

Supporting Information

Authors: Ole Winther and Anders Krogh
Title: Teaching computers to fold proteins

Fixed parameters

Definition of backbone lengths and angles

```
#define R_NC      1.46      // AA
#define R_CC      1.52
#define R_CN      1.33
#define R_NH      1.03
#define R_CCb     1.53
#define R_CO      1.23

#define C_CNC     0.5255   // 121.7^o
#define C_NCC     0.3584   // 111.0^o
#define C_CCN     0.4478   // 116.6^o

#define S_CNC     0.8508   // 121.7^o
#define S_NCC     0.9336   // 111.0^o
#define S_CCN     0.8942   // 116.6^o

#define C_HNC     -0.4726   // 118.2^o
#define C_NCCb    0.3420   // 110.0
#define C_CCC     -0.3420   // 110.0
#define C_CCO     0.5165   // 121.1^o
#define C_OCN     -0.5476   // 123.2^o
#define C_CNH     0.4924   // 119.5^o

#define S_HNC     0.8813   // 118.2^o
#define S_NCCb    0.9397   // 110.0^o
#define S_CCC     0.9397   // 110.0^o
#define S_CCO     0.8563   // 121.1^o
#define S_OCN     0.8368   // 123.2^o
#define S_CNH     0.8704   // 119.5
```

Adjustable parameters

Amino acids

$$a_i = \{ \text{ALA, ARG, ASN, ASP, CYS, GLN, GLU, GLY, HIS, ILE, LEU, LYS, MET, PHE, PRO, SER, THR, TRP, TYR, VAL} \} .$$

C_α to side chain distances

4.755 3.410 1.897 3.847 1.609 1.600 3.192 2.311 1.437 3.481 3.341 3.596 2.104 2.333 1.581 3.135 2.732 1.472 2.316 1.539

Initial value is 2.6.

Local Energy

Torsional – 2 parameters ϵ_ϕ and ϵ_ψ .

0.073 0.069

Initial value is 0.1.

$H(i) - R(i) - 20$ interactions, first row ϵ_i^{H-R} , second row σ_{ij}^{H-R}

1.620 1.188 0.898 1.126 0.906 0.974 1.711 0.827 0.991 1.469 1.381 1.263 1.037 1.260 0.902 1.558 1.349 0.875 1.234 1.094
4.695 3.616 2.072 4.453 0.874 1.724 3.440 3.769 1.983 4.181 3.726 3.914 2.928 2.344 0.823 3.638 3.621 0.557 3.162 2.402

Initial values are 1 and 3.

$R(i) - O(i) - 20$ interactions, first row ϵ_i^{R-O} , second row σ_{ij}^{R-O} .

0.951 0.934 1.315 0.983 1.034 1.025 0.897 1.026 0.955 0.921 0.901 0.937 1.039 0.934 0.972 0.891 1.175 1.178 1.404 0.898
2.657 2.492 2.271 3.264 3.108 3.433 2.590 3.493 1.722 2.361 2.166 2.631 4.063 3.580 3.229 1.947 3.974 3.175 3.528 2.973

Initial values are 1 and 3.

$H(i) - H(i+1) - 1$ interaction, ϵ_i^{H-H} and σ_i^{H-H} .

0.165 0.617

Initial values are 0.1 and 1.

$O(i) - H(i+2) - 1$ interaction, ϵ_i^{O-H} and σ_i^{O-H} .

0.108 1.066

Initial values are 0.1 and 1.

$O(i) - O(i+1) - 1$ interaction, ϵ_i^{O-O} and σ_i^{O-O} .

0.104 3.116

Initial values are 0.1 and 1.

Hydrogen bond

1 interaction, ϵ_{hb} and σ_{hb} .

1.418 1.912

Initial values are 2 and 2.

Hydrophobic, surface and related interactions

$C_{\alpha}(i) - C_{\alpha}(j) - 20 \times 20$ interaction matrix, first row ϵ_{ij}^{α} , second row σ_{ij}^{α} .

