Supplementary Material

Table S1. Masses and sizes of the particles in the coarse grained protein model (including lipid and water).

Name	Type	Mass (amu)	Radius (nm)
Backbone	BB	56.04	0.2512
(Gly)	BG	57.05	0.2512
(Pro)	BP	55.04	0.2512
Ala	SA	15.04	0.1816
Cys	SC	47.10	0.2107
Asp	SD	58.04	0.2403
Glu	SE	72.06	0.2767
Phe	SF	91.13	0.3198
His	SH	82.10	0.2888
Ile	SI	57.12	0.2902
Lys	SK	73.14	0.2926
Leu	SL	57.11	0.2894
Met	SM	75.15	0.2921
Asn	SN	58.06	0.2542
Pro	SP	42.08	0.2467
Gln	SQ	72.09	0.2828
Arg	SR	101.15	0.3198
Ser	SS	31.03	0.1984
Thr	ST	45.06	0.2369
Val	SV	43.09	0.2620
Trp	SW	130.17	0.3445
Tyr	SY	107.13	0.3200
Lipid (head)	H	56.11	0.2525
Lipid (tail)	T	56.11	0.2525
Water	W	72.05	0.2586

Table S2. Parameters for all bond interactions in the coarse grained protein model (including lipid and water).

Particles	Bond length (nm)	Force constant (kJ/mol/nm^2)
B*-B*	0.384	15733
BB-SA	0.077	5905
BB-SC	0.123	12748
BB-SD	0.171	14202
BB-SE	0.225	15704
BB-SF	0.223	17286
BB-SH	0.212	16591
BB-SI	0.176	14090
BB-SK	0.252	15805
BB-SL	0.194	14090
BB-SM	0.216	15991
BB-SN	0.167	14205
BB-SQ	0.225	15706
BB-SR	0.302	17964
BB-SS	0.117	9949
BB-ST	0.140	12442
BB-SV	0.140	12134
BB-SW	0.261	19515
BB-SY	0.248	18328
BP-SP	0.135	16761
SC-SC	0.289	4187
H-H	0.473	3156
H-T	0.473	3156
T-T	0.473	3156

Table S3. Parameters for all angle potential interactions. The first two rows are for the double angle potential and the last row is for the harmonic angle potential.

Particles	θ_1	θ_2	$V_{\mathrm{A}}(\theta_1)$ (kJ/mol)	$V_{\mathrm{A}}(\theta_2)$ (kJ/mol)	$V_{\mathrm{A}}(\xi)$ (kJ/mol)
B*-B*-B*	91.25°	123.25°	0.0	23.0	23.7
B*-B*-S*	118°	135°	0.0	0.0	0.003

Particles	θ_0	Force constant (kJ/mol/rad^2)
T-T-T	180.0°	5.408

Table S4. Non-bonded interaction energies for the coarse grained model. All energies are in units of kJ/mol. To represent the use of the truncated shifted Lennard-Jones potential (with only a repulsive part) a R is used and the associated energy is 1.97 kJ/mol.

