Structure *16*

Supplemental Data

Ab Initio Folding of Proteins with All-Atom

Discrete Molecular Dynamics

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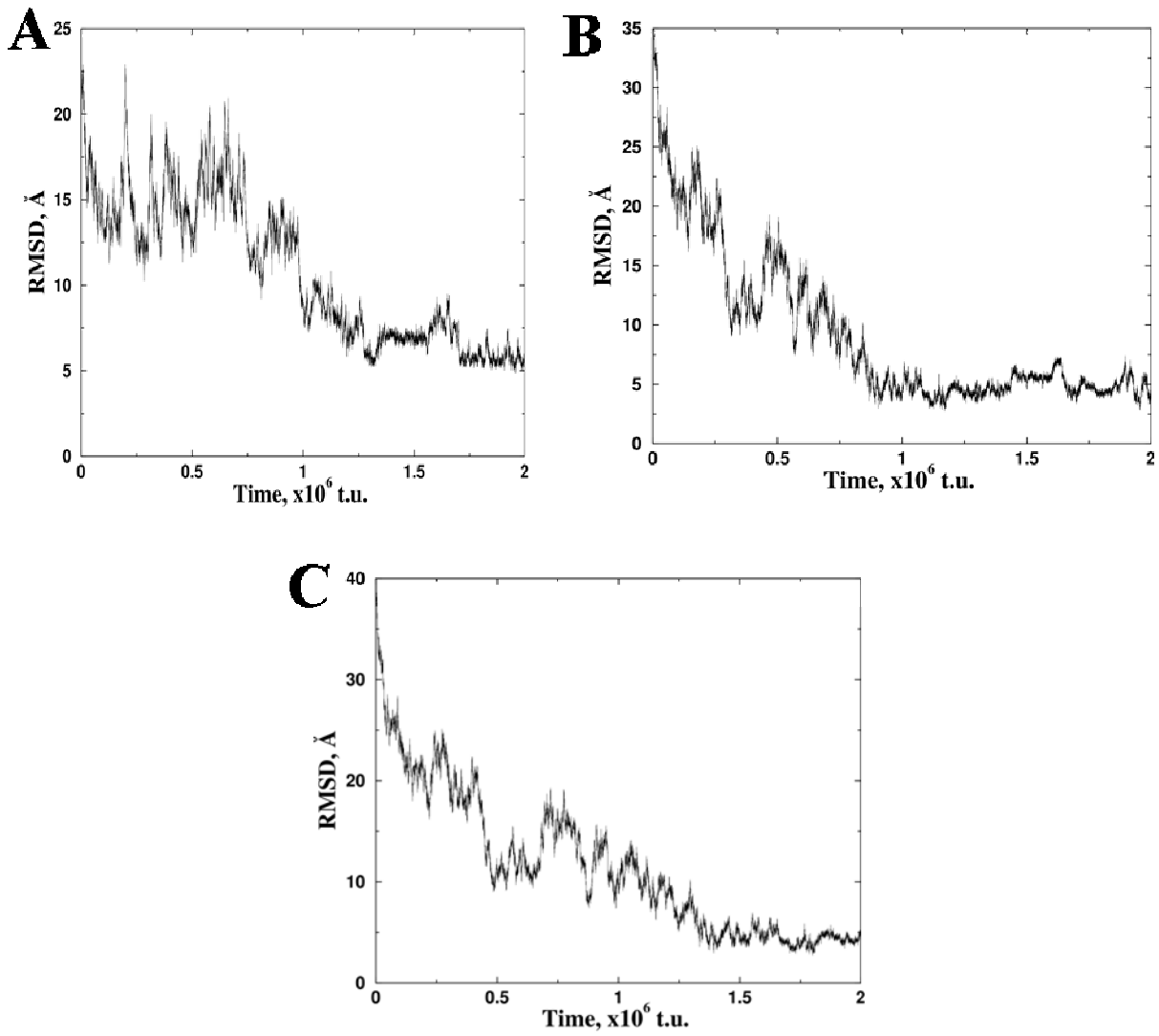

Figure S1. Several Folding Trajectories from REXDMD Simulations
The RMSD as the function of simulation time is presented for GB1 domain (A), bacterial ribosomal protein L20 (B), and the engrailed homeodomain (C). Only the trajectories from the successfully folded replicas are shown.