| | | | | | | | | | | | | | | | | | | | |
|-------|--------|-------|-------|--------|-------|-------|-------|--------|-------|-------|--------|-------|-------|--------|--------|-------|-------|-------|-------|
| 0.185 | 0.061 | 0.206 | 0.095 | 0.182 | 0.223 | 0.176 | 0.213 | 0.157 | 0.154 | 0.178 | 0.179 | 0.271 | 0.140 | 0.095 | 0.236 | 0.139 | 0.170 | 0.118 | 0.027 |
| 3.835 | 1.940 | 5.564 | 5.905 | 8.645 | 6.409 | 5.981 | 4.775 | 4.810 | 0.998 | 5.643 | 0.981 | 5.224 | 5.933 | 3.875 | 5.390 | 2.579 | 3.779 | 3.489 | 2.027 |
| 0.061 | 0.200 | 0.179 | 0.173 | 0.200 | 0.200 | 0.187 | 0.196 | 0.191 | 0.246 | 0.203 | 0.296 | 0.010 | 0.231 | 0.189 | 0.301 | 0.167 | 0.200 | 0.150 | 0.267 |
| 1.940 | 4.500 | 4.544 | 4.622 | 4.500 | 4.500 | 4.564 | 4.453 | 3.629 | 5.357 | 4.284 | 5.466 | 2.004 | 6.149 | 12.214 | 6.083 | 3.824 | 4.500 | 4.831 | 5.516 |
| 0.206 | 0.179 | 0.145 | 0.181 | 0.220 | 0.203 | 0.167 | 0.204 | 0.201 | 0.160 | 0.158 | 0.172 | 0.173 | 0.055 | 0.200 | 0.200 | 0.183 | 0.206 | 0.200 | 0.170 |
| 5.564 | 4.544 | 3.422 | 4.042 | 5.841 | 6.149 | 1.861 | 4.867 | 6.561 | 1.881 | 2.155 | 2.916 | 4.834 | 6.410 | 4.500 | 4.500 | 4.900 | 5.076 | 4.500 | 2.738 |
| 0.095 | 0.173 | 0.181 | 0.044 | 0.182 | 0.312 | 0.174 | 0.209 | 0.174 | 0.173 | 0.056 | 0.135 | 0.276 | 0.169 | 0.174 | 0.210 | 0.162 | 0.175 | 0.140 | 0.097 |
| 5.905 | 4.622 | 4.042 | 2.003 | 3.948 | 4.886 | 4.998 | 5.517 | 5.837 | 2.869 | 5.594 | 4.279 | 6.497 | 1.161 | 2.276 | 4.820 | 5.470 | 3.148 | 1.815 | 4.557 |
| 0.182 | 0.200 | 0.220 | 0.182 | 0.200 | 0.233 | 0.234 | 0.190 | 0.191 | 0.182 | 0.153 | 0.186 | 0.216 | 0.214 | 0.229 | 0.200 | 0.221 | 0.200 | 0.244 | 0.200 |
| 8.645 | 4.500 | 5.841 | 3.948 | 4.500 | 5.868 | 5.423 | 3.488 | 4.177 | 4.222 | 4.879 | 10.545 | 5.771 | 4.943 | 6.382 | 4.500 | 6.353 | 4.500 | 3.874 | 4.500 |
| 0.223 | 0.200 | 0.203 | 0.312 | 0.233 | 0.200 | 0.198 | 0.187 | 0.429 | 0.183 | 0.163 | 0.143 | 0.220 | 0.205 | 0.186 | 0.228 | 0.181 | 0.183 | 0.233 | 0.161 |
| 6.409 | 4.500 | 6.149 | 4.886 | 5.868 | 4.500 | 5.101 | 4.538 | 5.023 | 4.009 | 5.748 | 5.120 | 5.261 | 5.975 | 3.192 | 5.014 | 2.970 | 9.807 | 5.708 | 5.412 |