	B*	SA	SC	SD	SE	SF	SH	SI	SK	SL	SM	SN	SP	SQ	SR	SS	ST	SV	SW	SY	H	T	W
B*	5.04	R	1.97	3.93	3.93	R	3.93	R	3.93	R	R	3.93	1.97	3.93	3.93	3.93	3.93	R	R	R	1.00	R	1.97
SA	R	4.60	5.98	1.46	1.00	5.48	3.14	6.40	R	5.82	5.86	1.76	4.02	2.05	1.42	2.64	3.14	5.86	4.69	4.23	0.50	1.97	R
SC	1.97	5.98	7.03	3.51	2.97	7.15	5.52	7.61	2.01	6.95	7.28	3.56	5.52	4.06	3.10	4.98	5.06	6.82	6.19	5.65	0.50	0.50	0.50
SD	3.93	1.46	3.51	R	R	2.55	2.09	3.22	R	2.30	2.30	R	1.67	R	1.88	0.29	0.92	2.38	2.89	2.34	0.50	R	1.97
SE	3.93	1.00	2.97	R	R	2.30	1.05	3.22	R	2.30	2.59	R	1.38	R	1.55	R	0.38	2.43	2.64	1.84	0.50	R	1.97
SF	R	5.48	7.15	2.55	2.30	7.15	5.06	7.61	1.67	7.28	7.24	3.14	5.02	3.31	3.31	4.02	4.39	6.95	6.69	5.86	1.00	1.97	R
SH	3.93	3.14	5.52	2.09	1.05	5.06	3.97	4.98	R	4.60	5.23	1.59	3.39	0.96	1.46	2.34	2.93	4.23	4.81	4.02	1.97	R	R
SI	R	6.40	7.61	3.22	3.22	7.61	4.98	8.20	2.72	7.78	7.57	3.31	5.65	3.85	4.14	4.81	5.23	7.70	6.82	6.44	0.50	1.97	R
SK	3.93	R	2.01	R	R	1.67	R	2.72	R	1.92	1.42	R	0.67	R	R	R	R	1.88	2.05	1.30	0.50	R	1.97
SL	R	5.82	6.95	2.30	2.30	7.28	4.60	7.78	1.92	7.20	7.24	3.05	5.23	3.26	3.43	4.27	4.35	7.11	6.44	5.82	0.50	1.97	R
SM	R	5.86	7.28	2.30	2.59	7.24	5.23	7.57	1.42	7.24	7.32	3.10	5.23	3.68	3.35	4.23	4.64	6.82	6.65	6.03	0.50	1.00	R
SN	3.93	1.76	3.56	R	R	3.14	1.59	3.31	R	3.05	3.10	R	2.13	R	R	0.59	0.92	3.05	3.14	2.26	0.50	R	1.97
SP	1.97	4.02	5.52	1.67	1.38	5.02	3.39	5.65	0.67	5.23	5.23	2.13	5.15	2.34	2.05	3.26	3.35	5.15	4.98	4.60	0.50	R	1.97
SQ	3.93	2.05	4.06	R	R	3.31	0.96	3.85	R	3.26	3.68	R	2.34	R	R	0.42	1.00	3.14	3.18	2.51	0.50	R	1.97
SR	3.93	1.42	3.10	1.88	1.55	3.31	1.46	4.14	R	3.43	3.35	R	2.05	R	R	0.88	1.34	2.89	3.56	2.80	0.50	R	1.97
SS	3.93	2.64	4.98	0.29	R	4.02	2.34	4.81	R	4.27	4.23	0.59	3.26	0.42	0.88	1.26	2.30	4.18	3.39	2.89	0.50	0.50	0.50
ST	3.93	3.14	5.06	0.92	0.38	4.39	2.93	5.23	R	4.35	4.64	0.92	3.35	1.00	1.34	2.30	2.34	4.52	3.60	3.22	0.50	0.50	0.50
SV	R	5.86	6.82	2.38	2.43	6.95	4.23	7.70	1.88	7.11	6.82	3.05	5.15	3.14	2.89	4.18	4.52	6.95	6.15	5.40	0.50	1.97	R
SW	R	4.69	6.19	2.89	2.64	6.69	4.81	6.82	2.05	6.44	6.65	3.14	4.98	3.18	3.56	3.39	3.60	6.15	5.90	5.15	1.97	R	R
SY	R	4.23	5.65	2.34	1.84	5.86	4.02	6.44	1.30	5.82	6.03	2.26	4.60	2.51	2.80	2.89	3.22	5.40	5.15	4.43	1.97	R	R
H	1.00	0.50	0.50	0.50	0.50	1.00	1.97	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	1.97	1.97	3.93	R	3.93
T	R	1.97	0.50	R	R	1.97	R	1.97	R	1.97	1.00	R	R	R	R	0.50	0.50	1.97	R	R	R	1.97	R
W	1.97	R	0.50	1.97	1.97	R	R	R	1.97	R	R	1.97	1.97	1.97	1.97	0.50	0.50	R	R	R	3.93	R	3.93