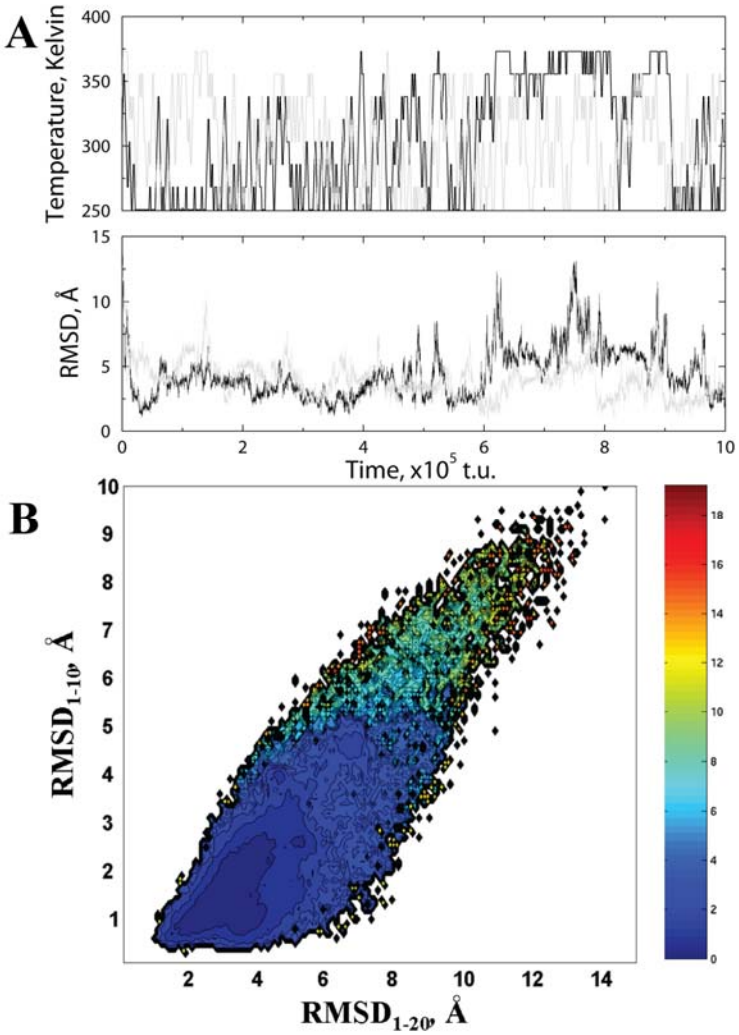

Figure S2. All-Atom DMD Simulation of Trp-Cage Folding
(A) Temperature (upper panel) and RMSD (lower panel) as a function of time during representative simulation trajectories. Only two replicas are presented for illustration purposes. The temperature in each replica is changed randomly (random walk) during replica exchange simulations. (B) The contour plot of the 2D-PMF at T=300K is plotted as the function of the RMSD of the N-terminal a-helix ($RMSD_{1-10}$) and the whole structure ($RMSD_{1-20}$). The free energy difference between two consecutive contours is 0.6 kcal/mol.

Table S1. The Parameters for Bonded and Angled Constraints

The average constraint length and its variance between two atom types is given as d_{AB} and σ_{AB} respectively. The parameters for a dihedral constraint are d_{min}, d_0, d_1, d_2, d_{max} (1). For the dihedral potential, we use an energy step dE = 1.2kcal/mol (Figure 1b).

Common constraints (ALA and GLY; GLY does not have the C_β atom.)

Type	Atom *A*	Atom *B*	d_{AB}, Å	σ_{AB}/d_{AB}
Bond	*N*	*H*	1.00	0.020
	N	C_α	1.46	0.020
	C_α	*C*	1.52	0.020
	C	*O*	1.23	0.020
	C_α	C_β	1.53	0.010
Angle	C_α	*H*	2.15	0.020
	N	C_β	2.46	0.012
	N	*C*	2.46	0.015
	C_α	*O*	2.40	0.020
	C	C_β	2.50	0.014

VAL

Type	Atom *A*	Atom *B*	d_{AB}, Å	σ_{AB}/d_{AB}
Bond	C_β	$C_{\gamma 1}$	1.53	0.010
	C_β	$C_{\gamma 2}$	1.53	0.010
Angle	C_α	$C_{\gamma 1}$	2.55	0.014
	C_α	$C_{\gamma 2}$	2.55	0.014
	$C_{\gamma 1}$	$C_{\gamma 2}$	2.50	0.012

Dihedral	d_{min},	d_0, Å	d_1, Å	d_2, Å	d_{max}, Å
N-C_α-C_β-$C_{\gamma 1}$	2.00	2.78	3.35	3.72	5.50

LEU

Type	Atom *A*	Atom *B*	d_{AB}, Å	σ_{AB}/d_{AB}
Bond	C_β	C_γ	1.52	0.010
	C_γ	$C_{\delta 1}$	1.52	0.010
	C_γ	$C_{\delta 2}$	1.52	0.010
Angle	C_α	C_γ	2.55	0.014
	C_β	$C_{\delta 1}$	2.52	0.014
	C_β	$C_{\delta 2}$	2.52	0.014
	$C_{\delta 1}$	$C_{\delta 2}$	2.38	0.010

Dihedral	d_{min},	d_0, Å	d_1, Å	d_2, Å	d_{max}, Å
N-C_α-C_β-C_γ	2.00	2.78	3.35	3.72	5.50
C_α-C_β-C_γ-$C_{\delta 1}$	2.00	2.79	3.75	3.80	5.50

ILE

Type	Atom *A*	Atom *B*	d_{AB}, Å	σ_{AB}/d_{AB}
Bond	C_β	$C_{\gamma 1}$	1.52	0.010
	C_β	$C_{\gamma 2}$	1.52	0.010
	$C_{\gamma 1}$	$C_{\delta 1}$	1.52	0.010
Angle	C_α	$C_{\gamma 1}$	2.55	0.014
	C_α	$C_{\gamma 2}$	2.52	0.014
	C_β	$C_{\delta 1}$	2.52	0.014
	$C_{\gamma 1}$	$C_{\gamma 2}$	2.52	0.014

