.158932442606	0.935831516684
H616	H	0.753584784897	0.675025675991	0.121145814270
H617	H	0.255421097292	0.163654284146	0.892544680258
H618	H	0.748865492911	0.674174763708	0.165828076394
H619	H	0.121193397063	0.130596272322	0.847281964925
H620	H	0.884170071425	0.619361701697	0.199395266900
H621	H	0.086772444997	0.278766121572	0.872727530049
H622	H	0.927867357455	0.761766232599	0.171948864537
H623	H	0.105371337001	0.227580901549	0.800370142805
H624	H	0.914328510648	0.717669608230	0.245781405751
H625	H	0.091170149197	0.319008245832	0.814421478325
H626	H	0.927849281426	0.806868856004	0.228890734301
H627	H	0.169273252827	0.357747844892	0.862481304912
H628	H	0.846512826250	0.848245970876	0.185512081888
H629	H	0.244522720094	0.330723592313	0.854462079712
H630	H	0.772478303476	0.819342324318	0.194786839851
H631	H	0.958014645814	0.785614237943	0.551918495211
H632	H	0.043091105823	0.544337968985	0.515722514995
H633	H	0.004736998668	0.559656159088	0.484050744308
H634	H	0.965418170630	0.954475406408	0.530134152236
H635	H	0.014242570534	0.773320607378	0.530813460642
H636	H	0.034854108063	0.023449702848	0.506153740449
H637	H	0.009582922144	0.896092473252	0.543348687743
H638	H	0.023623440137	0.140934913000	0.469148779438
H639	H	0.068808733088	0.094657437834	0.515178993483

H640	H	0.993996843497	0.282629018265	0.484629643636
H641	H	0.057712624193	0.214264156200	0.468247953897
H642	H	0.036067530472	0.341654411157	0.499902743189
H643	H	0.578512487570	0.745958765190	0.209730965722
H644	H	0.420009366472	0.511742947918	0.151580941355
H645	H	0.486244618149	0.482614303817	0.152623018857
H646	H	0.561464555381	0.923514030894	0.165198287092
H647	H	0.517329199662	0.778240914204	0.194593042512
H648	H	0.522183830587	0.025704123731	0.192698015655
H649	H	0.566443227782	0.889800380712	0.200441606778
H650	H	0.502353049452	0.156357139734	0.167993613068
H651	H	0.510212928477	0.098445079920	0.212938590052
H652	H	0.539411134366	0.354803881859	0.132170829707
H653	H	0.496729448472	0.239186558267	0.178948453039
H654	H	0.526871833685	0.385740542426	0.169447114792
H655	H	0.726930251966	0.097694320941	0.919826514703
H656	H	0.281851726578	0.535294456779	0.126090625962
H657	H	0.773881778488	0.035212538326	0.912545766441
H658	H	0.212512837598	0.526631653929	0.123897933555
H659	H	0.248182450794	0.149927239037	0.822379036406
H660	H	0.750726536978	0.648666145248	0.227662625417
H661	H	0.281196229001	0.087015023432	0.805058463415
H662	H	0.722129584274	0.587478754392	0.248462855213
H663	H	0.330799123043	0.155016451399	0.848566768614
H664	H	0.649138028386	0.640504451322	0.219586101277
H665	H	0.348578120015	0.184460852888	0.885235761868
H666	H	0.606407034213	0.643601369082	0.187959323305
H667	H	0.295245819702	0.340591346176	0.745422344243
H668	H	0.709296357877	0.836969792142	0.298102348050
H669	H	0.295195859257	0.427965577343	0.751505583010
H670	H	0.711926058434	0.923449352987	0.290269881768
H671	H	0.228657512320	0.399053815462	0.666915572594
H672	H	0.773772521574	0.899517551064	0.376825849817
H673	H	0.239954253337	0.419530003386	0.704542096645
H674	H	0.765274653141	0.917198448845	0.338793897627
H675	H	0.219313977372	0.533472084884	0.676038817024
H676	H	0.782913920346	0.029719562551	0.366890243612
H677	H	0.257064683978	0.601802976960	0.687643908898
H678	H	0.744375583900	0.098118691024	0.356991387816
H679	H	0.317369404483	0.587165040340	0.733640547136
H680	H	0.688496990992	0.084411039417	0.303383366204
H681	H	0.271827738641	0.652950844209	0.730314864903
H682	H	0.733461688405	0.147890475435	0.313015685760
H683	H	0.378890007161	0.499534602484	0.760835383004
H684	H	0.630590114990	0.995465653644	0.282383691868
H685	H	0.326650036516	0.530371850606	0.782784594022
H686	H	0.674778796185	0.007197200615	0.251973934470
H687	H	0.671179390836	0.299954971820	0.820087933237
H688	H	0.342662867703	0.801030383735	0.228723218261
H689	H	0.711844468483	0.333514860863	0.848078736055
H690	H	0.316031352093	0.838730885761	0.196429733924
H691	H	0.896320975449	0.529846890203	0.774191847240
H692	H	0.108826690132	0.018475025931	0.273385567392
H693	H	0.888796350688	0.552515009285	0.735663574593
H694	H	0.112584390646	0.044767227148	0.311569022695
H695	H	0.737992962090	0.557788575045	0.723650359227
H696	H	0.265257582208	0.056573231077	0.323036557876
H697	H	0.790975304597	0.549747279579	0.750427712214
H698	H	0.214461345797	0.040945520473	0.296084839204
H699	H	0.725454418214	0.501290997105	0.670342634164
H700	H	0.271782600379	0.010347456347	0.375754852488
H701	H	0.704925568262	0.585028808876	0.665779817738
H702	H	0.291740637721	0.093367394393	0.381999938205

H703	H	0.019591712108	0.156429422428	0.570820354824
H704	H	0.982083088512	0.733301082459	0.479394002024
H705	H	0.989486998235	0.103366968420	0.595909257004
H706	H	0.031464775313	0.681688628702	0.493920474130
H707	H	0.545007320867	0.213161137966	0.793240949283
H708	H	0.525735563438	0.810774814067	0.246856109709
H709	H	0.583242312522	0.269901098187	0.774332595022
H710	H	0.474995935141	0.775700000235	0.267266899696
H711	H	0.492771818128	0.312232448234	0.755685106123
H712	H	0.549345671232	0.830368298104	0.302648874250
H713	H	0.491509607341	0.349452147397	0.720002076515
H714	H	0.534263953790	0.848027191386	0.339501063103
H715	H	0.473107557329	0.491084255987	0.786592270513
H716	H	0.521714421241	0.986009627478	0.286490686062
H717	H	0.465755921414	0.436932028706	0.755396104118
H718	H	0.563457135017	0.935727145406	0.310333752222
H719	H	0.307421776622	0.205433951921	0.753974828155
H720	H	0.695189032076	0.699453914307	0.293921661755
H721	H	0.336059866824	0.234413510023	0.721827295966
H722	H	0.661053905786	0.742018129890	0.320972854145
H723	H	0.124308136062	0.154258446498	0.563498817867
H724	H	0.878135751103	0.687396322178	0.469839898166
H725	H	0.101108308046	0.204274099775	0.533212517416
H726	H	0.889463153627	0.744466008086	0.497876338709
H727	H	0.078064600190	0.003238001829	0.623646323951
H728	H	0.924138151308	0.516630129497	0.427270484138
H729	H	0.137656960643	0.029320220948	0.608305463448
H730	H	0.860419192172	0.545106376370	0.436698739465
H731	H	0.238970910366	0.858353367538	0.676778551252
H732	H	0.765624421252	0.357672181211	0.375207958471
H733	H	0.197282049433	0.788405486993	0.682034246419
H734	H	0.805617284888	0.287326945222	0.368329714289
H735	H	0.253891653676	0.981917523607	0.521561495635
H736	H	0.745852243238	0.543304108851	0.493448089681
H737	H	0.312599617517	0.013145251061	0.539972185852
H738	H	0.676968744180	0.533495475785	0.499805858953
H739	H	0.348951934926	0.798984676521	0.759216793483
H740	H	0.659844957350	0.280433190200	0.294761542838
H741	H	0.383302196710	0.740020306417	0.780163878777
H742	H	0.636627084695	0.201883565950	0.302128096053
H743	H	0.258464583752	0.849683900697	0.768233598257
H744	H	0.744190651829	0.343300879501	0.281606586912
H745	H	0.258670991736	0.825394124830	0.729035587860
H746	H	0.745134366951	0.323596880300	0.321420158055
H747	H	0.467415831210	0.580483769807	0.748466006336
H748	H	0.550821674980	0.076581847336	0.313941605916
H749	H	0.477410199343	0.650018640828	0.769982162098
H750	H	0.547298039864	0.145053437681	0.290854201414
H751	H	0.509599379754	0.095417873817	0.822862959002
H752	H	0.551392214586	0.595550018080	0.223982548652
H753	H	0.499560205973	0.008575255990	0.824895006875
H754	H	0.517443244370	0.517523481029	0.223335744463
H755	H	0.509021389006	0.719009016901	0.823806430988
H756	H	0.522505414161	0.205927210961	0.237938275025
H757	H	0.441254812439	0.691836112350	0.821740168746
H758	H	0.581735543466	0.160761755304	0.234361999720
H759	H	0.576651424387	0.772205863113	0.914219251275
H760	H	0.443332227004	0.348653228176	0.147946152267
H761	H	0.583217290964	0.792314704158	0.875403620786
H762	H	0.390834606961	0.330080545753	0.173613188694
H763	H	0.126827441193	0.696519328907	0.658327690767
H764	H	0.878177860516	0.194361658277	0.388673318882
H765	H	0.093048604013	0.758807073368	0.678849170246