| 0.176 | 0.187 | 0.167 | 0.174 | 0.234 | 0.198 | 0.507 | 0.184 | 0.165 | 0.267 | 0.588 | 0.121 | 0.163 | 0.043 | 0.181 | 0.172 | 0.145 | 0.184 | 0.162 | 0.162 |
| 5.981 | 4.564 | 1.861 | 4.998 | 5.423 | 5.101 | 6.111 | 2.959 | 6.531 | 5.760 | 4.355 | 1.705 | 0.828 | 6.713 | 3.671 | 3.022 | 3.889 | 4.425 | 6.210 | 4.577 |
| 0.213 | 0.196 | 0.204 | 0.209 | 0.190 | 0.187 | 0.184 | 0.168 | 0.240 | 0.012 | 0.116 | 0.162 | 0.291 | 0.118 | 0.200 | 0.231 | 0.116 | 0.196 | 0.148 | 0.145 |
| 4.775 | 4.453 | 4.867 | 5.517 | 3.488 | 4.538 | 2.959 | 6.129 | 4.560 | 1.999 | 6.468 | 2.410 | 2.752 | 6.686 | 4.500 | 6.576 | 6.076 | 4.283 | 8.909 | 5.833 |
| 0.157 | 0.191 | 0.201 | 0.174 | 0.191 | 0.429 | 0.165 | 0.240 | 0.208 | 0.174 | 0.289 | 0.205 | 0.186 | 0.231 | 0.172 | 0.192 | 0.290 | 0.182 | 0.168 | 0.166 |
| 4.810 | 3.629 | 6.561 | 5.837 | 4.177 | 5.023 | 6.531 | 4.560 | 5.297 | 5.322 | 3.740 | 4.979 | 5.442 | 5.713 | 10.519 | 3.789 | 5.210 | 5.878 | 3.746 | 5.526 |
| 0.154 | 0.246 | 0.160 | 0.173 | 0.182 | 0.183 | 0.267 | 0.012 | 0.174 | 0.076 | 0.144 | 0.078 | 0.225 | 0.194 | 0.163 | 0.142 | 0.069 | 0.112 | 0.251 | 0.227 |
| 0.998 | 5.357 | 1.881 | 2.869 | 4.222 | 4.009 | 5.760 | 1.999 | 5.322 | 3.265 | 1.022 | 4.518 | 4.543 | 1.130 | 2.679 | 1.910 | 6.981 | 6.520 | 4.567 | 5.496 |
| 0.178 | 0.203 | 0.158 | 0.056 | 0.153 | 0.163 | 0.588 | 0.116 | 0.289 | 0.144 | 0.136 | 0.086 | 0.228 | 0.132 | 0.143 | 0.093 | 0.069 | 0.162 | 0.345 | 0.203 |
| 5.643 | 4.284 | 2.155 | 5.594 | 4.879 | 5.748 | 4.355 | 6.468 | 3.740 | 1.022 | 5.730 | 5.658 | 5.104 | 1.865 | 4.857 | 2.965 | 4.851 | 2.599 | 5.555 | 6.689 |
| 0.179 | 0.296 | 0.172 | 0.135 | 0.186 | 0.143 | 0.121 | 0.162 | 0.205 | 0.078 | 0.086 | 0.104 | 0.450 | 0.215 | 0.310 | 0.094 | 0.129 | 0.162 | 0.116 | 0.130 |
| 0.981 | 5.466 | 2.916 | 4.279 | 10.545 | 5.120 | 1.705 | 2.410 | 4.979 | 4.518 | 5.658 | 5.512 | 3.709 | 3.889 | 5.184 | 2.779 | 4.518 | 2.402 | 3.976 | 5.715 |
| 0.271 | 0.010 | 0.173 | 0.276 | 0.216 | 0.220 | 0.163 | 0.291 | 0.186 | 0.225 | 0.228 | 0.450 | 0.211 | 0.431 | 0.188 | 0.188 | 0.141 | 0.200 | 0.191 | 0.208 |
| 5.224 | 2.004 | 4.834 | 6.497 | 5.771 | 5.261 | 0.828 | 2.752 | 5.442 | 4.543 | 5.104 | 3.709 | 6.776 | 4.914 | 4.139 | 4.504 | 3.535 | 4.500 | 4.191 | 6.092 |