Dihedral	d_{min},	d_0, Å	d_1, Å	d_2, Å	d_{max}, Å
N-C_α-C_β-$C_{\gamma 1}$	2.00	2.78	3.35	3.72	5.50
C_α-C_β-$C_{\gamma 1}$-$C_{\delta 1}$	2.00	2.79	3.75	3.80	5.50

MET

Type	Atom *A*	Atom *B*	d_{AB}, Å	σ_{AB}/d_{AB}
Bond	C_β	C_γ	1.52	0.010
	C_γ	S_δ	1.81	0.013
	S_δ	C_ε	1.79	0.024
Angle	C_α	C_γ	2.55	0.014
	C_β	S_δ	2.77	0.019
	C_γ	C_ε	2.76	0.021

Dihedral	d_{min},	d_0, Å	d_1, Å	d_2, Å	d_{max}, Å
N-C_α-C_β-C_γ	2.00	2.78	3.35	3.72	5.50
C_α-C_β-C_γ-S_δ	2.00	2.98	3.67	4.03	5.50
C_β-C_γ-S_δ-C_ε	2.00	2.60	3.70	3.90	5.50

CYS

Type	Atom *A*	Atom *B*	d_{AB}, Å	σ_{AB}/d_{AB}
Bond	C_β	S_γ	1.81	0.011
	S_γ	$H_{\gamma 1}$	1.34	0.020
Angle	C_α	S_γ	2.80	0.016
	C_β	$H_{\gamma 1}$	2.36	0.020

Dihedral	d_{min},	d_0, Å	d_1, Å	d_2, Å	d_{max}, Å
N-C_α-C_β-S_γ	2.00	2.95	3.51	3.99	5.50
C_α-C_β-S_γ-H_γ	2.00	2.72	3.11	3.72	5.50

HIS

Type	Atom *A*	Atom *B*	d_{AB}, Å	σ_{AB}/d_{AB}
Bond	C_β	C_γ	1.81	0.011
	C_γ	$N_{\delta 1}$	1.34	0.020
	$N_{\delta 1}$	$H_{\delta 1}$	1.00	0.020
	C_γ	$C_{\delta 2}$	1.37	0.010
	$N_{\delta 1}$	$C_{\varepsilon 1}$	1.36	0.007
	$C_{\delta 2}$	$N_{\varepsilon 2}$	1.37	0.013
	$C_{\varepsilon 1}$	$N_{\varepsilon 2}$	1.32	0.008
Angle	C_γ	$H_{\delta 1}$	2.12	0.020
	$C_{\varepsilon 1}$	$H_{\delta 1}$	2.12	0.020
	C_β	$N_{\delta 1}$	2.53	0.008
	C_β	$C_{\delta 2}$	2.59	0.007
	C_γ	$C_{\varepsilon 1}$	2.20	0.009
	C_γ	$N_{\varepsilon 2}$	2.20	0.009
	$N_{\delta 1}$	$N_{\varepsilon 2}$	2.15	0.010
	$C_{\delta 2}$	$C_{\varepsilon 1}$	2.19	0.008
	$N_{\delta 1}$	$C_{\delta 2}$	2.18	0.010

Dihedral	d_{min},	d_0, Å	d_1, Å	d_2, Å	d_{max}, Å
N-C_α-C_β-C_γ	2.00	2.78	3.35	3.72	5.50
C_α-C_β-C_γ-$N_{\delta 1}$	2.00	2.20	2.94	3.22	5.50
C_α-C_β-C_γ-$C_{\delta 2}$	2.00	2.20	3.08	3.32	5.50

PHE

Type	Atom *A*	Atom *B*	d_{AB}, Å	σ_{AB}/d_{AB}
Bond	C_β	C_γ	1.81	0.011
	C_γ	$C_{\delta 1}$	1.34	0.020
	C_γ	$C_{\delta 2}$	1.39	0.009
	$C_{\delta 1}$	$C_{\varepsilon 1}$	1.39	0.008
	$C_{\delta 2}$	$C_{\varepsilon 2}$	1.39	0.008
	$C_{\varepsilon 1}$	C_ζ	1.39	0.008
	$C_{\varepsilon 2}$	C_ζ	1.39	0.008
Angle	C_α	C_γ	2.55	0.014
	C_β	$C_{\delta 1}$	2.52	0.007
	C_β	$C_{\delta 2}$	2.52	0.007
	C_γ	$C_{\varepsilon 1}$	2.42	0.007
	C_γ	$C_{\varepsilon 2}$	2.42	0.007
	$C_{\delta 1}$	C_ζ	2.40	0.020
	$C_{\delta 2}$	C_ζ	2.40	0.020
	$C_{\delta 1}$	$C_{\delta 2}$	2.40	0.006
	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	2.40	0.008

Dihedral	d_{min},	d_0, Å	d_1, Å	d_2, Å	d_{max}, Å
N-C_α-C_β-C_γ	2.00	2.78	3.35	3.72	5.50