Double angle potential

In Figure 3(a) the general shape of the double angle potential is shown, indicating all parameters. In this part of the supplementary material the functions that describe the double angle potential are derived. From the curve some important observations can be made. For instance, the reference angle ξ lies in between the two other reference angles: $\theta_1 < \xi < \theta_2$. Because the curve has a maximum at $V(\xi)$, it follows that $V(\theta_1)$ and $V(\theta_2)$ are the minima of the polynomial. Thus, the form of the derivative of the fourth power polynomial $V'(\theta)$ describing the double angle potential is easily determined

$$V'(\theta) = A\,(\theta - \theta_1)\,(\theta - \theta_2)\,(\theta - \xi)\ ,$$

where A is a yet undetermined constant. The above equation can be expanded to become

$$V'(\theta) \;=\; A\left[\theta^3 \;-\; (\theta_1 + \theta_2 + \xi)\,\theta^2 \;+\; (\theta_1\theta_2 + \theta_1\xi + \theta_2\xi)\,\theta \;-\; (\theta_1\theta_2\xi)\right] .$$

Integrating this equation gives the desired fourth power polynomial

$$V(\theta) \;=\; A\left[\tfrac{1}{4}\theta^4 \;-\; \tfrac{1}{3}(\theta_1 + \theta_2 + \xi)\,\theta^3 \;+\; \tfrac{1}{2}(\theta_1\theta_2 + \theta_1\xi + \theta_2\xi)\,\theta^2 \;-\; (\theta_1\theta_2\xi)\,\theta\right] + \;D\ ,$$

where D is an arbitrary constant of integration and is not yet determined. Renaming the part within the square brackets in the above equation as $g(\theta)$ allows to simplify the integrated function to

$$V(\theta) \;=\; A\,g(\theta) \;+\; D\ .$$

In the above equations some constants (A and D) still need to be determined. Based upon the parameters supplied to the double angle potential, the following set of equations can be expressed

$$V(\theta_1) \;=\; A\,g(\theta_1) \;+\; D \qquad \text{and} \qquad V(\xi) \;=\; A\,g(\xi) \;+\; D$$

¿From the first equation the constant A can be isolated

$$A \;=\; \frac{V(\theta_1) \;-\; D}{g(\theta_1)}\ ,$$

which can subsequently be reinserted into the second equation to give

$$D \;=\; \frac{g(\theta_1)\,V(\xi) - g(\xi)\,V(\theta_1)}{g(\theta_1) - g(\xi)}\ .$$

with another substitution this yields

$$A \;=\; \frac{V(\xi) - V(\theta_1)}{g(\xi) - g(\theta_1)}\ .$$

Although the constants A and D are now expressed in terms of the fourth power polynomial $g(\theta)$ and the parameters θ_1, $V(\theta_1)$ and $V(\xi)$, the variable $g(\xi)$ is still unknown, since ξ is an unknown parameter of $V(\theta)$. In order to compute the variable $g(\xi)$, it is necessary to determine ξ. For this purpose it is useful to take a close look at the derivative function $V'(\theta)$ again. While constructing the fourth power polynomial belonging to this derivative, $V'(\theta)$ has been integrated completely. However, integrating parts of the derivative (for example between θ_1 and ξ) allows for the computation of ξ. Therefore, the following two equations can be constructed

$$A\,I_1 = A\int_{\theta_1}^{\xi} (\theta-\theta_1)\,(\theta-\theta_2)\,(\theta-\xi)\,d\theta \qquad \text{and} \qquad A\,I_2 = A\int_{\xi}^{\theta_2} (\theta-\theta_1)\,(\theta-\theta_2)\,(\theta-\xi)\,d\theta$$

where I_1 and I_2 are the areas under the curve (normalized with respect to the constant A). Since integrating the derivative finally gives the full fourth order polynomial, the area under the curve can be alternatively expressed as

$$A\,I_1 = V(\xi) - V(\theta_1) \qquad \text{and} \qquad A\,I_2 = V(\theta_2) - V(\xi)$$

from which the constant A can be calculated in two ways

$$A = \frac{V(\xi) - V(\theta_1)}{I_1} \qquad \text{and} \qquad A = \frac{V(\theta_2) - V(\xi)}{I_2}$$