| 0.140 | 0.231 | 0.055 | 0.169 | 0.214 | 0.205 | 0.043 | 0.118 | 0.231 | 0.194 | 0.132 | 0.215 | 0.431 | 0.199 | 0.192 | 0.159 | 0.178 | 0.178 | 0.284 | 0.182 |
| 5.933 | 6.149 | 6.410 | 1.161 | 4.943 | 5.975 | 6.713 | 6.686 | 5.713 | 1.130 | 1.865 | 3.889 | 4.914 | 6.675 | 5.003 | 2.576 | 5.385 | 2.936 | 4.220 | 2.796 |
| 0.095 | 0.189 | 0.200 | 0.174 | 0.229 | 0.186 | 0.181 | 0.200 | 0.172 | 0.163 | 0.143 | 0.310 | 0.188 | 0.192 | 0.200 | 0.087 | 0.190 | 0.200 | 0.112 | 0.161 |
| 3.875 | 12.214 | 4.500 | 2.276 | 6.382 | 3.192 | 3.671 | 4.500 | 10.519 | 2.679 | 4.857 | 5.184 | 4.139 | 5.003 | 4.500 | 10.970 | 4.432 | 4.500 | 4.054 | 4.298 |
| 0.236 | 0.301 | 0.200 | 0.210 | 0.200 | 0.228 | 0.172 | 0.231 | 0.192 | 0.142 | 0.093 | 0.094 | 0.188 | 0.159 | 0.087 | 0.258 | 0.431 | 1.445 | 0.073 | 0.160 |
| 5.390 | 6.083 | 4.500 | 4.820 | 4.500 | 5.014 | 3.022 | 6.576 | 3.789 | 1.910 | 2.965 | 2.779 | 4.504 | 2.576 | 10.970 | 3.519 | 4.571 | 1.479 | 4.676 | 3.464 |
| 0.139 | 0.167 | 0.183 | 0.162 | 0.221 | 0.181 | 0.145 | 0.116 | 0.290 | 0.069 | 0.069 | 0.129 | 0.141 | 0.178 | 0.190 | 0.431 | 0.100 | 0.160 | 0.363 | 0.090 |
| 2.579 | 3.824 | 4.900 | 5.470 | 6.353 | 2.970 | 3.889 | 6.076 | 5.210 | 6.981 | 4.851 | 4.518 | 3.535 | 5.385 | 4.432 | 4.571 | 6.190 | 6.434 | 5.554 | 1.867 |
| 0.170 | 0.200 | 0.206 | 0.175 | 0.200 | 0.183 | 0.184 | 0.196 | 0.182 | 0.112 | 0.162 | 0.162 | 0.200 | 0.178 | 0.200 | 1.445 | 0.160 | 0.177 | 0.163 | 0.325 |
| 3.779 | 4.500 | 5.076 | 3.148 | 4.500 | 9.807 | 4.425 | 4.283 | 5.878 | 6.520 | 2.599 | 2.402 | 4.500 | 2.936 | 4.500 | 1.479 | 6.434 | 4.980 | 2.929 | 4.359 |
| 0.118 | 0.150 | 0.200 | 0.140 | 0.244 | 0.233 | 0.162 | 0.148 | 0.168 | 0.251 | 0.345 | 0.116 | 0.191 | 0.284 | 0.112 | 0.073 | 0.363 | 0.163 | 0.176 | 0.268 |
| 3.489 | 4.831 | 4.500 | 1.815 | 3.874 | 5.708 | 6.210 | 8.909 | 3.746 | 4.567 | 5.555 | 3.976 | 4.191 | 4.220 | 4.054 | 4.676 | 5.554 | 2.929 | 5.975 | 5.510 |
| 0.027 | 0.267 | 0.170 | 0.097 | 0.200 | 0.161 | 0.162 | 0.145 | 0.166 | 0.227 | 0.203 | 0.130 | 0.208 | 0.182 | 0.161 | 0.160 | 0.090 | 0.325 | 0.268 | 0.203 |
| 2.027 | 5.516 | 2.738 | 4.557 | 4.500 | 5.412 | 4.577 | 5.833 | 5.526 | 5.496 | 6.689 | 5.715 | 6.092 | 2.796 | 4.298 | 3.464 | 1.867 | 4.359 | 4.510 | 5.651 |