H766	H	0.910359574205	0.257626873327	0.368131855741
H767	H	0.932150941292	0.697717992336	0.644025248405
H768	H	0.039560580148	0.171750219248	0.410391364801
H769	H	0.950919667842	0.710970967469	0.679939709462
H770	H	0.062269675972	0.205896792945	0.376326789034
H771	H	0.894319816487	0.525298185140	0.828956645240
H772	H	0.116346033204	0.006045458119	0.219992595677
H773	H	0.955637531458	0.482887001293	0.829292321001
H774	H	0.054356299206	0.965680398118	0.221115951793
H775	H	0.692049079335	0.457780206177	0.853585832910
H776	H	0.324488196349	0.965198394528	0.178312161826
H777	H	0.762380133395	0.471344484548	0.849298136181
H778	H	0.256891560812	0.966141682914	0.190584119341
H779	H	0.888562291862	0.448323338578	0.012887770250
H780	H	0.109017748765	0.927219355079	0.037943627530
H781	H	0.942923149724	0.497305682823	0.001695954549
H782	H	0.058971965186	0.983525418684	0.048476327784
H783	H	0.062505974613	0.468668782021	0.004870435332
H784	H	0.942518833906	0.004857842254	0.036619656804
H785	H	0.043254158862	0.516740379992	0.036096613029
H786	H	0.990083589503	0.046395476855	0.013325709437
H787	H	0.955910831753	0.620793892855	0.084523901746
H788	H	0.018015784061	0.109922392499	0.963369495877
H789	H	0.983539194289	0.653750900534	0.051690204852
H790	H	0.988373331640	0.155845801216	0.992780769033
H791	H	0.948492718256	0.537374812900	0.133521839244
H792	H	0.048273769843	0.047990539925	0.909057619253
H793	H	0.992294031445	0.599975182188	0.144521978583
H794	H	0.016562822502	0.120334924388	0.897593397694
H795	H	0.104179720661	0.541642805593	0.084463588870
H796	H	0.875584671798	0.075314977511	0.923444510937
H797	H	0.039052086327	0.559465592691	0.093801444158
H798	H	0.941587430734	0.097513860476	0.925353152768
H799	H	0.314193450610	0.753102077547	0.049943681520
H800	H	0.592053018171	0.307483475951	0.029756146051
H801	H	0.369231270206	0.796182364845	0.034929669674
H802	H	0.600734069817	0.269043503924	0.064957736025
H803	H	0.278197009882	0.660983387468	0.878005430720
H804	H	0.725394441796	0.125644545579	0.159668489203
H805	H	0.268895569019	0.590634893612	0.857102689185
H806	H	0.715936517104	0.045014125667	0.172044574232
H807	H	0.340502942025	0.617895173336	0.825057721213
H808	H	0.656852757845	0.071555030231	0.206902453032
H809	H	0.347842216777	0.534030830513	0.835726890173
H810	H	0.630803365403	0.991246728560	0.199533280873
H811	H	0.980947718670	0.406940065346	0.879384149336
H812	H	0.035955484255	0.897639953595	0.170580970605
H813	H	0.993861211075	0.361874328719	0.847598437469
H814	H	0.021919487829	0.842320130884	0.198921453555
H815	H	0.073084863130	0.419642115650	0.874131286289
H816	H	0.940563491483	0.909180253261	0.177363833572
H817	H	0.095382477192	0.392623400373	0.908380502837
H818	H	0.920503297823	0.878576076575	0.143441820574
H819	H	0.080501831973	0.585282895278	0.876639819660
H820	H	0.828042696494	0.064955979712	0.161599055904
H821	H	0.104049840251	0.522886355288	0.899024378696
H822	H	0.880219555459	0.009720693572	0.158117942073
H823	H	0.632328656799	0.308426526732	0.873573693379
H824	H	0.608150004158	0.388432883854	0.876821770392
H825	H	0.455239938476	0.658174216123	0.086253177704
H826	H	0.460626893949	0.699543346406	0.051244811775
H827	H	0.383949497280	0.738669153979	0.953360533281
H828	H	0.353920114321	0.716596559099	0.918170507331

H829	H	0.391306235860	0.226078977064	0.994854172743
H830	H	0.338329797772	0.172725684617	0.986534059443
H831	H	0.437625681734	0.604735555752	0.951528481974
H832	H	0.391391328439	0.566696149532	0.927222246356
H833	H	0.578775838853	0.927353423695	0.040742644800
H834	H	0.548883192809	0.951887658755	0.005481595426
H835	H	0.295672804156	0.562913372300	0.904998252457
H836	H	0.308201576260	0.510696805552	0.937765849419
H837	H	0.526399409222	0.254864981560	0.090116315555
H838	H	0.541377508683	0.235029565629	0.127738167191
H839	H	0.451434699747	0.644658715158	0.901594297107
H840	H	0.477798546219	0.674563294086	0.866701229044
H841	H	0.512343720753	0.335549928642	0.997823007114
H842	H	0.567977152986	0.383029597654	0.986725466575
H843	H	0.449006729148	0.999925583370	0.092261089935
H844	H	0.495650661220	0.064983691671	0.094388022049
H845	H	0.422252664421	0.921847891801	0.030378469486
H846	H	0.477581960263	0.872128176040	0.034864742433
H847	H	0.425951465704	0.030662839801	0.175373280191
H848	H	0.407419003736	0.041599270420	0.138437417034
H849	H	0.573544429989	0.684030722447	0.951684836608
H850	H	0.518905677129	0.700603530247	0.927282846838
H851	H	0.652708156553	0.958498070438	0.085806041157
H852	H	0.650198192419	0.873670970618	0.074529017756
H853	H	0.617464544925	0.090303223581	0.899198074487
H854	H	0.595150157713	0.015687703021	0.884763514767
H855	H	0.557126487968	0.285723565886	0.921713611526
H856	H	0.565282432909	0.209668312445	0.939343502925
H857	H	0.406634004677	0.746863183229	0.094340436171
H858	H	0.346340433408	0.753546425328	0.112123097262
H859	H	0.426878483986	0.064639063665	0.933493888185
H860	H	0.465012331808	0.111168739417	0.961050612712
H861	H	0.523977478643	0.670188566456	0.013360584686
H862	H	0.483640079234	0.737281863152	0.000333761308
H863	H	0.616427855132	0.079761138223	0.094380697248
H864	H	0.576377708143	0.151511704302	0.096191290057
H865	H	0.333955806784	0.383434712080	0.948194927367
H866	H	0.396487531561	0.392975309265	0.930622830282
H867	H	0.422849813473	0.933727444040	0.134365928867
H868	H	0.414964691523	0.863840760239	0.111015515484
H869	H	0.548019557144	0.508830962774	0.075590363644
H870	H	0.528970298813	0.584440437978	0.092468431755
H871	H	0.472407420778	0.165651689027	0.901470437496
H872	H	0.433474952167	0.185316453994	0.869399250835
H873	H	0.405015043858	0.113407249526	0.073073525187
H874	H	0.371749800985	0.161219625872	0.043060687194
H875	H	0.643278560523	0.771320280108	0.106933543379
H876	H	0.605927285828	0.799772161207	0.136598220053
H877	H	0.706817674415	0.024020427481	0.964661186772
H878	H	0.706019624609	0.006010905072	0.003287839871
H879	H	0.587767871582	0.570828205186	0.926211862153
H880	H	0.540640216732	0.595784997000	0.898874963034
H881	H	0.530973054891	0.646066450000	0.131958759212
H882	H	0.474958315061	0.597609797462	0.137984636716
H883	H	0.320027386107	0.654339082431	0.972731526926
H884	H	0.322706790539	0.690528807189	0.007986037629
H885	H	0.646206444586	0.780452592044	0.041514589059
H886	H	0.672278808063	0.723655444783	0.067626600215
H887	H	0.390374200375	0.170111230294	0.934420355070
H888	H	0.363875441777	0.250477032106	0.932323743737
H889	H	0.674645889192	0.148796051872	0.998246832979
H890	H	0.685453988013	0.227387169058	0.985277368893
H891	H	0.574684234378	0.761205376743	0.007167999240