C_α-C_β-C_γ-$C_{\delta1}$	2.00	2.20	2.90	3.16	5.50
C_α-C_β-C_γ-$C_{\delta2}$	2.00	2.20	2.90	3.16	5.50

TYR

Type	Atom *A*	Atom *B*	d_{AB}, Å	σ_{AB}/d_{AB}
Bond	C_β	C_γ	1.52	0.011
	C_γ	$C_{\delta1}$	1.39	0.020
	C_γ	$C_{\delta2}$	1.39	0.010
	$C_{\delta1}$	$C_{\varepsilon1}$	1.39	0.006
	$C_{\delta2}$	$C_{\varepsilon2}$	1.41	0.008
	$C_{\varepsilon1}$	C_ζ	1.38	0.007
	$C_{\varepsilon2}$	C_ζ	1.38	0.007
	C_ζ	O_η	1.37	0.007
	O_η	HO	1.00	0.020
Angle	C_α	C_γ	2.80	0.016
	C_β	$C_{\delta1}$	2.36	0.020
	C_β	$C_{\delta2}$	2.53	0.007
	C_γ	$C_{\varepsilon1}$	2.42	0.007
	C_γ	$C_{\varepsilon2}$	2.42	0.007
	$C_{\delta1}$	C_ζ	2.40	0.020
	$C_{\delta2}$	C_ζ	2.40	0.020
	$C_{\delta1}$	$C_{\delta2}$	2.40	0.006
	$C_{\varepsilon1}$	O_η	2.39	0.009
	$C_{\varepsilon2}$	O_η	2.39	0.009
	C_ζ	*HO*	1.96	0.020

Dihedral	d_{min},	d_0, Å	d_1, Å	d_2, Å	d_{max}, Å
N-C_α-C_β-C_γ	2.00	2.78	3.35	3.72	5.50
C_α-C_β-C_γ-$C_{\delta1}$	2.00	2.20	2.90	3.16	5.50
C_α-C_β-C_γ-$C_{\delta2}$	2.00	2.20	2.90	3.16	5.50

TRP

Type	Atom *A*	Atom *B*	d_{AB}, Å	σ_{AB}/d_{AB}
Bond	C_β	C_γ	1.81	0.011
	C_γ	$C_{\delta 1}$	1.34	0.020
	C_γ	$C_{\delta 2}$	1.00	0.020
	$C_{\delta 1}$	$N_{\varepsilon 1}$	1.37	0.010
	$C_{\delta 2}$	$C_{\varepsilon 2}$	1.36	0.007
	$C_{\delta 2}$	$C_{\varepsilon 3}$	1.37	0.013
	$N_{\varepsilon 1}$	$C_{\varepsilon 2}$	1.32	0.008
	$C_{\varepsilon 2}$	$C_{\zeta 2}$	1.40	0.009
	$C_{\varepsilon 3}$	$C_{\zeta 3}$	1.39	0.007
	$C_{\zeta 2}$	$C_{\eta 2}$	1.39	0.007
	$C_{\zeta 3}$	$C_{\eta 2}$	1.41	0.008
	$N_{\varepsilon 1}$	$H_{\varepsilon 1}$	1.00	0.002
Angle	C_α	C_γ	2.12	0.020
	C_β	$C_{\delta 1}$	2.12	0.020
	C_β	$C_{\delta 2}$	2.53	0.008
	C_γ	$N_{\varepsilon 1}$	2.59	0.007
	C_γ	$C_{\varepsilon 1}$	2.20	0.009
	C_γ	$C_{\varepsilon 2}$	2.20	0.009
	$C_{\delta 2}$	$C_{\zeta 2}$	2.15	0.010
	$C_{\delta 2}$	$C_{\zeta 3}$	2.19	0.008
	$C_{\delta 1}$	$C_{\varepsilon 2}$	2.18	0.010
	$C_{\delta 1}$	$C_{\delta 2}$	2.24	0.007
	$C_{\delta 2}$	$N_{\varepsilon 1}$	2.24	0.006
	$C_{\varepsilon 2}$	$C_{\eta 2}$	2.37	0.006
	$C_{\varepsilon 3}$	$C_{\eta 2}$	2.43	0.007
	$N_{\varepsilon 1}$	$C_{\zeta 1}$	2.51	0.007
	$C_{\varepsilon 2}$	$C_{\varepsilon 3}$	2.42	0.005
	$C_{\zeta 2}$	$C_{\zeta 3}$	2.42	0.006
	$C_{\delta 1}$	$H_{\varepsilon 1}$	2.16	0.020
	$C_{\varepsilon 2}$	$H_{\varepsilon 1}$	2.12	0.020

Dihedral	d_{min},	d_0, Å	d_1, Å	d_2, Å	d_{max}, Å
N-C_α-C_β-C_γ	2.00	2.78	3.35	3.72	5.50
C_α-C_β-C_γ-$C_{\delta 1}$	2.00	2.20	2.90	3.16	5.50
C_α-C_β-C_γ-$C_{\delta 2}$	2.00	2.20	2.90	3.16	5.50

SER

Type	Atom *A*	Atom *B*	d_{AB}, Å	σ_{AB}/d_{AB}
Bond	C_β	O_γ	1.42	0.008
	O_γ	H_γ	1.00	0.020
Angle	C_α	O_γ	2.42	0.014
	C_β	H_γ	1.98	0.020