Initial values are 0.2 and 4.5.

$R(i) - R(j)$: -20×20 interaction matrix, first row ϵ_{ij}^R , second row σ_{ij}^R .

| | | | | | | | | | | | | | | | | | | | |
|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 0.873 | 0.469 | 0.012 | 0.154 | 1.024 | 0.584 | 0.246 | 0.581 | 0.485 | 0.283 | 0.355 | 0.265 | 0.594 | 0.328 | 0.451 | 0.383 | 0.346 | 0.490 | 0.274 | 0.356 |
| 12.017 | 4.953 | 2.000 | 4.591 | 1.068 | 4.202 | 1.943 | 3.326 | 1.982 | 2.549 | 0.908 | 2.744 | 2.217 | 1.797 | 5.121 | 7.137 | 1.545 | 2.883 | 1.648 | 1.290 |
| 0.469 | 1.000 | 0.789 | 0.486 | 1.000 | 1.000 | 0.580 | 0.665 | 0.686 | 2.540 | 0.458 | 0.630 | 0.520 | 1.157 | 0.579 | 0.615 | 0.467 | 1.000 | 0.403 | 0.912 |
| 4.953 | 5.000 | 3.094 | 2.026 | 5.000 | 5.000 | 7.460 | 3.269 | 3.926 | 5.702 | 3.422 | 3.945 | 3.197 | 9.367 | 3.765 | 6.004 | 2.888 | 5.000 | 3.201 | 2.562 |
| 0.012 | 0.789 | 0.497 | 0.462 | 1.388 | 2.145 | 0.371 | 0.971 | 1.074 | 0.303 | 0.337 | 0.175 | 0.502 | 0.404 | 1.000 | 1.000 | 0.412 | 1.117 | 1.000 | 0.539 |
| 2.000 | 3.094 | 1.924 | 3.454 | 6.946 | 5.784 | 1.100 | 3.172 | 6.374 | 1.100 | 1.666 | 5.457 | 3.344 | 1.446 | 5.000 | 5.000 | 4.219 | 4.096 | 5.000 | 1.819 |
| 0.154 | 0.486 | 0.462 | 0.388 | 0.487 | 0.466 | 0.643 | 0.601 | 0.554 | 0.453 | 0.542 | 0.233 | 0.444 | 0.340 | 0.469 | 0.222 | 0.453 | 0.433 | 0.263 | 0.289 |
| 4.591 | 2.026 | 3.454 | 1.311 | 3.894 | 2.112 | 2.583 | 3.561 | 2.667 | 1.613 | 0.648 | 3.953 | 2.348 | 6.472 | 2.210 | 2.251 | 5.466 | 2.667 | 1.264 | 1.417 |
| 1.024 | 1.000 | 1.388 | 0.487 | 1.000 | 1.260 | 1.788 | 0.693 | 1.995 | 0.602 | 0.408 | 0.739 | 0.804 | 0.426 | 2.917 | 1.000 | 0.560 | 1.000 | 1.647 | 1.000 |
| 1.068 | 5.000 | 6.946 | 3.894 | 5.000 | 7.798 | 7.294 | 3.245 | 6.206 | 2.786 | 2.179 | 3.005 | 2.982 | 6.450 | 6.040 | 5.000 | 5.596 | 5.000 | 4.575 | 5.000 |
| 0.584 | 1.000 | 2.145 | 0.466 | 1.260 | 1.000 | 0.846 | 0.618 | 1.481 | 0.511 | 0.420 | 0.722 | 1.574 | 1.785 | 0.711 | 1.074 | 0.615 | 0.792 | 0.509 | 0.514 |
| 4.202 | 5.000 | 5.784 | 2.112 | 7.798 | 5.000 | 2.965 | 2.198 | 1.587 | 4.749 | 3.102 | 3.101 | 5.762 | 6.352 | 2.221 | 4.840 | 6.427 | 3.388 | 2.442 | 3.504 |
| 0.246 | 0.580 | 0.371 | 0.643 | 1.788 | 0.846 | 0.409 | 0.662 | 0.708 | 0.389 | 0.336 | 0.324 | 0.435 | 0.299 | 0.812 | 0.380 | 0.419 | 0.565 | 0.611 | 0.294 |
| 1.943 | 7.460 | 1.100 | 2.583 | 7.294 | 2.965 | 2.010 | 1.881 | 5.652 | 0.981 | 0.568 | 0.996 | 1.656 | 1.420 | 3.517 | 2.134 | 2.528 | 3.033 | 2.116 | 4.730 |

0.581 0.665 0.971 0.601 0.693 0.618 0.662 0.578 0.915 0.379 0.528 0.254 0.654 0.605 1.000 0.548 0.569 0.795 0.722 0.566
3.326 3.269 3.172 3.561 3.245 2.198 1.881 2.756 1.237 1.676 1.889 2.679 1.538 1.697 5.000 2.331 2.010 4.675 3.196 1.670

0.485 0.686 1.074 0.554 1.995 1.481 0.708 0.915 1.229 0.403 0.410 0.366 0.686 0.531 0.857 0.841 0.012 0.699 0.376 0.613
1.982 3.926 6.374 2.667 6.206 1.587 5.652 1.237 6.108 2.405 1.632 5.183 2.077 2.264 3.638 6.981 1.994 2.833 2.612 1.943

0.283 2.540 0.303 0.453 0.602 0.511 0.389 0.379 0.403 0.309 0.222 0.198 0.697 0.223 0.203 0.296 0.336 0.629 0.313 1.110
2.549 5.702 1.100 1.613 2.786 4.749 0.981 1.676 2.405 1.146 0.789 1.272 8.318 0.771 3.258 1.176 3.123 1.576 0.989 0.036

0.355 0.458 0.337 0.542 0.408 0.420 0.336 0.528 0.410 0.222 0.250 0.667 0.418 0.276 0.367 0.302 0.284 0.335 0.691 0.326
0.908 3.422 1.666 0.648 2.179 3.102 0.568 1.889 1.632 0.789 1.052 4.118 1.316 0.995 1.779 2.806 1.539 1.565 0.878 3.535