Since these two equations yield an equality, the quotient $Q = I_1/I_2$ is given by

$$Q = \frac{I_1}{I_2} = \frac{V(\xi) - V(\theta_1)}{V(\theta_2) - V(\xi)}\,,$$

which uses the three known parameters $V(\theta_1)$, $V(\theta_2)$ and $V(\xi)$. Consequently, the value of Q is also known. Inserting the simplified form of the fourth power polynomial eliminates the constants A and D embedded within $V(\theta_1)$, $V(\theta_2)$ and $V(\xi)$ from the expression of the quotient and gives

$$Q = \frac{g(\xi) - g(\theta_1)}{g(\theta_2) - g(\xi)}\,.$$

Rearranging the above equation gives us an expression for the variable $g(\xi)$ in terms of the quotient Q, and the variables $g(\theta_1)$ and $g(\theta_2)$

$$g(\xi) = \frac{Q\,g(\theta_2) + g(\theta_1)}{Q+1}\,.$$

Since, this equality has only one unknown parameter, namely ξ, it is possible to determine this parameter.

The first step is to move all terms to one side, resulting in a quartic equation in ξ,

$$Q\,g(\theta_2) + g(\theta_1) - (Q+1)\,g(\xi) = 0\,.$$

Now the definition for $g(\theta)$ can be used to expand each of the three functions in terms of θ_1, θ_2, ξ and Q only. After rearranging the resulting quartic equation in ξ is given by

$$-\tfrac{1}{12}(Q+1)\,\xi^4 + \tfrac{1}{6}(Q+1)(\theta_1+\theta_2)\,\xi^3 - \tfrac{1}{2}(Q+1)\,\theta_1\theta_2\,\xi^2 \\ + \left[\tfrac{1}{2}\left(Q\theta_1\theta_2^2 + \theta_1^2\theta_2\right) - \tfrac{1}{6}\left(Q\theta_2^3 + \theta_1^3\right)\right]\xi + \left[\tfrac{1}{12}\left(Q\theta_2^4 + \theta_1^4\right) - \tfrac{1}{6}\left(Q\theta_1\theta_2^3 + \theta_1^3\theta_2\right)\right] = 0\,.$$

Although this equation can be solved in the general case, using for instance Ferrari's method, its computation is very tedious and laborious. However, from the choice that $V(\theta)$ has two minima, and one maximum, it follows that the maximum has to be located in between the two minima: $\theta_1 < \xi < \theta_2$. From this requirement it can be seen that the quartic equation has a solution.

In order to compute the location of ξ the Newton-Raphson numerical analysis method can be used. This method is an efficient algorithm for finding approximations of the roots a real-valued function $f(x)$. The basic idea of the method is to start with an initial guess x_0 which is reasonably close to the true zero. The tangent of the function $f(x)$ at x_0 is given by $f'(x_0)$, which is equal to $\tan\phi$, where ϕ is the angle the tangent line makes with the x-axis. Using elementary algebra it can be shown that $\tan\phi = f(x_0) / (x_0 - x_1)$, where x_1 is the point where the tangent line crosses the x-axis. Consequently, it follows

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} \, .$$

The zero of the tangent, x_1, typically is a better approximation to the function's root. Arrived at this point all steps can be repeated until convergence, and the root of the function is found. Using the Newton-Raphson method on the previously determined quartic equation gives a very good estimate for ξ. Typically only a few iterations are needed for the method to converge.