H892	H	0.596264296621	0.841172528014	0.005599366144
H893	H	0.578599273718	0.899144429843	0.109265903670
H894	H	0.512499082457	0.884931717410	0.122899678111
H895	H	0.533938762646	0.121517188415	0.006835962094
H896	H	0.481788389704	0.173667891605	0.015354111981
H897	H	0.640234577242	0.146999264158	0.952188503149
H898	H	0.584963043730	0.091760026703	0.949370223355
H899	H	0.526824421545	0.410510978538	0.043804479237
H900	H	0.477191551412	0.444464914686	0.066807957502
H901	H	0.450749351647	0.813674702898	0.957383589109
H902	H	0.431114157161	0.827531178497	0.995924608455
H903	H	0.529870492593	0.181566334702	0.853382892772
H904	H	0.585066888219	0.130714706915	0.847853161721
H905	H	0.265782222135	0.542136376349	0.062676124517
H906	H	0.288135384245	0.576910009923	0.028194732290
H907	H	0.431593392189	0.762424557119	0.152873709986
H908	H	0.406535551431	0.784171665830	0.187587487904
H909	H	0.442159769011	0.049442723429	0.015830626683
H910	H	0.372001082687	0.031750774339	0.015913049369
H911	H	0.582177888320	0.888203251442	0.903426034024
H912	H	0.538841930270	0.930232225373	0.879246546766
H913	H	0.335187930457	0.341302311478	0.889160006034
H914	H	0.341804040707	0.289184962691	0.858420278118
H915	H	0.490576384836	0.873254906720	0.911726492442
H916	H	0.467025208931	0.793139170398	0.903891909591
H917	H	0.556116866362	0.437980339661	0.941527879239
H918	H	0.607816994351	0.385511183933	0.932572075512
H919	H	0.448953811042	0.209132156917	0.061742247866
H920	H	0.458342448780	0.287580592000	0.049696692054
H921	H	0.609038559149	0.186093241227	0.028985194195
H922	H	0.598414666748	0.111250417945	0.045925802182
H923	H	0.740225926286	0.924159525591	0.032543061086
H924	H	0.797438989219	0.958685200709	0.047562924493
H925	H	0.376320922184	0.423867906377	0.858601618252
H926	H	0.368102839055	0.489506670207	0.883194866262
H927	H	0.335922799892	0.652737817251	0.079971018530
H928	H	0.272859225485	0.644606179153	0.096685953374
H929	H	0.389854283993	0.427193655845	0.062131674902
H930	H	0.362510196893	0.505923209048	0.057989477444
H931	H	0.718570457110	0.026348617435	0.078176289852
H932	H	0.711218978397	0.049172070617	0.117352982200
H933	H	0.372323854847	0.425199235616	0.140241806995
H934	H	0.371903837422	0.477317025656	0.108642252215
H935	H	0.526018518551	0.343199961630	0.875591215818
H936	H	0.471033728102	0.294678714297	0.882064102292
H937	H	0.283233356367	0.470691687763	0.997603801610
H938	H	0.348935003361	0.457607547875	0.985479704538
H939	H	0.483176026076	0.267274639389	0.961646276317
H940	H	0.423339678491	0.313761371727	0.963226934482
H941	H	0.466071018725	0.485158806781	0.924441399960
H942	H	0.476099239645	0.402050231572	0.909630959598
H943	H	0.623288729515	0.680283571294	0.139343218535
H944	H	0.622588478562	0.589104598728	0.142055306979
H945	H	0.554575651297	0.573405324266	0.035426708244
H946	H	0.509817460869	0.562599579783	0.004779857324
H947	H	0.446735090260	0.440548066324	0.974101396392
H948	H	0.427018427053	0.496737388662	0.002876045329
H949	H	0.607608708191	0.001040879794	0.973181019882
H950	H	0.557060312703	0.979284186320	0.946393756854
H951	H	0.428307603079	0.607828150733	0.031871865275
H952	H	0.381729798745	0.604187419743	0.002655443646
H953	H	0.681900859427	0.602388738626	0.058396047241
H954	H	0.629119620500	0.613966489830	0.081751616739

H955	H	0.607248054702	0.592587145361	0.981695380712
H956	H	0.666485599182	0.608048787111	0.959316604946
H957	H	0.577088483917	0.479973693529	0.842369403006
H958	H	0.598058389104	0.504468687533	0.877387909141
H959	H	0.351796147394	0.324509876128	0.041803379240
H960	H	0.401698674069	0.370444401456	0.021661689845
H961	H	0.464592450602	0.499717360633	0.844107697276
H962	H	0.494196405862	0.569946394299	0.828058202856
H963	H	0.416596171075	0.679716753262	0.244867409153
H964	H	0.409904643214	0.675366844523	0.191223269894
H965	H	0.423009792523	0.598099672437	0.205432610247
H966	H	0.451537766145	0.878704224101	0.238044252302
H967	H	0.477752250929	0.650307013794	0.255705794660
H968	H	0.443013901642	0.987092779880	0.249686517351
H969	H	0.471602878691	0.920858457316	0.206521073033
H970	H	0.347237462957	0.284605266119	0.225990692518
H971	H	0.466850977367	0.065140594886	0.260786275876
H972	H	0.388517432140	0.416460078039	0.219243603213
H973	H	0.417972081876	0.294128077790	0.220463960900
H974	H	0.424636751830	0.477980402516	0.200700870053
C1	C	0.719550514019	0.834193587097	0.945238302822
C2	C	0.288866045517	0.312270938925	0.110235996614
C3	C	0.743972165007	0.835338082578	0.909731866793
C4	C	0.254223871921	0.321812341877	0.142958803689
C5	C	0.769580210343	0.841064866918	0.972624759153
C6	C	0.244883868984	0.308758735263	0.079898254195
C7	C	0.809427427518	0.908770450562	0.969158952593
C8	C	0.209074086108	0.380032418478	0.075602311347
C9	C	0.767887612963	0.912972556268	0.861558690953
C10	C	0.217041167960	0.404486023102	0.185570757933
C11	C	0.828789600157	0.949705489086	0.868838206266
C12	C	0.156402140760	0.431132526083	0.171796126892
C13	C	0.727854486809	0.959096779085	0.837129584291
C14	C	0.239415666120	0.467091261799	0.210010496448
C15	C	0.667522497899	0.920294395296	0.831051610311
C16	C	0.258352774691	0.436716987778	0.244173971185
C17	C	0.937342953428	0.945792982683	0.857643871427
C18	C	0.047696819536	0.426022971232	0.184641462049
C19	C	0.965537082687	0.961116497359	0.823451471118
C20	C	0.024114556248	0.444418497004	0.219831068287
C21	C	0.973505098100	0.884137206466	0.875287760234
C22	C	0.009945665343	0.362952619952	0.169243209453
C23	C	0.014592726447	0.045198931476	0.785642774569
C24	C	0.984226338318	0.533341874161	0.258919925502
C25	C	0.083418756788	0.050010482050	0.785757767026
C26	C	0.915403049982	0.539596003860	0.260958465877
C27	C	0.984317914120	0.115943359305	0.772575308301
C28	C	0.016054314848	0.604208521045	0.270617330168
C29	C	0.177845287074	0.025248500303	0.756917043994
C30	C	0.823698675622	0.516736804517	0.292851710384
C31	C	0.203736550737	0.102366345342	0.751258161131
C32	C	0.798417925899	0.593792096248	0.298929783574
C33	C	0.190939658752	0.972660706439	0.727641137085
C34	C	0.813299528555	0.464851971913	0.322762168613
C35	C	0.136443194120	0.982727770538	0.704052335009
C36	C	0.869907047994	0.474630271304	0.344711958433
C37	C	0.083688632998	0.988218263033	0.728249021465
C38	C	0.920288190578	0.480773563517	0.319008836186
C39	C	0.182814378894	0.230159037436	0.734601534124
C40	C	0.820568780740	0.721978575028	0.313179267312
C41	C	0.128333655448	0.279856995431	0.740388555733
C42	C	0.875555713159	0.769628957210	0.305914628027
C43	C	0.209031870818	0.243861511272	0.699882814493

C44	C	0.793900718849	0.740989036714	0.347223776503
C45	C	0.095828158711	0.406925529917	0.750178319928
C46	C	0.907327487506	0.896873823276	0.294320412664
C47	C	0.057270434648	0.418440029746	0.718236558709
C48	C	0.948320415894	0.905771474076	0.325523551051
C49	C	0.124239806162	0.478558291129	0.764498337637
C50	C	0.875969817479	0.969264574435	0.283512955408
C51	C	0.139238501247	0.466186177438	0.802090690304
C52	C	0.846432438232	0.959955259041	0.248458004651
C53	C	0.083121692189	0.544976796820	0.758828837006
C54	C	0.919434901437	0.034343355211	0.285260348170
C55	C	0.169349191727	0.530434012709	0.820572763389
C56	C	0.811042128447	0.027187506372	0.236141730649
C57	C	0.046505589383	0.425943952405	0.657891596022
C58	C	0.960241348692	0.918910913997	0.386017574801
C59	C	0.009157433009	0.355453830932	0.652763919960
C60	C	0.996311931167	0.848319240003	0.393348346071
C61	C	0.082777538212	0.449593830201	0.626615818998
C62	C	0.923499574891	0.948821480879	0.416017721007
C63	C	0.052696998759	0.425353434651	0.593404760955
C64	C	0.951283239059	0.929595419951	0.450472244394
C65	C	0.092026123633	0.533606756427	0.627864044881
C66	C	0.916218345252	0.032630657467	0.411643087227
C67	C	0.995893239212	0.223569136080	0.660318672732
C68	C	0.009829966275	0.716336358807	0.386144179564
C69	C	0.939958635648	0.233186116741	0.682728612534
C70	C	0.066215541920	0.725409501954	0.363844915125
C71	C	0.032556476112	0.154328041374	0.668802717230
C72	C	0.973217095225	0.647098651300	0.377530773838
C73	C	0.897585538507	0.287882434615	0.734226881799
C74	C	0.110071831532	0.775482596205	0.312067988519
C75	C	0.853974729780	0.342078852234	0.716908486821
C76	C	0.151252649613	0.832505350200	0.329365567377
C77	C	0.921794186768	0.321337764986	0.767360165772
C78	C	0.089057298410	0.804536854776	0.277386077967
C79	C	0.873412434679	0.355001923904	0.789982068649
C80	C	0.139526970450	0.836856611293	0.255522550911
C81	C	0.826467674254	0.302092733456	0.804147382448
C82	C	0.187358402575	0.783603328215	0.242366744488
C83	C	0.830674724008	0.183100358367	0.835221578646
C84	C	0.188156988334	0.674525706404	0.204116858840
C85	C	0.838698373012	0.452025719268	0.683338516280
C86	C	0.162066619895	0.945170476146	0.361625867493
C87	C	0.800892423934	0.410658543648	0.656370898283
C88	C	0.202959955742	0.908622343166	0.388593228087
C89	C	0.874151761777	0.515190666475	0.667246205541
C90	C	0.123976674390	0.006287651638	0.377549597832
C91	C	0.799661004496	0.319143923960	0.611668636602
C92	C	0.213298083182	0.824491509355	0.435438364043
C93	C	0.752433266165	0.267905275395	0.627046570533
C94	C	0.253837252879	0.764522521543	0.420614472414
C95	C	0.845035913490	0.275102828644	0.591234948185
C96	C	0.176069142951	0.797379143040	0.465189270226
C97	C	0.882945547770	0.325014332383	0.568433987552
C98	C	0.160214563554	0.862948677841	0.487924838762
C99	C	0.726874241680	0.185405316506	0.673532483120
C100	C	0.278507608698	0.682991085882	0.374044841314
C101	C	0.668619258698	0.226085436364	0.682395795417
C102	C	0.336628302681	0.723472025687	0.364460972694
C103	C	0.758635262849	0.153477392961	0.705143752402
C104	C	0.246794983494	0.647587901978	0.343187874850
C105	C	0.721608083824	0.094419480306	0.721941470821
C106	C	0.285085950917	0.588362769055	0.327336827106