Dihedral	d_{min},	d_0, Å	d_1, Å	d_2, Å	d_{max}, Å
N-C_α-C_β-O_γ	2.00	2.65	3.19	3.60	5.50
C_α-C_β-O_γ-H_γ	2.00	2.46	2.77	3.27	5.50

THR

Type	Atom *A*	Atom *B*	d_{AB}, Å	σ_{AB}/d_{AB}
Bond	C_β	$O_{\gamma 1}$	1.42	0.008
	$O_{\gamma 1}$	$H_{\gamma 1}$	1.34	0.020
	C_β	$C_{\gamma 2}$	1.52	0.010
Angle	C_α	$O_{\gamma 1}$	2.42	0.014
	C_β	$H_{\gamma 1}$	1.98	0.020
	C_α	$C_{\gamma 2}$	2.53	0.013
	$O_{\gamma 1}$	$C_{\gamma 2}$	2.41	0.014

Dihedral	d_{min},	d_0, Å	d_1, Å	d_2, Å	d_{max}, Å
N-C_α-C_β-$O_{\gamma 1}$	2.00	2.65	3.19	3.60	5.50
C_α-C_β-O_γ-$H_{\gamma 1}$	2.00	2.46	2.77	3.27	5.50

ASN

Type	Atom *A*	Atom *B*	d_{AB}, Å	σ_{AB}/d_{AB}
Bond	C_β	C_γ	1.52	0.008
	C_γ	$O_{\delta 1}$	1.24	0.012
	C_γ	$N_{\delta 2}$	1.33	0.008
	$N_{\delta 2}$	$H_{\delta 1}$	1.00	0.020
	$N_{\delta 2}$	$H_{\delta 2}$	1.00	0.020
Angle	C_α	C_γ	2.55	0.014
	C_β	$O_{\delta 1}$	2.39	0.011
	C_β	$N_{\delta 2}$	2.42	0.011
	$O_{\delta 1}$	$N_{\delta 2}$	2.24	0.011
	C_γ	$H_{\delta 1}$	2.02	0.020
	C_γ	$H_{\delta 2}$	2.02	0.020

Dihedral	d_{min},	d_0, Å	d_1, Å	d_2, Å	d_{max}, Å
N-C_α-C_β-C_γ	2.00	2.78	3.35	3.72	5.50
C_α-C_β-C_γ-$O_{\delta 1}$	2.00	2.67	2.94	3.02	5.50
C_β-C_γ-$N_{\delta 2}$-$H_{\delta 1}$	2.00	2.53	2.58	3.32	5.50
C_β-C_γ-$N_{\delta 2}$-$H_{\delta 2}$	2.00	2.53	2.58	3.32	5.50

GLN

Type	Atom *A*	Atom *B*	d_{AB}, Å	σ_{AB}/d_{AB}
Bond	C_β	C_γ	1.52	0.008
	C_γ	C_δ	1.52	0.010
	C_δ	$O_{\varepsilon 1}$	1.24	0.012
	C_δ	$N_{\varepsilon 2}$	1.33	0.008
	$N_{\varepsilon 2}$	$H_{\varepsilon 1}$	1.00	0.020
	$N_{\varepsilon 2}$	$H_{\varepsilon 2}$	1.00	0.020
Angle	C_α	C_γ	2.55	0.014
	C_β	C_δ	2.55	0.014
	C_δ	$O_{\varepsilon 1}$	2.39	0.011
	C_δ	$N_{\varepsilon 2}$	2.42	0.011
	$O_{\varepsilon 1}$	$N_{\varepsilon 2}$	2.24	0.011
	C_δ	$H_{\varepsilon 1}$	2.02	0.020
	C_δ	$H_{\varepsilon 2}$	2.02	0.020

Dihedral	d_{min},	d_0, Å	d_1, Å	d_2, Å	d_{max}, Å
N-C_α-C_β-C_γ	2.00	2.78	3.35	3.72	5.50
C_α-C_β-C_γ-C_δ	2.00	2.79	3.75	3.80	5.50
C_β-C_γ-C_δ-$O_{\varepsilon 1}$	2.00	2.65	3.20	3.30	5.50
C_γ-C_δ-$N_{\varepsilon 2}$-$H_{\varepsilon 1}$	2.00	2.53	2.58	3.32	5.50
C_γ-C_δ-$N_{\varepsilon 2}$-$H_{\varepsilon 2}$	2.00	2.53	2.58	3.32	5.50

LYS

Type	Atom *A*	Atom *B*	d_{AB}, Å	σ_{AB}/d_{AB}
Bond	C_β	C_γ	1.52	0.010
	C_γ	C_δ	1.52	0.010
	C_δ	C_ε	1.52	0.010
	C_ε	N_ζ	1.49	0.010
	N_ζ	$H_{\zeta 1}$	1.00	0.020
	N_ζ	$H_{\zeta 2}$	1.00	0.020
	N_ζ	$H_{\zeta 3}$	1.00	0.020
Angle	C_α	C_γ	2.55	0.014
	C_β	C_δ	2.52	0.014
	C_γ	C_ε	2.52	0.014
	C_δ	N_ζ	2.50	0.016
	C_ε	$H_{\zeta 1}$	2.01	0.020
	C_ε	$H_{\zeta 2}$	2.01	0.020
	C_ε	$H_{\zeta 3}$	2.01	0.020