0.265 0.630 0.175 0.233 0.739 0.722 0.324 0.254 0.366 0.198 0.667 0.337 0.820 0.404 0.941 0.208 0.581 0.315 0.312 0.382
2.744 3.945 5.457 3.953 3.005 3.101 0.996 2.679 5.183 1.272 4.118 1.761 5.533 1.036 5.201 1.937 1.100 2.067 1.744 1.510

0.594 0.520 0.502 0.444 0.804 1.574 0.435 0.654 0.686 0.697 0.418 0.820 1.388 0.545 0.598 0.669 0.247 1.000 0.749 0.880
2.217 3.197 3.344 2.348 2.982 5.762 1.656 1.538 2.077 8.318 1.316 5.533 6.579 0.909 4.209 0.971 3.517 5.000 2.860 4.112

0.328 1.157 0.404 0.340 0.426 1.785 0.299 0.605 0.531 0.223 0.276 0.404 0.545 0.583 0.480 0.505 0.288 0.730 0.656 0.613
1.797 9.367 1.446 6.472 6.450 6.352 1.420 1.697 2.264 0.771 0.995 1.036 0.909 2.283 2.377 1.538 2.776 5.272 4.945 9.808

0.451 0.579 1.000 0.469 2.917 0.711 0.812 1.000 0.857 0.203 0.367 0.941 0.598 0.480 1.000 0.430 0.507 1.000 0.578 0.323
5.121 3.765 5.000 2.210 6.040 2.221 3.517 5.000 3.638 3.258 1.779 5.201 4.209 2.377 5.000 2.540 2.496 5.000 4.121 8.236

0.383 0.615 1.000 0.222 1.000 1.074 0.380 0.548 0.841 0.296 0.302 0.208 0.669 0.505 0.430 0.698 0.677 0.506 0.284 0.299
7.137 6.004 5.000 2.251 5.000 4.840 2.134 2.331 6.981 1.176 2.806 1.937 0.971 1.538 2.540 6.524 1.138 1.838 1.108 2.167

0.346 0.467 0.412 0.453 0.560 0.615 0.419 0.569 0.012 0.336 0.284 0.581 0.247 0.288 0.507 0.677 0.393 0.553 0.396 0.312
1.545 2.888 4.219 5.466 5.596 6.427 2.528 2.010 1.994 3.123 1.539 1.100 3.517 2.776 2.496 1.138 3.142 2.427 1.519 1.208

0.490 1.000 1.117 0.433 1.000 0.792 0.565 0.795 0.699 0.629 0.335 0.315 1.000 0.730 1.000 0.506 0.553 0.611 0.714 0.600
2.883 5.000 4.096 2.667 5.000 3.388 3.033 4.675 2.833 1.576 1.565 2.067 5.000 5.272 5.000 1.838 2.427 3.264 1.727 5.483

0.274 0.403 1.000 0.263 1.647 0.509 0.611 0.722 0.376 0.313 0.691 0.312 0.749 0.656 0.578 0.284 0.396 0.714 0.596 0.513
1.648 3.201 5.000 1.264 4.575 2.442 2.116 3.196 2.612 0.989 0.878 1.744 2.860 4.945 4.121 1.108 1.519 1.727 1.151 0.961

0.356 0.912 0.539 0.289 1.000 0.514 0.294 0.566 0.613 1.110 0.326 0.382 0.880 0.613 0.323 0.299 0.312 0.600 0.513 0.578
1.290 2.562 1.819 1.417 5.000 3.504 4.730 1.670 1.943 0.036 3.535 1.510 4.112 9.808 8.236 2.167 1.208 5.483 0.961 1.866

Initial values are 1 and 5.

Surface – 20*5 parameters ϵ_i^{surf} , s_i , b_i , $\sigma_i^{\text{surf},0}$ and σ_i^{surf} .

