

Power method for calculating the B-factors (PowerB)

The calculation of B_i^{GNM} requires complete eigenvalue decomposition of the Kirchhoff matrix Γ , the computing time of which scales with N^3 , making the solution intractable for large networks. Because Γ has one zero eigenvalue (λ_0), its decomposition can be written as

$$\Gamma = 0 \times \mathbf{u}_0 \mathbf{u}_0^T + \sum_{j=1}^{N-1} \lambda_j \mathbf{u}_j \mathbf{u}_j^T \quad (\text{S1})$$

If we perturb Γ by adding a small number, $\varepsilon = 10^{-4}$, to the first element, Γ_{11} , the new matrix, Γ' , becomes invertible. Let us denote the inverse of Γ' by A ; the N eigenvalues of A can be ordered as: $|\lambda'_0| > |\lambda'_1| \geq |\lambda'_2| \geq \dots \geq |\lambda'_{N-1}|$ where λ'_0 is the dominant eigenvalue

(replacing $1/\lambda_0$). Because A has dominant eigenvalue, it is possible to employ the power method (Wilkinson, 1965) to solve for a subset of dominant eigenvectors. Mainly, the product of A with any N -dimensional vector, \mathbf{X}_0 , is expressed in terms of A 's eigenvalues, λ'_i , and associated eigenvectors, \mathbf{v}_i , as

$$\mathbf{A}\mathbf{X}_0 = \sum_{i=0}^{N-1} C_i \lambda'_i \mathbf{v}_i \quad (\text{S2})$$

and repeating this multiplication k times, we obtain $\mathbf{A}^k \mathbf{X}_0 \approx \lambda'_0{}^k C_0 \mathbf{v}_0$, as $(\lambda'_i / \lambda'_0)^k \rightarrow 0$ for large k , and $i \neq 0$. The normalized eigenvector \mathbf{v}_0 is obtained from \mathbf{X}_0 using

$$\mathbf{v}_0 = \frac{\mathbf{A}^k \mathbf{X}_0}{|\mathbf{A}^k \mathbf{X}_0|} \quad (\text{S3})$$

and the eigenvalue is deduced from the inner product of Equation 4 with a normalized random vector \mathbf{Y} using the ratio

$$\frac{\mathbf{A}^{k+1} \mathbf{X}_0 \cdot \mathbf{Y}}{\mathbf{A}^k \mathbf{X}_0 \cdot \mathbf{Y}} = \frac{\lambda'_0{}^{k+1}}{\lambda'_0{}^k} = \lambda'_0 \quad (\text{S4})$$

provided that \mathbf{X}_0 and \mathbf{Y} are not orthogonal. This method can be used to estimate the leading eigenvalues and eigenvectors for a fixed number of iterations (e.g. $k = 100$) through a deflation process, when the difference between consecutive iterations is smaller than a threshold ($\delta = 10^{-7}$). The convergence rate depends upon the ratio of the dominant eigenvalue to the next largest eigenvalue, but in general, the computing time is in the order of N^2 for the first 10 modes.

We note that the pseudo-inverse of Γ is related to A simply by $\Gamma^{-1} \cong A - \lambda'_0 \mathbf{u}_0 \mathbf{u}_0^T$ which provides us with an efficient method to estimate B_i^{GNM} using

$$B_i^{GNM} \cong \frac{8\pi^2 k_B T}{\gamma} [A - \lambda'_0 \mathbf{u}_0 \mathbf{u}_0^T]_{ii} \quad (\text{S5})$$

We term this fast algorithm for calculating B_i^{GNM} the *PowerB* method.