Dihedral	d_{min},	d_0, Å	d_1, Å	d_2, Å	d_{max}, Å
N-C_α-C_β-C_γ	2.00	2.78	3.35	3.72	5.50
C_α-C_β-C_γ-C_δ	2.00	2.79	3.75	3.80	5.50
C_β-C_γ-C_δ-C_ε	2.00	2.80	3.40	3.60	5.50

C_γ-C_δ-C_ε-N_ζ	2.00	2.62	3.45	3.65	5.50
C_δ-C_ε-N_ζ-$H_{\zeta 1}$	2.00	2.55	2.85	3.33	5.50

ARG

Type	Atom *A*	Atom *B*	d_{AB}, Å	σ_{AB}/d_{AB}
Bond	C_β	C_γ	1.52	0.010
	C_γ	C_δ	1.52	0.010
	C_δ	N_ε	1.46	0.008
	N_ε	C_ζ	1.33	0.010
	C_ζ	$N_{\eta 1}$	1.33	0.007
	C_ζ	$N_{\eta 2}$	1.33	0.007
	N_ε	H_ε	1.00	0.020
	$N_{\eta 1}$	$H_{\eta 11}$	1.00	0.020
	$N_{\eta 1}$	$H_{\eta 12}$	1.00	0.020
	$N_{\eta 2}$	$H_{\eta 21}$	1.00	0.020
	$N_{\eta 2}$	$H_{\eta 22}$	1.00	0.020
Angle	C_α	C_γ	2.55	0.014
	C_β	C_δ	2.52	0.014
	C_γ	N_ε	2.47	0.017
	N_ε	$N_{\eta 1}$	2.31	0.010
	N_ε	$N_{\eta 2}$	2.31	0.010
	$N_{\eta 1}$	$N_{\eta 2}$	2.30	0.008
	C_δ	H_ε	2.16	0.020
	C_ζ	H_ε	2.04	0.020
	$H_{\eta 11}$	$H_{\eta 12}$	1.77	0.020
	C_ζ	$H_{\eta 11}$	2.04	0.020
	C_ζ	$H_{\eta 12}$	2.04	0.020
	$H_{\eta 21}$	$H_{\eta 22}$	1.77	0.020
	C_ζ	$H_{\eta 21}$	2.04	0.020
	C_ζ	$H_{\eta 22}$	2.04	0.020

Dihedral	d_{min},	d_0, Å	d_1, Å	d_2, Å	d_{max}, Å
N-C_α-C_β-C_γ	2.00	2.78	3.35	3.72	5.50
C_α-C_β-C_γ-C_δ	2.00	2.79	3.75	3.80	5.50
C_β-C_γ-C_δ-N_ε	2.00	2.68	3.50	3.68	5.50
C_γ-C_δ-N_ε-C_ζ	2.00	3.01	3.42	3.52	5.50
C_δ-N_ε-C_ζ-$N_{\eta 1}$	2.00	2.80	2.85	3.65	5.50
C_δ-N_ε-C_ζ-$N_{\eta 1}$	2.00	2.80	2.85	3.65	5.50
C_δ-N_ε-C_ζ-$N_{\eta 2}$	2.00	2.80	2.85	3.65	5.50
N_ε-C_ζ-$N_{\eta 1}$-$H_{\eta 11}$	2.00	2.48	2.53	3.18	5.50
N_ε-C_ζ-$N_{\eta 1}$-$H_{\eta 12}$	2.00	2.48	2.53	3.18	5.50
N_ε-C_ζ-$N_{\eta 2}$-$H_{\eta 21}$	2.00	2.48	2.53	3.18	5.50
N_ε-C_ζ-$N_{\eta 2}$-$H_{\eta 22}$	2.00	2.48	2.53	3.18	5.50

ASP

Type	Atom *A*	Atom *B*	d_{AB}, Å	σ_{AB}/d_{AB}
Bond	C_β	C_γ	1.52	0.008
	C_γ	$O_{\delta 1}$	1.24	0.012
	C_γ	$O_{\delta 2}$	1.24	0.012
Angle	C_α	C_γ	2.55	0.014
	C_β	$O_{\delta 1}$	2.39	0.011
	C_β	$O_{\delta 2}$	2.42	0.011
	$O_{\delta 1}$	$O_{\delta 2}$	2.42	0.011

Dihedral	d_{min},	d_0, Å	d_1, Å	d_2, Å	d_{max}, Å
$N\text{-}C_\alpha\text{-}C_\beta\text{-}C_\gamma$	2.00	2.78	3.35	3.72	5.50
$C_\alpha\text{-}C_\beta\text{-}C_\gamma\text{-}O_{\delta 1}$	2.00	2.67	2.94	3.02	5.50