-0.143 1.399 0.750 0.777 -0.610 0.800 1.147 -0.002 0.020 -0.684 -0.593 2.058 -0.650 -0.613 0.497 0.394 0.320 -0.390 0.277 -0.554
1.000 1.001 1.000 1.001 1.000 1.000 1.002 1.000 1.000 0.999 0.999 1.002 1.000 0.999 1.001 1.001 1.000 1.000 1.000 0.999
1.000 1.000 1.000 1.000 1.000 1.000 1.001 1.000 1.000 0.999 1.000 1.001 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000
5.998 5.998 5.998 5.993 6.001 5.994 5.998 6.002 5.995 5.995 6.000 5.988 6.000 5.999 5.989 5.998 5.995 5.999 5.997 5.992
1.259 1.388 60.601 2.473 1.855 1.585 1.165 1.581 1.878 0.593 5.444 3.676 5.982 0.643 4.402 2.316 1.287 1.891 1.754 2.173

Initial values are for ϵ_i^{surf} taken from Ref. [1] table xx and for the others: 1.0, 1.0, 6.0 and 6.0.

References

- [1] T. E. Creighton, Proteins: Structures and Molecular Properties, W. H. Freeman & Co., 2nd ed. (1992).

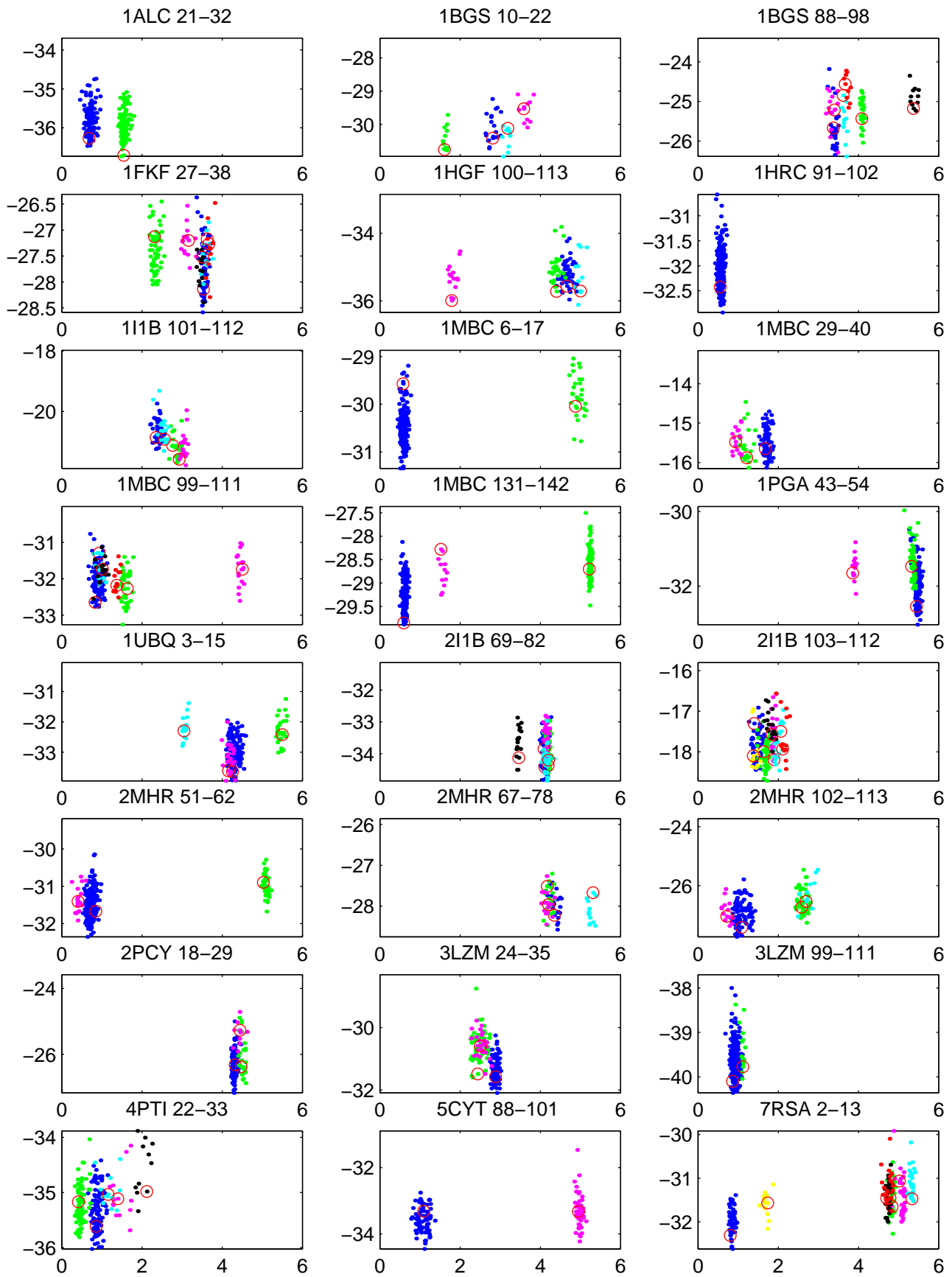


Figure 1: Decoy plots – energy versus RMSD for $T = 0.1$. Cluster RMSD cut-off is 0.5 \AA . Cluster centers are marked with a circle. Blue codes for the largest cluster.

