Table S3 summarizes scores and weights in the energy function in BCL::Fold; amino acid clash score (aa\_clash), amino acid distance score (aa\_dist), amino acid environment potential and the counterpart for the unfolded fraction of the model (aa\_neigh & aa\_neigh\_unf), SSE clash score (sse\_clash), SSE packing score (sse\_pack), β-strand pairing score (strand\_pair), loop score (loop), loop closure score (loop\_closure), radius of gyration score (rgyr), contact order score (co) contact order score, SSE prediction scores and the counterparts for the unfolded fraction of the model using methods JUFO (sse\_JUFO & ss\_JUFO\_unf and PSIPRED (ss\_PSIPRED & ss\_PSIPRED\_unf).

|  |  |
| --- | --- |
| **energy function** | **weight** |
| aa\_clash | 500.00 |
| aa\_dist | 0.35 |
| aa\_neigh | 50.00 |
| aa\_neigh\_unf | 50.00 |
| sse\_clash | 500.00 |
| sse\_pack | 8.00 |
| strand\_pair | 20.00 |
| loop | 10.00 |
| loop\_closure | 500.00 |
| rgyr | 5.00 |
| co | 0.50 |
| ss\_JUFO\* | 5.00 |
| ss\_JUFO\_unf\* | 5.00 |
| ss\_PSIPRED\* | 20.00 |
| ss\_SIPRED\_unf\* | 20.00 |

**Table S3: Weightset for the energy function in BCL::Fold**