GLU

Type	Atom *A*	Atom *B*	d_{AB}, Å	σ_{AB}/d_{AB}
Bond	C_β	C_γ	1.52	0.008
	C_γ	C_δ	1.52	0.010
	C_δ	$O_{\varepsilon 1}$	1.24	0.012
	C_δ	$O_{\varepsilon 2}$	1.24	0.012
Angle	C_α	C_γ	2.55	0.014
	C_β	C_δ	2.55	0.014
	C_δ	$O_{\varepsilon 1}$	2.39	0.011
	C_δ	$O_{\varepsilon 2}$	2.42	0.011
	$O_{\varepsilon 1}$	$O_{\varepsilon 2}$	2.42	0.011

Dihedral	d_{min},	d_0, Å	d_1, Å	d_2, Å	d_{max}, Å
$N\text{-}C_\alpha\text{-}C_\beta\text{-}C_\gamma$	2.00	2.78	3.35	3.72	5.50
$C_\alpha\text{-}C_\beta\text{-}C_\gamma\text{-}C_\delta$	2.00	2.79	3.75	3.80	5.50
$C_\beta\text{-}C_\gamma\text{-}C_\delta\text{-}O_{\varepsilon 1}$	2.00	2.65	3.20	3.30	5.50

PRO

Type	Atom *A*	Atom *B*	d_{AB}, Å	σ_{AB}/d_{AB}
Bond	C_β	C_γ	1.50	0.013
	C_γ	C_δ	1.51	0.011
	N	C_δ	1.48	0.020
Angle	C_α	C_γ	2.38	0.032
	C_α	C_δ	2.43	0.008
	C_β	C_δ	2.38	0.018

Dihedral	d_{min},	d_0, Å	d_1, Å	d_2, Å	d_{max}, Å
$C\text{-}C_\alpha\text{-}C_\beta\text{-}C_\gamma$	2.00	2.97	3.51	3.58	5.50

Inter-residue constraints:

Atom A_i	Atom B_{i+1}	d_{AB}, Å	σ_{AB}/d_{AB}
C_α	N	2.425	0.014
C	H	2.020	0.020
C	N	1.329	0.020
C	C_α	2.435	0.014
C_α	C_α	3.830	0.015
O	C_α	2.694	0.035

Table S2. The non-bonded interactions in all-atom DMD simulations are assigned between different atoms types. In Section A, we list the types of atoms that are used in DMD simulations. Simple descriptions are given after each atom type. In Section B, we provide the interaction potentials between all pairs of atoms in Section A. The potential between two atoms is defined by the hardcore distance (d_{hc}) and a set of potential steps $\{d_i, e_i\}$, where $hdc<d_0<d_1<...<d_N$, $e_i=E(d_{i-1},di) - E(d_i,d_{i+1})$ and $E(d_N,\infty)=0$. The energy is in the unit of kcal/mol and the distance is in the unit of angstrom, Å. Hence, the format of the potential is "type1 type2 d_{hc} d_0 e_0 d_1 e_1 ... d_N e_N".

A. Atom types. Here, we introduce additional atom types for the backbone. The backbone related pairwise interactions are tweaked to reproduce the backbone dihedral angle distributions.

```
CR    carbonyl carbon
CA    aliphatic carbon
CA1   aliphatic carbon with 1 hydrogen
CA2   aliphatic carbon with 2 hydrogens
CA3   aliphatic carbon with 3 hydrogens
CM1   aromatic carbon with 1 hydrogen
NCK   charged nitrogen for lys
NCR   charged nitrogen for arg
NZ    peptide nitrogen
NR    nitrogen in aromatic ring with no hydrogens
NZNP  peptide nitrogen
NZNQ  nitrogen for asn and glu
OC    charged oxygen
OZ    carbonyl and charged oxygen
OW    water oxygen
OZH   serine
SG    sulfur
SGNP  sulfur S-S bond and met

OZB   backbone carbonyl
NZB   backbone nitrogen
CRB   backbone carbonyl carbon
```