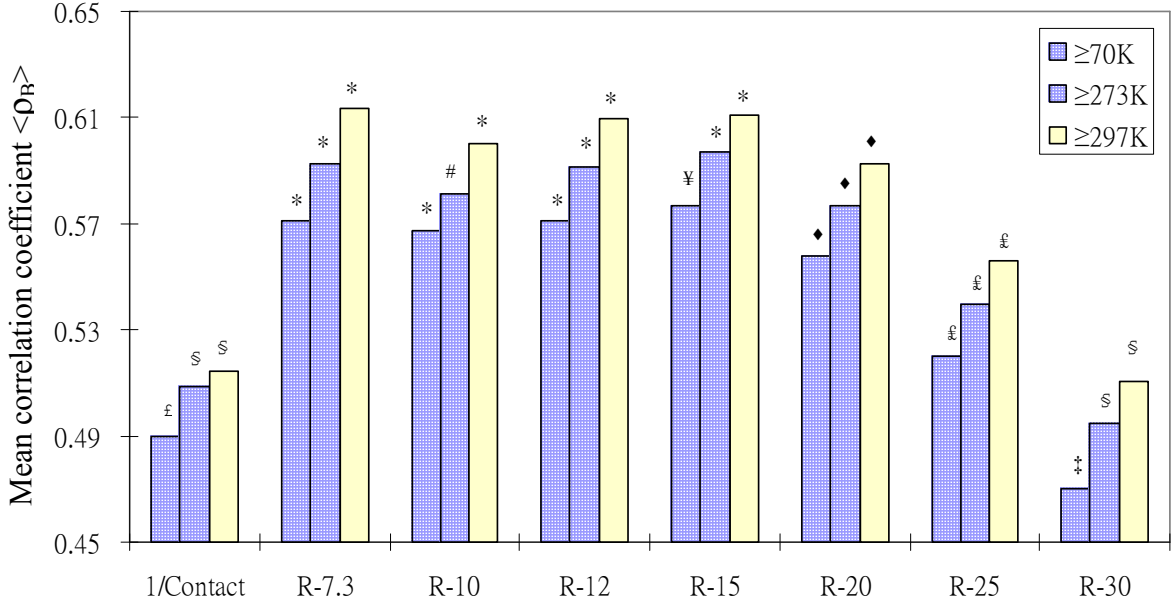


Figure S1. Correlation coefficients $\langle \rho_B \rangle$ between experimental and theoretical B-factors. Results are shown as a function of cutoff distance (r_c) for discrete values along the abscissa and X-ray diffraction temperatures (XDT), averaged over 1250 non homologous proteins. The different colored bars refer to subsets of structures determined at XDT ≥ 70 K (all structures; blue bars), XDT ≥ 273 K (235 structures; dark red), and XDT ≥ 297 K (59 structures; yellow). The first set of results (labeled as 1/Contact) refers to the correlation $\langle \rho \rangle$ between B^{exp} and the inverse residue coordination number ($1/\Gamma_{ii}$) averaged over all proteins, based on a cutoff distance of 7.3 Å. The average $\langle \rho_B \rangle$ are computed using *PowerB* approach. The mean $\langle \rho_B \rangle$ values of different groups are considered statistically identical by a paired student t-test if the symbols above the group columns are the same. Groups with different symbols have statistically different mean values.

These results show that the GNM results are rather insensitive to r_c in the range $7.3 \leq r_c \leq 15$ Å. Another interesting observation is the higher correlation with experiments observed in the case of higher XDTs, indicating that the GNM results agree better with experiments when the structures are subject to less constrained (or larger) fluctuations. At $r_c = 7.3$ Å, the force/spring constant averaged over all structures is found to be $k_B T / \gamma =$

$1.10 \pm 0.50 \text{ \AA}^2$ in close agreement with the result of $k_B T / \gamma = 0.87 \pm 0.46 \text{ \AA}^2$ obtained for a set of 113 monomeric proteins (28). This spring constant provides a measure of a generic ‘stiffness’ that controls residue fluctuations in folded proteins.

Supplemental Table 1. 1250 proteins used in the study of cutoff distances (*Figure S1*)