C107	C	0.679114688017	0.111682112000	0.746611716947
C108	C	0.327303620843	0.605575144176	0.302525115008
C109	C	0.728162285114	0.020556167520	0.711963868370
C110	C	0.280416750079	0.514912425042	0.338285855923
C111	C	0.643726784221	0.056247206126	0.760797475053
C112	C	0.364340462230	0.550703818180	0.289298691237
C113	C	0.692932773633	0.964955713005	0.726099199161
C114	C	0.317812866029	0.460082791926	0.325254272895
C115	C	0.650354444472	0.983041946867	0.750371101745
C116	C	0.360310146699	0.478281871600	0.300973525606
C117	C	0.622258726980	0.332145491944	0.708258421855
C118	C	0.381342174166	0.831830788653	0.338610222791
C119	C	0.582967108589	0.355022529338	0.677793305710
C120	C	0.418908103588	0.855662088441	0.369584701584
C121	C	0.637805214340	0.399161398127	0.730183821566
C122	C	0.362363317854	0.898022488092	0.317120312386
C123	C	0.665497773716	0.379919739676	0.764405702299
C124	C	0.342229297604	0.876939746636	0.281502119065
C125	C	0.576915816246	0.391061490231	0.618650513467
C126	C	0.422590414670	0.892294257637	0.428581188864
C127	C	0.544218584632	0.321647870787	0.605464082691
C128	C	0.457066533818	0.824164179947	0.441678463114
C129	C	0.618051871676	0.427048110943	0.592111079013
C130	C	0.380508956730	0.925258808545	0.455423000677
C131	C	0.589046328402	0.424879959001	0.556966011442
C132	C	0.410061390412	0.923500377949	0.490490136853
C133	C	0.633339355225	0.506087064152	0.602803346428
C134	C	0.362029191829	0.003791945846	0.445523896643
C135	C	0.551119036965	0.189128842840	0.593212202876
C136	C	0.453915801207	0.691652997632	0.453943509679
C137	C	0.494912669410	0.167957458930	0.613628874299
C138	C	0.508809303640	0.671262468655	0.432312850514
C139	C	0.601971289045	0.131332909020	0.595378225496
C140	C	0.404072501639	0.632403925901	0.453795019764
C141	C	0.446856611249	0.170028889076	0.668679437578
C142	C	0.554184952364	0.676353737926	0.376662936340
C143	C	0.393574728078	0.223027251162	0.664157261846
C144	C	0.606173861116	0.731632598712	0.379948345713
C145	C	0.469045015960	0.170193136629	0.705538540773
C146	C	0.529604455315	0.671814515498	0.340361952428
C147	C	0.512955736370	0.107309554353	0.713948510905
C148	C	0.491655985702	0.602395669664	0.333984638077
C149	C	0.482603030000	0.032047045077	0.717710810513
C150	C	0.528513112612	0.531567781510	0.331342915065
C151	C	0.396847470806	0.992170255461	0.754634199390
C152	C	0.613784669403	0.490794585511	0.295104110956
C153	C	0.351128043214	0.339959354520	0.644738632478
C154	C	0.647490069045	0.848275142449	0.400311192641
C155	C	0.294304243279	0.308846849927	0.627211526903
C156	C	0.704100207685	0.815409492823	0.417156744784
C157	C	0.371271189969	0.411516760424	0.627573821602
C158	C	0.626390200499	0.917194293386	0.419301620306
C159	C	0.413096247562	0.462113911958	0.648596727428
C160	C	0.591515086190	0.973845576117	0.397785734961
C161	C	0.429813236697	0.528169687335	0.626431959611
C162	C	0.565922007837	0.032404784706	0.421497359837
C163	C	0.384443289568	0.486474432150	0.681729078369
C164	C	0.631566619100	0.008394426643	0.370912150991
C165	C	0.242943320984	0.229078705550	0.586547052103
C166	C	0.752638996066	0.734133735801	0.458347337554
C167	C	0.222276473789	0.160803334660	0.606032565909
C168	C	0.768125595759	0.660721293975	0.441382892799
C169	C	0.259790569085	0.207380646786	0.550502582591

C170	C	0.736398578218	0.722030389947	0.495135596125
C171	C	0.328598774495	0.199494831099	0.551615988971
C172	C	0.667877709661	0.712445436687	0.494313461961
C173	C	0.349489998184	0.258490696901	0.576575989897
C174	C	0.647275446920	0.768268123130	0.467829055382
C175	C	0.241033790026	0.073913534345	0.652284364819
C176	C	0.755300898960	0.578271752522	0.393089926546
C177	C	0.273787636999	0.002263169271	0.644248751205
C178	C	0.729388857071	0.506106741183	0.406185063673
C179	C	0.351632722946	0.940697111419	0.610967967822
C180	C	0.651419568695	0.446585200216	0.439591483857
C181	C	0.374590708474	0.901358150302	0.642893828227
C182	C	0.632333128053	0.401596523354	0.408506614607
C183	C	0.407848938839	0.967345861822	0.591706834514
C184	C	0.592437634945	0.470455687728	0.456912450574
C185	C	0.442677382097	0.903140285844	0.576728698284
C186	C	0.560140334317	0.404794240265	0.472432844964
C187	C	0.393949487320	0.788972076758	0.674922440475
C188	C	0.616375929535	0.285195940500	0.379659109895
C189	C	0.459502409160	0.809112009629	0.682505882439
C190	C	0.550893136604	0.303944520586	0.371264897938
C191	C	0.388275260892	0.707187311583	0.665150774868
C192	C	0.622845221083	0.205197320897	0.391593083369
C193	C	0.330246639459	0.706217746313	0.643943699031
C194	C	0.679534429363	0.207931429975	0.413949093742
C195	C	0.332036979825	0.778367346022	0.623816945686
C196	C	0.675923723054	0.282783937809	0.431853095768
C197	C	0.536585254449	0.819104648374	0.726456757351
C198	C	0.476779678419	0.317760139095	0.326347359979
C199	C	0.578426901301	0.765039025013	0.708402301715
C200	C	0.431410658120	0.265347470666	0.342621942173
C201	C	0.544609859316	0.809982861241	0.764740778545
C202	C	0.472086101365	0.311231340583	0.287989141453
C203	C	0.513608923882	0.869002671505	0.785954769031
C204	C	0.509943296472	0.367045851804	0.268608875308
C205	C	0.525992444607	0.862819175120	0.823779203268
C206	C	0.509543366523	0.355211477950	0.230710017999
C207	C	0.597804137780	0.640457246659	0.688613347115
C208	C	0.404255003135	0.142005066579	0.360674445723
C209	C	0.615244106351	0.661953967299	0.652575326393
C210	C	0.386260077611	0.163344014757	0.396586193800
C211	C	0.568244893351	0.564115953789	0.689816094467
C212	C	0.428942831142	0.063199684675	0.358857709393
C213	C	0.584684623526	0.714735897679	0.598374389235
C214	C	0.415425630630	0.215689235584	0.451193609850
C215	C	0.623784849447	0.784502582194	0.599137792709
C216	C	0.378040062195	0.286877240781	0.450111593819
C217	C	0.525998505873	0.726400254102	0.577940508190
C218	C	0.473566163657	0.225815014125	0.472277727963
C219	C	0.497059895327	0.654439890233	0.564751012400
C220	C	0.502755506372	0.153034938877	0.484210676975
C221	C	0.431776475596	0.668210478803	0.552750050458
C222	C	0.568316566329	0.166462110951	0.495823252522
C223	C	0.534947504555	0.618812582731	0.537154505603
C224	C	0.465535030135	0.115253927551	0.511529685911
C225	C	0.651880903819	0.897793944730	0.626992260955
C226	C	0.354956121940	0.402432131703	0.422511281050
C227	C	0.716434316149	0.877025421145	0.638469046923
C228	C	0.290970816244	0.384392684783	0.409489409831
C229	C	0.623667146668	0.957210214660	0.649029422531
C230	C	0.384652796202	0.460509426463	0.400364907123
C231	C	0.783130521508	0.788246907082	0.667629188744
C232	C	0.225591436537	0.300178554931	0.376923291877