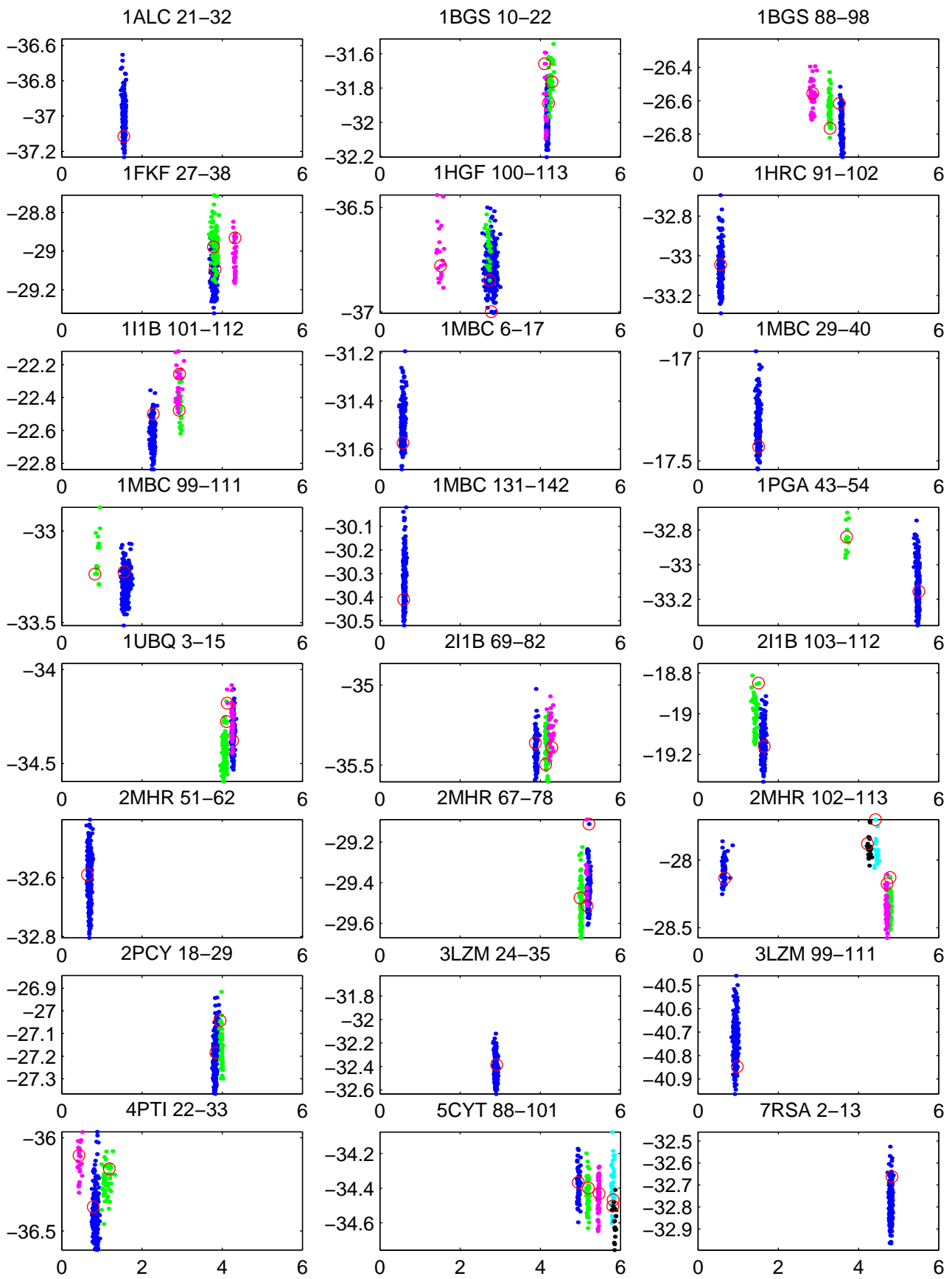


Figure 2: Decoy plots – energy versus RMSD for $T = 0.025$. Cluster RMSD cut-off is 0.5 \AA . Cluster centers are marked with a circle. Blue codes for the largest cluster.