12as, 1a0b, 1a12, 1a1x, 1a28, 1a32, 1a3k, 1a49, 1a4i, 1a53, 1a6j, 1a6m, 1a76, 1a79, 1a7w, 1a8d, 1a8e, 1a8h, 1a8l, 1a8p, 1aa7, 1ad6, 1ado, 1af7, 1afr, 1agq, 1ah7, 1ail, 1aj2, 1aj8, 1ajs, 1ak0, 1ako, 1amf, 1amm, 1amx, 1aoc, 1aq0, 1aqt, 1ass, 1atz, 1au1, 1aui, 1ava, 1avq, 1ayo, 1az9, 1azs, 1b00, 1b0y, 1b2p, 1b33, 1b35, 1b3a, 1b3u, 1b4p, 1b5e, 1b5p, 1b63, 1b74, 1b77, 1b7g, 1b8a, 1b8o, 1b9h, 1b9w, 1baz, 1bbz, 1bd0, 1bd3, 1bd8, 1bea, 1beb, 1beh, 1bf2, 1bf6, 1bfd, 1bfg, 1bgv, 1bhe, 1bht, 1bif, 1bis, 1bja, 1bk5, 1bkr, 1bm8, 1bn8, 1bol, 1bou, 1bqk, 1bqs, 1br9, 1brf, 1brt, 1bt4, 1btn, 1bu7, 1bwv, 1bxa, 1bxr, 1byq, 1byr, 1c02, 1c0p, 1c1k, 1c1l, 1c30, 1c39, 1c4q, 1c52, 1c5e, 1c5k, 1c7j, 1c7k, 1c7q, 1c7s, 1c8k, 1c8u, 1c96, 1c9o, 1ca1, 1cbf, 1cc8, 1ccw, 1ccz, 1cdk, 1cfr, 1cfz, 1chk, 1cip, 1cjc, 1cjw, 1cjsx, 1cnz, 1coz, 1cp2, 1cpq, 1cq3, 1cqk, 1cqx, 1cqy, 1cru, 1cs6, 1ctq, 1cun, 1cv8, 1cvr, 1cwv, 1cy5, 1cz3, 1cz9, 1cza, 1d09, 1d0c, 1d0q, 1d1m, 1d1q, 1d2o, 1d2u, 1d3b, 1d4o, 1d4t, 1d4v, 1d7p, 1d7u, 1d9c, 1dbf, 1dbt, 1dce, 1dci, 1dd4, 1ddz, 1de6, 1del, 1dfx, 1dgw, 1dj0, 1djn, 1djt, 1dk0, 1dk8, 1dkq, 1dlj, 1dlw, 1dmh, 1dmr, 1dmt, 1dos, 1doz, 1dp0, 1dp4, 1dq3, 1dqa, 1dqe, 1dqg, 1dqi, 1dqp, 1dqt, 1dqw, 1ds1, 1dtd, 1dvo, 1dx5, 1dxe, 1dy9, 1dz3, 1dzf, 1dzi, 1dzk, 1e0b, 1e19, 1e1a, 1e29, 1e30, 1e39, 1e3u, 1e44, 1e4c, 1e59, 1e6i, 1e6p, 1e6u, 1e79, 1e9e, 1eai, 1eaj, 1eao, 1eaz, 1eb6, 1ebf, 1ecs, 1ed1, 1edg, 1edq, 1ee6, 1ee8, 1eej, 1eeo, 1eer, 1eex, 1efv, 1efy, 1eg3, 1ega, 1ehd, 1ei1, 1ei9, 1ej2, 1ekg, 1el6, 1elk, 1em9, 1eo9, 1eoi, 1eok, 1ep3, 1ep9, 1eqf, 1erz, 1es5, 1esj, 1esw, 1ete, 1eu3, 1eu8, 1eua, 1euc, 1eum, 1euv, 1evh, 1ew0, 1ew4, 1ew6, 1ex1, 1ex2, 1ex7, 1ext, 1ey4, 1eyh, 1eyq, 1eys, 1eyv, 1ezg, 1ezv, 1f00, 1f08, 1f0j, 1f0k, 1f20, 1f24, 1f2d, 1f2t, 1f2u, 1f2v, 1f39, 1f3m, 1f46, 1f4l, 1f5m, 1f5v, 1f60, 1f7d, 1f7s, 1f82, 1f8e, 1f8m, 1f8y, 1fbq, 1fc3, 1fc9, 1fcj, 1fcu, 1fcz, 1ffv, 1fi2, 1fil, 1fj2, 1fjr, 1fk5, 1fkn, 1fl0, 1fl2, 1fle, 1flm, 1flt, 1fm0, 1fm4, 1fn0, 1fn9, 1fnf, 1fns, 1fob, 1fp2, 1fp3, 1fqj, 1fr2, 1fr3, 1fs7, 1fsg, 1ft5, 1fth, 1ftr, 1fur, 1fw1, 1fw9, 1fxk, 1fxq, 1fy7, 1fzc, 1g0o, 1g0s, 1g12, 1g1k, 1g1t, 1g29, 1g2a, 1g2q, 1g2w, 1g3q, 1g40, 1g4y, 1g5b, 1g5c, 1g5t, 1g61, 1g6g, 1g6h, 1g6s, 1g6u, 1g71, 1g72, 1g73, 1g79, 1g8a, 1g8e, 1g8k, 1g8l, 1g8q, 1g97, 1ga6, 1gak, 1gc5, 1gcq, 1gd0, 1gd8, 1gdv, 1gef, 1gg6, 1gjw, 1gk1, 1gk2, 1gk8, 1gl4, 1gmu, 1gn0, 1gnu, 1gny, 1go4, 1got, 1gp0, 1gp2, 1gpe, 1gpi, 1gpq, 1gpu, 1gpw, 1gqi, 1gqn, 1gqv, 1gqy, 1gs5, 1gs9, 1gtz, 1gu2, 1gu3, 1gu7, 1gui, 1gux, 1gv4, 1gvc, 1gvj, 1gvn, 1gvp, 1gvr, 1gwy, 1gxj, 1gxm, 1gxy, 1gy6, 1gyj, 1gzf, 1gzs, 1h03, 1h09, 1h0o, 1h1y, 1h2b, 1h2c, 1h2w, 1h34, 1h3o, 1h3q, 1h4g, 1h4i, 1h4k, 1h4p, 1h4r, 1h4y, 1h59, 1h6d, 1h6h, 1h6l, 1h6t, 1h6w, 1h70, 1h7e, 1h7w, 1h8e, 1h8p, 1h8u, 1h9s, 1ha4, 1hb6, 1hbk, 1hbn, 1hd2,

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Supplemental Table 2. Set of 64 nucleotide/nucleotide-protein complexes.