C233	C	0.817493422175	0.759342812251	0.636924794253
C234	C	0.188342032251	0.271619274231	0.406580742519
C235	C	0.776311690257	0.728195954163	0.694460917252
C236	C	0.233883884670	0.242828277326	0.349151039698
C237	C	0.821126148860	0.687517836874	0.586198512957
C238	C	0.177658190708	0.194048922344	0.454883485171
C239	C	0.830849607332	0.752532924238	0.561960071362
C240	C	0.165977900461	0.257383325415	0.479486969163
C241	C	0.792316967862	0.620258793393	0.568565617773
C242	C	0.203721876405	0.125546739015	0.472753651614
C243	C	0.799511093668	0.548112244006	0.588114499488
C244	C	0.195260307370	0.055576841485	0.451911789996
C245	C	0.799480486087	0.869927224166	0.538066457986
C246	C	0.198873286572	0.369620621244	0.508107213647
C247	C	0.852849767287	0.920082973342	0.547767862808
C248	C	0.146286656302	0.419886980185	0.496834248087
C249	C	0.741361405972	0.916829847482	0.533856841309
C250	C	0.257394233930	0.415439565079	0.512525254699
C251	C	0.749683124310	0.975369367968	0.507177624344
C252	C	0.249762598417	0.476346707219	0.538023242612
C253	C	0.759189898511	0.954467056572	0.473761118709
C254	C	0.244763922856	0.458634918399	0.572127405899
C255	C	0.754111351259	0.050573730660	0.514994505130
C256	C	0.243816906666	0.550704097419	0.528834541394
C257	C	0.773332358118	0.005675038735	0.449040887963
C258	C	0.234453396550	0.512282263647	0.596361806083
C259	C	0.768492067849	0.102831561127	0.490557593269
C260	C	0.233339510259	0.605366893046	0.552794117899
C261	C	0.779266999889	0.080737335355	0.457354659404
C262	C	0.228079780794	0.586692828984	0.586896837693
C263	C	0.899064181380	0.993165162773	0.593623013676
C264	C	0.106753258500	0.497591266854	0.451774995122
C265	C	0.958461837452	0.964826460560	0.608624459815
C266	C	0.045187885737	0.466552165686	0.441364218831
C267	C	0.867994520143	0.038847803551	0.621471757470
C268	C	0.133090938205	0.539839264142	0.421597011070
C269	C	0.811021227837	0.077899956059	0.609054035645
C270	C	0.188239098254	0.585429357969	0.431654882299
C271	C	0.010754185165	0.859208328926	0.634419246960
C272	C	0.993384167631	0.363848912775	0.412608516251
C273	C	0.002434744357	0.862015286615	0.672562179059
C274	C	0.000174005100	0.362778811341	0.374379330735
C275	C	0.937264162551	0.898539090853	0.719234280885
C276	C	0.064010073444	0.394859379599	0.326714774271
C277	C	0.915510399871	0.819468140020	0.727748578066
C278	C	0.083259237974	0.314055078574	0.319913887866
C279	C	0.886074171936	0.953283253564	0.726627795399
C280	C	0.116656557839	0.446430332441	0.317821051774
C281	C	0.892090268552	0.732943810342	0.772687350836
C282	C	0.098321086556	0.222254337376	0.275933371811
C283	C	0.843042880188	0.737668300907	0.799175951734
C284	C	0.145157217820	0.225039179214	0.248257537867
C285	C	0.950075723008	0.692923157709	0.785942797936
C286	C	0.039156479837	0.181436317783	0.264992633368
C287	C	0.976577574793	0.727479428285	0.818335645637
C288	C	0.012572717665	0.210136652484	0.231391895071
C289	C	0.995898923719	0.688681701459	0.757525619422
C290	C	0.995015613584	0.185403226153	0.294257898302
C291	C	0.027601791208	0.682323921123	0.834677253089
C292	C	0.962212733055	0.162014883478	0.216373303509
C293	C	0.770835814340	0.665050737714	0.831782893335
C294	C	0.218277058116	0.153845193721	0.216431238107
C295	C	0.799813727479	0.608592506051	0.855449687020

C296	C	0.197205633194	0.093880420283	0.192253996089
C297	C	0.706348651714	0.636641460732	0.822697414688
C298	C	0.283261514345	0.136924753573	0.229041127408
C299	C	0.676549874223	0.678027391737	0.793124907774
C300	C	0.300071135293	0.186937543762	0.258841765541
C301	C	0.666820052478	0.639408246921	0.854200374037
C302	C	0.326878526526	0.142544512326	0.199394354196
C303	C	0.622392578263	0.635569082445	0.778690795656
C304	C	0.362547776427	0.172230341555	0.274014910891
C305	C	0.823928731837	0.573831550574	0.913098437254
C306	C	0.171016102304	0.064063539887	0.134130607726
C307	C	0.773017589721	0.561230607667	0.937964530687
C308	C	0.223656030117	0.064359935898	0.109505307972
C309	C	0.884182967798	0.595889127566	0.931025257664
C310	C	0.108745305796	0.080787636310	0.116944076250
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C312	C	0.110579223988	0.150563155321	0.094748663555
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C314	C	0.059210520346	0.083239414776	0.143694227155
C315	C	0.933106056098	0.685192857753	0.973990502911
C316	C	0.052138545788	0.166307863723	0.074968849134
C317	C	0.724847840240	0.480482481814	0.979051527181
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C320	C	0.259044217906	0.034229772476	0.032519684015
C321	C	0.729353258252	0.396646917447	0.986242614200
C322	C	0.298553466041	0.919842237143	0.063194540078
C323	C	0.786787813143	0.370215536215	0.968600851269
C324	C	0.241385605521	0.878171020569	0.073728036177
C325	C	0.797347042265	0.425543131984	0.940193013536
C326	C	0.214116218118	0.926809909458	0.101146713296
C327	C	0.806124144175	0.595842758093	0.046935856329
C328	C	0.175693724481	0.083030424095	0.999683645380
C329	C	0.792185727240	0.678668862384	0.042949252200
C330	C	0.190140179877	0.164903307371	0.006253887665
C331	C	0.808773606675	0.801264011382	0.070834858751
C332	C	0.182723708779	0.292091309507	0.983088618151
C333	C	0.869225373278	0.838879185753	0.062887892964
C334	C	0.121501919009	0.332155857847	0.984188092958
C335	C	0.788244444790	0.828090716459	0.105565204332
C336	C	0.219762493648	0.320127448414	0.953355733897
C337	C	0.979884199049	0.822038193826	0.066479482047
C338	C	0.011119699149	0.314862906962	0.977019135353
C339	C	0.013275531755	0.801234495101	0.034449529237
C340	C	0.972877101762	0.295413422008	0.007464593444
C341	C	0.010620375839	0.789826805733	0.098415383714
C342	C	0.987994216519	0.284029356574	0.943043746905
C343	C	0.070937739157	0.826124996946	0.106550719857
C344	C	0.925344851681	0.311334397287	0.933538781822
C345	C	0.045925003247	0.847670807317	0.980152003804
C346	C	0.942188377766	0.340639633233	0.062537959920
C347	C	0.113567703903	0.834327929888	0.985909547281
C348	C	0.873294921955	0.340752832613	0.058534567092
C349	C	0.039095904081	0.917975621791	0.959071275746
C350	C	0.960919301035	0.404270132247	0.085710629858
C351	C	0.206548695304	0.781335311723	0.965180739632
C352	C	0.776797633481	0.287437658410	0.074070788899
C353	C	0.237359219567	0.852825892061	0.953238742240
C354	C	0.751274206335	0.353820673582	0.093419188630
C355	C	0.216628787572	0.715980902498	0.941058207209
C356	C	0.761308752965	0.212418637195	0.090369081258
C357	C	0.166450867153	0.724767953937	0.914603582251
C358	C	0.813188297968	0.200764522425	0.115756751873

C359	C	0.112526290529	0.750255372424	0.935173215077
C360	C	0.868518710973	0.232100518417	0.098097033743
C361	C	0.330644141399	0.927127398585	0.955919250014
C362	C	0.660922475103	0.431593481710	0.100041646215
C363	C	0.346368182642	0.941635494095	0.919247834621
C364	C	0.655717173193	0.432816465065	0.138221449102
C365	C	0.337787941186	0.896885367636	0.860673499117
C366	C	0.661468411534	0.364637820924	0.191374232604
C367	C	0.276384708010	0.906807174311	0.842330582108
C368	C	0.722610167264	0.387595767460	0.206855948495
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C370	C	0.637177014572	0.291345381527	0.205020271024
C371	C	0.351556390108	0.756347411752	0.850294624504
C372	C	0.663953970583	0.217861106881	0.193586789439
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C374	C	0.827892504407	0.423123100532	0.197356547150
C375	C	0.143674767404	0.987860190944	0.872666702091
C376	C	0.848914487714	0.483623752369	0.173187574966
C377	C	0.123429935477	0.863788787713	0.844092717009
C378	C	0.873169561570	0.359845675118	0.201494755433
C379	C	0.141472440256	0.813689046983	0.815767619124
C380	C	0.857239005221	0.310293614720	0.230372663506
C381	C	0.185529610537	0.758503767447	0.819468119200
C382	C	0.813967783295	0.254110350554	0.227338253907
C383	C	0.114842307751	0.823770118560	0.784005839706
C384	C	0.883453672590	0.323431684248	0.261980910795
C385	C	0.201576269732	0.714294198857	0.792357962340
C386	C	0.797880448796	0.211940849755	0.255072840577
C387	C	0.130505401927	0.780353430415	0.756579033657
C388	C	0.868348634612	0.281406481358	0.289956045028
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C390	C	0.826218194157	0.224297551872	0.286310917662
C391	C	0.176192893907	0.098205157859	0.903596115745
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C393	C	0.134762604744	0.163479299407	0.896062290678
C394	C	0.867775208069	0.653995884485	0.151030366532
C395	C	0.239378665470	0.127064551646	0.912518586851
C396	C	0.756071065863	0.639856048893	0.143431174774
C397	C	0.082320057036	0.236437445470	0.853259826992
C398	C	0.931647855588	0.719726071897	0.191555501929
C399	C	0.014001666864	0.222031934449	0.849782406600
C400	C	0.999835512813	0.702286394005	0.193299101904
C401	C	0.112083541858	0.266132576468	0.821293239347
C402	C	0.905935913039	0.753445101637	0.224035221490
C403	C	0.180248976256	0.274369560987	0.827249806398
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N3	N	0.738307731771	0.900027665418	0.893436021761
N4	N	0.257891393806	0.387536641263	0.158519124419
N5	N	0.875078237985	0.923401094681	0.851353353944
N6	N	0.110220792700	0.404619344290	0.189529112027
N7	N	0.993235281397	0.026023602299	0.818869737004
N8	N	0.001921853876	0.512261804958	0.225216740218
N9	N	0.111416653234	0.024329390087	0.758287357642
N10	N	0.889864917354	0.516066253699	0.289618005269
N11	N	0.165328191039	0.154041628654	0.739637899035
N12	N	0.837275705666	0.645191540681	0.310060821647
N13	N	0.142211764317	0.350901850302	0.746048337812
N14	N	0.861882466190	0.840004490235	0.299040785740
N15	N	0.084429720830	0.421124517503	0.688198230726
N16	N	0.922237424305	0.911470775788	0.355820087140
N17	N	0.033488970689	0.289938369417	0.661604120564

N18	N	0.972403920756	0.782621124959	0.384314030398
N19	N	0.947983825300	0.266323776938	0.712901356045
N20	N	0.058454915822	0.754630557449	0.332756312728
N21	N	0.855402672976	0.247402355384	0.826179401643
N22	N	0.160513336392	0.733158479771	0.217450473710
N23	N	0.772044049820	0.169487130703	0.829294396239
N24	N	0.247882283613	0.665477901603	0.206711898196
N25	N	0.866413560218	0.130907911309	0.849047446382
N26	N	0.153426311504	0.623084118015	0.188600672275
N27	N	0.878084581805	0.400391425783	0.701054028787
N28	N	0.124868645455	0.889640407847	0.344896565687
N29	N	0.830650142914	0.362666979759	0.637399187760
N30	N	0.176561576990	0.861993715336	0.410090394455
N31	N	0.933556604104	0.292796612545	0.557124706129
N32	N	0.101397209491	0.870559793829	0.494490101458
N33	N	0.768009950096	0.234219223283	0.656004896065
N34	N	0.238049926131	0.733849204958	0.391089705003
N35	N	0.675593930073	0.291824182583	0.698021957856
N36	N	0.329230588413	0.788425711795	0.348467263850
N37	N	0.703386972536	0.429095460716	0.777664284413
N38	N	0.310328035340	0.928321627739	0.264981497032
N39	N	0.611180819676	0.375777340121	0.649590931210
N40	N	0.389230229911	0.876089380142	0.397429786869
N41	N	0.577069286099	0.259217136181	0.604173695762
N42	N	0.425912534484	0.760405786365	0.442918494491
N43	N	0.496682595442	0.185811316820	0.646417413390
N44	N	0.505368739749	0.690357572446	0.399787138616
N45	N	0.447316347069	0.030614402291	0.748423896608
N46	N	0.564965112964	0.532645543461	0.300953802649
N47	N	0.366577087608	0.954963189159	0.730958461764
N48	N	0.640745640606	0.450989102880	0.319015120305
N49	N	0.376608049687	0.992981249577	0.786379833803
N50	N	0.636188890928	0.490612176492	0.263806888604
N51	N	0.400668378683	0.287059105413	0.647917465156
N52	N	0.598556391842	0.794633697095	0.396714209111
N53	N	0.298117209230	0.264025291570	0.600287847991
N54	N	0.698809331321	0.770639881028	0.444011279522
N55	N	0.257329392008	0.136599132272	0.631645703679
N56	N	0.739244824691	0.643001236540	0.412536118479
N57	N	0.315926976652	0.004464228250	0.620268432312
N58	N	0.684354655598	0.511355451345	0.428597966512
N59	N	0.368954294497	0.827842044279	0.645415680869
N60	N	0.639784539936	0.328274698817	0.408228632458
N61	N	0.474139835227	0.810516374101	0.715436174179
N62	N	0.538018169035	0.305139315614	0.338241810309
N63	N	0.558013994303	0.695774591347	0.703161266033
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N65	N	0.571174439886	0.688645294901	0.632290530353
N66	N	0.429783366830	0.189406933093	0.417409063505
N67	N	0.613081552350	0.833800128976	0.623775580624
N68	N	0.392053045458	0.336992687797	0.426288785850
N69	N	0.723823057593	0.817469488110	0.657833363715
N70	N	0.284353211502	0.326318379943	0.389232508658
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N72	N	0.212848252499	0.218364111841	0.426306939069
N73	N	0.790973720947	0.808730249909	0.561498430449
N74	N	0.208660115498	0.308814446556	0.484569442156
N75	N	0.859119641106	0.935563192763	0.580956353265
N76	N	0.148857292047	0.442966332786	0.464570986579
N77	N	0.962198963825	0.892291133505	0.615043747915
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N79	N	0.956015061998	0.902174324243	0.684427790515
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N81	N	0.905140062099	0.806660432406	0.760427274925
N82	N	0.087025491919	0.297039126788	0.287144330507
N83	N	0.810923077840	0.675182363854	0.803406978166
N84	N	0.174064852295	0.160882990978	0.242881676719
N85	N	0.804116988755	0.627006420390	0.887908456550
N86	N	0.185920997196	0.115929162419	0.160789309824
N87	N	0.768660678423	0.494207213712	0.952229743657
N88	N	0.234196550781	0.002031669369	0.091896185188
N89	N	0.791219720600	0.552447054358	0.017473570627
N90	N	0.199413043545	0.038470054330	0.026738814068
N91	N	0.812054907449	0.720830255744	0.068770474075
N92	N	0.175297614622	0.212150954036	0.981481419587
N93	N	0.918217060047	0.794931964684	0.063679081551
N94	N	0.072052829028	0.288299572009	0.983821815960
N95	N	0.015559136291	0.856171087354	0.011750199439
N96	N	0.970342304232	0.349878954069	0.030200403117
N97	N	0.140999886065	0.790320731158	0.963795669648
N98	N	0.842761238506	0.289083967466	0.075410683986
N99	N	0.295933438856	0.860789116852	0.963052199682
N100	N	0.693096218665	0.369478848027	0.085895741079
N101	N	0.330866652906	0.889219419281	0.896684504455
N102	N	0.660058310869	0.367643321748	0.154802419319
N103	N	0.226868734705	0.906570481276	0.861403459911
N104	N	0.768855313427	0.396986692590	0.186033457450
N105	N	0.180642911382	0.046277929308	0.876063368688
N106	N	0.812482227343	0.543009283000	0.172010427783
N107	N	0.115003137240	0.171707489821	0.864680988499
N108	N	0.894491497113	0.657513276077	0.181187035233
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O1	O	0.768112167378	0.779790456872	0.897747982614
O2	O	0.222875723795	0.269957540121	0.153199720216
O3	O	0.739822106898	0.841190785146	0.004029396113
O4	O	0.280302165936	0.294449312092	0.050925242328
O5	O	0.834013260654	0.000879028994	0.889916377557
O6	O	0.151999735450	0.478099186172	0.148855379954
O7	O	0.721234236691	0.032393399165	0.849107870723
O8	O	0.282498355898	0.512867111661	0.194103449912
O9	O	0.962451739818	0.913219932739	0.801123753768
O10	O	0.026893681791	0.396824953918	0.242268228354
O11	O	0.112271959529	0.077069693142	0.809743526009
O12	O	0.884570748696	0.565922950438	0.237578180369
O13	O	0.258628142783	0.113144106618	0.756330466267
O14	O	0.743275994627	0.605230068068	0.294686653953
O15	O	0.075745909995	0.255540968200	0.739187874687
O16	O	0.927887410780	0.744471783471	0.307095669367
O17	O	0.162646867739	0.243262556057	0.674643008881
O18	O	0.839526198778	0.742151138767	0.372871151610
O19	O	0.001695159366	0.424222694570	0.721163867512
O20	O	0.003866399441	0.907396364498	0.321855692958
O21	O	0.957026090485	0.360690643702	0.641230890887
O22	O	0.047472482290	0.853545643858	0.406287543916
O23	O	0.889836650655	0.211155290654	0.672516852164
O24	O	0.116466878068	0.706277020127	0.374964066681
O25	O	0.798457576436	0.332205754291	0.718758308607
O26	O	0.207068425166	0.825224889994	0.327993023414
O27	O	0.745241633751	0.421748819660	0.652845703621
O28	O	0.258310258214	0.922520753008	0.390334881986
O29	O	0.908437948093	0.553543369972	0.692152671478
O30	O	0.084807092699	0.039259508705	0.353216853940
O31	O	0.702939479273	0.258194505924	0.612595046091
O32	O	0.301172047119	0.748133312889	0.436072823462
O33	O	0.865740158160	0.387636525630	0.560912053570