PDBid	residues	nucleotides	Resolution (Å)	name
1cx0	95	72	2.30	Hepatitis δ virus ribozyme
1drz	95	72	2.30	Hepatitis δ virus ribozyme
1m5k	184	226	2.40	rProtein A – hairpin ribozyme complex
1u6b	95	222	3.10	Group I intron
1hr2	0	315	2.25	P4-P6 ribozyme domain
1l8v	0	314	2.80	P4-P6 ribozyme domain
1u9s	0	155	2.90	Ribonuclease P
1y0q	0	234	3.60	Group I ribozyme
1gid	0	316	2.50	P4-P6 ribozyme domain
1nbs	0	270	3.15	Ribonuclease P
1y26	0	72	2.10	A-riboswitch
1egk	0	108	3.10	Nucleic acid four-way junction
1ehz	0	76	1.93	Phenylalanine tRNA
1evv	0	76	2.00	Phenylalanine tRNA
1fir	0	76	3.30	HIV reverse-transcription primer tRNA
1i9v	0	76	2.60	tRNA-neomycin B complex
1tn2	0	77	3.00	Phenylalanine tRNA
1tra	0	76	3.00	Phenylalanine tRNA
2tra	0	74	3.00	Aspartic acid tRNA
3tra	0	72	3.00	Aspartic acid tRNA
4tra	0	76	3.00	Phenylalanine tRNA
1yfg	0	75	3.00	Initiator tRNA
1qf6	641	77	2.90	Threonyl-tRNA synthetase-tRNA
1qu3	880	76	2.90	Isoleucyl-tRNA synthetase-tRNA
1qu2	917	76	2.20	Isoleucyl-tRNA synthetase-tRNA
1c0a	586	79	2.40	Aspartyl-tRNA synthetase-tRNA
1efw	1160	146	3.00	Aspartyl-tRNA synthetase-tRNA
1f7u	607	76	2.20	Arginyl-tRNA synthetase-tRNA
1ffy	917	76	2.20	Isoleucyl-tRNA synthetase-tRNA
1h4s	948	69	2.85	Prolyl-tRNA synthetase-tRNA
1j1u	300	74	1.95	Trosyl-tRNA synthetase-tRNA
1j2b	1152	148	3.30	tRNA-Guanine tansglycosylase-tRNA
1o0c	530	75	2.70	Glutaminyl-tRNA synthetase
1rc7	220	41	2.15	Ribonuclease III – dsRNA complex
1u0b	461	74	2.30	Cysteinyl-tRNA synthetase-tRNA
1h3e	428	84	2.90	Tyrosyl-tRNA synthetase-tRNA
1qtq	530	75	2.25	Glutaminyl-tRNA synthetase-tRNA
1gtr	529	75	2.50	Glutaminyl-tRNA synthetase-tRNA
1ser	793	65	2.90	Seryl-tRNA synthetase-tRNA
1asy	980	150	2.90	Aspartyl-tRNA synthetase-tRNA
1qrs	529	75	2.60	Glutaminyl-tRNA synthetase-tRNA
1b23	406	75	2.60	EF-TU – Cys-tRNA complex

1m5o	187	226	2.20	rProtein A-ribozyme complex
1vby	167	73	2.90	rProtein A – hepatitis δ virus ribozyme
1vc0	95	73	2.50	rProtein A – hepatitis δ virus ribozyme
1vc5	167	70	3.40	rProtein A – hepatitis δ virus ribozyme
1sj3	95	73	2.20	rProtein A – hepatitis δ virus ribozyme
1ttt	1218	231	2.70	EF-TU – Phe-tRNA complex
1l9a	87	126	2.90	SRP19 – SRP RNA complex
1lng	87	97	2.30	SRP19 – SRP RNA complex
1mfq	215	128	3.10	SRP19 – SRP RNA complex
1mms	203	116	2.57	rProtein L11 – rRNA fragment complex
1fg0	0	499	3.00	Domain V of 23S rRNA
1i94	2410	1514	3.20	30S ribosomal subunit
1j5e	2396	1513	3.05	30S ribosomal subunit
1n32	2389	2876	3.00	30S ribosomal subunit
1fjg	2404	1507	3.00	30S ribosomal subunit
1ffk	3656	2828	2.40	50S ribosomal subunit
1s72	3775	2876	2.40	50S ribosomal subunit
1jj2	3701	2876	2.40	50S ribosomal subunit
1j5a	385	2774	3.50	50S ribosomal subunit
1jzx	385	2774	3.10	50S ribosomal subunit
1yhq	3775	2876	2.40	50S ribosomal subunit
1yij	3775	2876	2.60	50S ribosomal subunit

References

Wilkinson, J. H. (1965) *The algebraic eigenvalue problem* Clarendon Press, Oxford.