O34	O	0.200902698794	0.904563381848	0.498388022754
O35	O	0.618408038506	0.199051392840	0.675825590160
O36	O	0.386854794431	0.696877126522	0.371434460619
O37	O	0.526930494269	0.353798521793	0.679740181734
O38	O	0.475062821892	0.854908371871	0.368979649258
O39	O	0.650094225557	0.322048515223	0.779507795319
O40	O	0.358431490808	0.817035039511	0.268989473109
O41	O	0.490267591390	0.324244148244	0.596633111778
O42	O	0.510769827360	0.828810896802	0.450709552479
O43	O	0.450721565940	0.137210435051	0.600026811531
O44	O	0.554015019674	0.640501266877	0.444971739667
O45	O	0.343649303827	0.204973172165	0.676160785057
O46	O	0.655934814490	0.714772730567	0.367411471787
O47	O	0.243726832779	0.326269852705	0.638525408175
O48	O	0.755018597492	0.830662173585	0.405702742080
O49	O	0.175279382056	0.129038953615	0.596586684951
O50	O	0.806565174953	0.620011253724	0.455111924847
O51	O	0.262251209692	0.945419146908	0.660180452098
O52	O	0.747887459989	0.446101948272	0.395766657813
O53	O	0.401780034573	0.938679111499	0.664542565267
O54	O	0.606072299122	0.434821700491	0.385131520722
O55	O	0.388986513495	0.019571984487	0.566597711710
O56	O	0.604979548316	0.527098218922	0.481058114802
O57	O	0.497093727105	0.816621860292	0.659681301755
O58	O	0.512356000214	0.312136593353	0.393583844445
O59	O	0.629330442701	0.785946316525	0.699784580732
O60	O	0.380951425266	0.289527382207	0.350445037656
O61	O	0.541404300499	0.801047943924	0.836415589083
O62	O	0.493164587855	0.291479360014	0.219476777852
O63	O	0.518751960647	0.921236587390	0.840934163277
O64	O	0.526226547230	0.407357383152	0.212090290161
O65	O	0.667671854791	0.652783341933	0.642404817385
O66	O	0.333388157959	0.154738773002	0.406129672797
O67	O	0.663615855696	0.793968939701	0.577977964408
O68	O	0.336890274799	0.296963801344	0.470388590257
O69	O	0.759240878825	0.915565742602	0.628245257904
O70	O	0.248219465515	0.424558953999	0.418473622134
O71	O	0.870085096320	0.779969095301	0.631605419465
O72	O	0.137937796904	0.297811737683	0.412470291141
O73	O	0.876063486684	0.752107741169	0.543697903188
O74	O	0.116592199699	0.260060679285	0.494454564030
O75	O	0.730628842418	0.636954271004	0.561779682767
O76	O	0.265296682569	0.139770081605	0.481021142579
O77	O	0.884885893150	0.946662591488	0.525766346122
O78	O	0.106507226568	0.439846007052	0.516257781990
O79	O	0.795983846022	0.132219956617	0.434523896355
O80	O	0.216126055702	0.640438246848	0.609494627996
O81	O	0.997977210808	0.010387908720	0.616971485918
O82	O	0.000792759354	0.508718821259	0.441694857972
O83	O	0.857347615982	0.992344528382	0.650084188297
O84	O	0.144732206900	0.490487607977	0.394219941617
O85	O	0.038713056464	0.828366706652	0.691229587305
O86	O	0.964001034404	0.326756965539	0.356637065796
O87	O	0.907523057074	0.772959284393	0.705422136334
O88	O	0.095095110405	0.270799620093	0.343038812447
O89	O	0.834919271012	0.794623584420	0.815975447105
O90	O	0.154749301832	0.282343521215	0.231900525240
O91	O	0.815754749882	0.546843588087	0.844308982554
O92	O	0.192437884225	0.028160278978	0.201846479067
O93	O	0.738549121320	0.613184379359	0.945695057210
O94	O	0.254196345079	0.120946115244	0.105257476335
O95	O	0.690386323641	0.540583701531	0.027977537735
O96	O	0.296579801980	0.054972739187	0.011341209993

O97	O	0.764561551178	0.702187962767	0.017729107046
O98	O	0.213323404723	0.183736653925	0.033415955255
O99	O	0.871368019605	0.906927923747	0.058267042243
O100	O	0.119642969816	0.400484527419	0.984620036997
O101	O	0.034181963825	0.738805777159	0.029721149602
O102	O	0.949352983658	0.233723469138	0.011307701819
O103	O	0.971495182994	0.799943438905	0.126234614584
O104	O	0.029572982874	0.306777838792	0.917960069633
O105	O	0.141683050704	0.866551496857	0.008931391529
O106	O	0.847622790364	0.388642621808	0.040957631497
O107	O	0.211250950908	0.897589962825	0.934491002701
O108	O	0.781423716137	0.387673912490	0.114909090243
O109	O	0.369940827734	0.001333731975	0.911566122791
O110	O	0.646679731775	0.491949924549	0.153041122358
O111	O	0.274344038273	0.916604779320	0.811307641748
O112	O	0.726762798612	0.399587237223	0.237739621680
O113	O	0.319096303848	0.743491801568	0.875686807143
O114	O	0.699452146486	0.215897862574	0.169030953628
O115	O	0.367112393840	0.707493434926	0.829038238525
O116	O	0.645004955224	0.162070959979	0.209886697317
O117	O	0.095907906121	0.980589660098	0.888442415534
O118	O	0.895068208522	0.477560379029	0.155919932512
O119	O	0.189460650076	0.678111117886	0.735518721583
O120	O	0.811220799962	0.179018120604	0.312306864943
O121	O	0.123438763174	0.208484248503	0.919109126017
O122	O	0.880457545230	0.696393674998	0.127252457524
O123	O	0.993656788429	0.159883289645	0.858998289649
O124	O	0.018528260194	0.639835109880	0.183408660050
O125	O	0.216055891924	0.234175819506	0.811758164740
O126	O	0.802638388687	0.722009863316	0.236075468329
O127	O	0.981810868098	0.273655086041	0.838100383499
O128	O	0.033857626050	0.752866476728	0.204421802353
O129	O	0.020920447105	0.583856199636	0.504344572065
O130	O	0.000886665045	0.798685489580	0.551357681108
O131	O	0.008274022299	0.948612265699	0.536403840048
O132	O	0.053646674085	0.066554093595	0.495597986785
O133	O	0.023865969095	0.188771122812	0.456912072343
O134	O	0.993638139165	0.331632340939	0.494902808577
O135	O	0.460512347420	0.521796717912	0.161894859135
O136	O	0.555273655738	0.792133853442	0.206501035530
O137	O	0.561278594134	0.938546141602	0.189545120764
O138	O	0.496149018095	0.069851169486	0.192960368591
O139	O	0.497405600723	0.206825803460	0.159119625053
O140	O	0.513069433511	0.386513944777	0.145465813165
O141	O	0.737447233474	0.047316347749	0.925722074042
O142	O	0.246555673191	0.551948284276	0.112929733815
O143	O	0.270647643737	0.103797202282	0.827700625050
O144	O	0.724203696641	0.605044420089	0.225103008270
O145	O	0.356938994796	0.190408666595	0.860936206816
O146	O	0.606888951117	0.652405223939	0.212824431751
O147	O	0.270752580479	0.386052266607	0.742456393783
O148	O	0.734478160591	0.881837032836	0.300993038721
O149	O	0.216107449938	0.434600901946	0.684309109976
O150	O	0.788765279556	0.932781265869	0.359049756386
O151	O	0.224044540800	0.586737773087	0.671841370919
O152	O	0.778380803318	0.083033814373	0.371572233698
O153	O	0.306679943521	0.630277343857	0.719526742868
O154	O	0.693537929040	0.127621568275	0.318390030677
O155	O	0.334482936317	0.508411793919	0.760351680438
O156	O	0.674068507901	0.002416914649	0.276827801825
O157	O	0.688670799380	0.288551357021	0.842749913730
O158	O	0.331603991788	0.791038008244	0.204582468326
O159	O	0.868465969447	0.552315906644	0.757634229283

O160	O	0.135076082318	0.043366152115	0.290206213021
O161	O	0.746679865646	0.554727719959	0.748118209514
O162	O	0.258632509323	0.046154782356	0.298833820098
O163	O	0.718202572925	0.548224702835	0.682520308598
O164	O	0.271190032505	0.060311426082	0.365836732280
O165	O	0.982604794288	0.150035517718	0.583981621307
O166	O	0.024820291370	0.733367433663	0.486927099877
O167	O	0.545568150526	0.241198236829	0.772168355190
O168	O	0.499078830455	0.822072115572	0.266001221468
O169	O	0.473655729744	0.352287742642	0.742498040875
O170	O	0.568382819714	0.847869327225	0.323830307767
O171	O	0.458110294977	0.488957527091	0.763147780886
O172	O	0.560632822893	0.985147493361	0.299145790847
O173	O	0.328720800732	0.248680396048	0.745183830165
O174	O	0.673365302092	0.745849983795	0.297442845629
O175	O	0.090605123566	0.161993473248	0.547350131439
O176	O	0.898514464459	0.734480030959	0.474176423189
O177	O	0.121891851425	0.995501906620	0.625123499233
O178	O	0.882470647501	0.520528419227	0.418844713127
O179	O	0.234510439394	0.812837492930	0.689884149752
O180	O	0.767933544512	0.312515629163	0.361707246857
O181	O	0.276178547235	0.027055514940	0.527332576098
O182	O	0.716795571819	0.534979507987	0.511238946669
O183	O	0.390308668594	0.781896801205	0.765325524469
O184	O	0.622478721009	0.250325421778	0.293935671484
O185	O	0.284029380881	0.840413028312	0.748944183561
O186	O	0.719426659011	0.337024323204	0.301493842148
O187	O	0.471052904553	0.634771624701	0.746628462528
O188	O	0.544353022154	0.130589817894	0.314598720517
O189	O	0.483298077543	0.054644482712	0.814946896802
O190	O	0.519149606561	0.565400970228	0.234824876733
O191	O	0.483683202677	0.673580662966	0.821233057784
O192	O	0.539639952594	0.156952367536	0.243350273729
O193	O	0.603691972090	0.796963482900	0.897734355122
O194	O	0.398999223452	0.339359134335	0.149620092511
O195	O	0.130480575802	0.728884587029	0.677756908036
O196	O	0.872775101079	0.227900101114	0.369763415997
O197	O	0.958008527096	0.675844262376	0.661499095882
O198	O	0.045169185540	0.161257099043	0.386319416900
O199	O	0.931953559301	0.519343071542	0.816503333168
O200	O	0.078204291741	0.004472329702	0.232256087211
O201	O	0.731487664889	0.432723238242	0.851842677955
O202	O	0.291562395496	0.933727194950	0.186374805874
O203	O	0.901034745439	0.484580945857	0.995790421564
O204	O	0.099588884595	0.966155885982	0.054537194200
O205	O	0.027220566490	0.487802411350	0.016841845079
O206	O	0.984115044012	0.004306839222	0.028995603579
O207	O	0.945234548194	0.639690532958	0.062033605886
O208	O	0.019298940710	0.117975907180	0.987883483337
O209	O	0.979241553116	0.571240817588	0.124588494854
O210	O	0.024483947201	0.089631397287	0.917720346251
O211	O	0.067754304382	0.564061412577	0.075128539547
O212	O	0.901013007934	0.118125220382	0.927652208786
O213	O	0.331466850091	0.770492378013	0.028823554039
O214	O	0.620996620528	0.276772640643	0.043442576058
O215	O	0.256993014525	0.612783571151	0.878653881783
O216	O	0.737742078240	0.073674137368	0.154855810818
O217	O	0.321809633958	0.568307516871	0.822501046424
O218	O	0.667474161614	0.017877243501	0.207008911436
O219	O	0.996874769985	0.413247536850	0.856847863269
O220	O	0.018227994720	0.895855275848	0.192831247192
O221	O	0.110402799773	0.416437014489	0.888066849735
O222	O	0.903929552377	0.904119809711	0.163051575185

O223	O	0.087318664702	0.572869866433	0.900134361581
O224	O	0.871989735767	0.062646272240	0.159415517047
O225	O	0.605669016926	0.338991302136	0.887860675754
O226	O	0.430979377051	0.675028213265	0.066398321033
O227	O	0.361244198235	0.699625073487	0.941240774949
O228	O	0.356134891834	0.201355767248	0.004853843879
O229	O	0.435813585557	0.576033293870	0.930814115356
O230	O	0.551413570107	0.911651916726	0.022150560856
O231	O	0.326270482618	0.530726629534	0.917182267045
O232	O	0.560494146287	0.254224950370	0.106811091285
O233	O	0.475456709208	0.684581943677	0.891008220913
O234	O	0.547400201152	0.363127972379	0.006978497553
O235	O	0.452097784246	0.053681827731	0.095397461036
O236	O	0.433093551946	0.868734280447	0.033936209447
O237	O	0.396240672924	0.013020935335	0.158435843044
O238	O	0.544113052264	0.722688539959	0.945119603421
O239	O	0.625973925325	0.919023382360	0.076571695785
O240	O	0.616072634833	0.061264499701	0.877900720956
O241	O	0.547555763491	0.259456525091	0.942404415380
O242	O	0.386620482600	0.776017068186	0.112023638596
O243	O	0.450316587926	0.110147284950	0.937382084013
O244	O	0.509595055580	0.720211219805	0.019505729089
O245	O	0.575956863426	0.099751010178	0.088529533056
O246	O	0.362959157159	0.357426006851	0.933905622276
O247	O	0.439243874430	0.909207986989	0.114229559243
O248	O	0.558030336851	0.562543162954	0.076610553086
O249	O	0.472375379239	0.196811978617	0.881107398294
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O251	O	0.639564872709	0.766088185065	0.131468441835
O252	O	0.681645625792	0.003217038468	0.982610268054
O253	O	0.564214812633	0.553324271661	0.906349184248
O254	O	0.489623208148	0.636861510985	0.122588043056
O255	O	0.313823932765	0.642472886876	0.996772486420
O256	O	0.667715895890	0.777811187386	0.063537808092
O257	O	0.352845888766	0.198592028328	0.929735163983
O258	O	0.694911632189	0.176229197920	0.980065196637
O259	O	0.611926968274	0.790200627575	0.002579250409
O260	O	0.556076651553	0.880455536982	0.128962684593
O261	O	0.489788793438	0.127818549206	0.002970317042
O262	O	0.606495823025	0.131233988346	0.936917335086
O263	O	0.518591641885	0.425570203095	0.067282649328
O264	O	0.432340515301	0.790410222631	0.977444975539
O265	O	0.558878228049	0.166118379297	0.835847382166
O266	O	0.290382352258	0.532985184218	0.042784490516
O267	O	0.442778320244	0.762432880748	0.176877878258
O268	O	0.412551888397	0.009619412817	0.019065616102
O269	O	0.557425097969	0.934081779594	0.902708214083
O270	O	0.329688988936	0.340036303264	0.864606627949
O271	O	0.457620240881	0.838410969039	0.916163349378
O272	O	0.595828368767	0.421214066857	0.949816394271
O273	O	0.482119495381	0.242657138675	0.054472912989
O274	O	0.607624367916	0.132582351347	0.023591965103
O275	O	0.754532445800	0.970317115280	0.043040397677
O276	O	0.389545326978	0.475536635568	0.862513351502
O277	O	0.299696183174	0.680446120687	0.085785032542
O278	O	0.395015998103	0.479243529887	0.070319982526
O279	O	0.689065511184	0.038512106383	0.095598376069
O280	O	0.357819335321	0.474744970571	0.132576752428
O281	O	0.482046644619	0.347123213575	0.878624253409
O282	O	0.306278679191	0.459671066008	0.977424370004
O283	O	0.450091709751	0.283030231786	0.977132604497
O284	O	0.470295831486	0.432655015850	0.930752501058
O285	O	0.601072692607	0.635137410077	0.147307312647

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O286   O     0.550306449618   0.580028820399   0.010501879163
O287   O     0.423611398325   0.444619770291   0.994988426698
O288   O     0.563872068541   0.006902477902   0.967407415948
O289   O     0.423179586067   0.586516856727   0.009124262978
O290   O     0.669953183180   0.633184086679   0.077892834078
O291   O     0.622041087609   0.613312151445   0.960284495513
O292   O     0.610985562322   0.472199884311   0.858314221571
O293   O     0.392686975640   0.346990637090   0.043402003588
O294   O     0.498331182384   0.516070714283   0.829887440251
O295   O     0.391214359104   0.635174058701   0.204182262490
O296   O     0.447820625944   0.686786231235   0.262524086238
O297   O     0.436830421502   0.915033327174   0.221164003455
O298   O     0.452787447051   0.018302960489   0.269686055889
O299   O     0.377460900350   0.316581172938   0.216111875432
O300   O     0.393305971434   0.470070794590   0.217540428620
S1   S     0.941351103191   0.850691100809   0.914571646238
S2   S     0.042493632907   0.316776860735   0.132962021345
S3   S     0.903097185098   0.102800769454   0.764277483404
S4   S     0.097964425046   0.591988483542   0.276566221533
S5   S     0.579722694863   0.036458206068   0.584971187223
S6   S     0.428763650376   0.538735078525   0.464456989352
S7   S     0.552652196222   0.993982066447   0.631161291304
S8   S     0.455436871585   0.496801600903   0.418147566243
S9   S     0.901445118690   0.051396585294   0.717273896802
S10   S     0.104799932424   0.546179432377   0.324713247361
S11   S     0.960363124356   0.937757835074   0.947186047034
S12   S     0.041388806464   0.401191067882   0.097608385108
#END
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