B. Interaction potentials.

```
CA1  OZB  3.030000 3.150000 0.522911 3.350000 0.176907 4.200000 0.038104 6.500000 0.013761
CA1P OZB  3.030000 3.150000 0.522911 3.350000 0.176907 4.200000 0.038104 6.500000 0.013761
CA2  OZB  3.070000 3.240000 0.555211 3.325000 0.183005 4.500000 -0.009721 6.500000 -0.001656
CA2P OZB  3.070000 3.240000 0.555211 3.325000 0.183005 4.500000 -0.009721 6.500000 -0.001656
CA3  OZB  3.080000 3.250000 0.562704 3.300000 0.168244
CA   OZB  2.890000 3.270000 0.605362 4.150000 0.142014
CM1  OZB  2.960000 3.130000 0.555512 3.235000 0.185509 4.300000 -0.016432
CM1P OZB  2.960000 3.130000 0.555512 3.235000 0.185509 4.300000 -0.016432
CRNP OZB  2.950000 3.110000 0.526147 3.470000 0.216817 4.210000 -0.044660 6.500000 -0.014468
CR   OZB  2.950000 3.120000 0.546242 3.515000 0.203210 4.250000 -0.029392 6.500000 -0.008252
NCK  OZB  2.480000 2.680000 0.371078 3.060000 0.142101 3.740000 0.124071 6.500000 0.100916
NCR  OZB  2.440000 2.570000 0.487853 2.970000 0.165959 4.090000 0.050739 6.500000 0.048288
NR   OZB  2.630000 2.750000 0.513916 3.045000 0.209952 3.640000 -0.066128
NZNP OZB  2.620000 2.730000 0.487731 2.965000 0.237678 3.570000 -0.077597 4.230000 -0.067413 6.500000 -0.017387
NZNQ OZB  2.460000 2.600000 0.436412 3.010000 0.158046 3.660000 0.075781 6.500000 0.045130
NZ   OZB  2.440000 2.570000 0.487407 2.970000 0.163084 4.080000 0.042117 6.500000 0.026910
OC   OZB  2.640000 2.780000 0.517125 3.180000 0.165380 4.620000 0.025642 6.500000 0.034427
OZB  OW   2.420000 2.560000 0.454142 2.980000 0.150144 3.330000 0.073228 6.500000 0.044704
OZB  OZ   2.620000 2.770000 0.511054 3.190000 0.169160 4.270000 0.034400 6.500000 0.021677
OZB  OZB  2.620000 2.770000 0.511054 3.190000 0.169160 4.270000 0.034400 6.500000 0.021677
OZB  OZH  2.420000 2.570000 0.449897 2.990000 0.168694 3.230000 0.100000 3.870000 0.077856 6.500000 0.038782
OZB  SG   2.710000 2.970000 0.460779 3.440000 0.183263 4.510000 0.071785 6.500000 0.030485
OZB  SGNP 2.680000 2.930000 0.490539 3.410000 0.171476 4.040000 0.064018 6.500000 0.031591
NZB  OZB  2.440000 2.570000 0.487407 2.650000 0.163084 4.080000 0.042117 6.500000 0.026910
CA1  NZB  3.150000 3.380000 0.493240 3.890000 0.178631 4.470000 0.053793 6.500000 0.024935
CA1P NZB  3.150000 3.380000 0.493240 3.890000 0.178631 4.470000 0.053793 6.500000 0.024935
CA2  NZB  3.150000 3.310000 0.513758 3.790000 0.172961 4.090000 0.028865 6.500000 0.012153
CA2P NZB  3.150000 3.310000 0.513758 3.790000 0.172961 4.090000 0.028865 6.500000 0.012153
CA3  NZB  3.160000 3.330000 0.487620 3.790000 0.161516 4.130000 0.042772 6.500000 0.024925
CA   NZB  3.050000 3.360000 0.530339 3.890000 0.178258 4.270000 0.033302 6.500000 0.008227
CM1  NZB  3.030000 3.190000 0.532889 3.650000 0.167914 3.890000 0.019127 6.500000 0.008818
CM1P NZB  3.030000 3.190000 0.532889 3.650000 0.167914 3.890000 0.019127 6.500000 0.008818
CRNP NZB  3.010000 3.150000 0.507610 3.485000 0.220317 4.210000 -0.054270 6.500000 -0.018200
CR   NZB  3.020000 3.170000 0.540154 3.605000 0.189060 4.300000 -0.019794
NCK  NZB  2.690000 2.810000 0.525426 3.210000 0.164171 4.730000 0.020653 6.500000 0.031425
NCR  NZB  2.680000 2.790000 0.557863 3.215000 0.165034 3.680000 -0.022955 6.500000 0.019716
NZB  NR   2.450000 2.550000 0.501008 2.805000 0.218441 3.330000 -0.057988 3.860000 -0.044978 6.500000 -0.001332
```

```
NZB  NZ   2.670000 2.780000 0.488896 3.045000 0.219862 3.620000 -0.050141 4.190000 -0.038520 6.500000 -0.003058
NZB  NZB  2.600000 2.65 0.120 2.70 0.120 2.75 0.120 3.620000 -0.050141 4.190000 -0.038520 6.500000 -0.003058
NZB  NZNP 2.650000 2.760000 0.475074 2.965000 0.243674 3.550000 -0.105817 4.240000 -0.093861 6.500000 -0.025448
NZB  NZNQ 2.680000 2.800000 0.546222 3.200000 0.157583 4.890000 0.005391 6.500000 0.011738
NZB  OC   2.460000 2.570000 0.505975 2.970000 0.161890 4.320000 0.029425 6.500000 0.029573
NZB  OW   2.440000 2.570000 0.487407 2.970000 0.163084 4.080000 0.042117 6.500000 0.026910
NZB  OZ   2.440000 2.570000 0.487407 2.970000 0.163084 4.080000 0.042117 6.500000 0.026910
NZB  OZH  2.440000 2.570000 0.488204 2.970000 0.167317 4.030000 0.026450 6.500000 0.018918
NZB  SG   2.810000 3.050000 0.431769 3.530000 0.197984 4.990000 0.080101 6.500000 0.030069
NZB  SGNP 2.760000 2.980000 0.479141 3.440000 0.166478 4.060000 0.064128 6.500000 0.032400
CRB  OZB  2.300000 2.637000 1.500000 2.780000 0.500000 4.250000 -0.029392 6.500000 -0.008252
CRB  NZB  3.020000 3.150000 0.630154 4.300000 -0.019794
CRB  CA1  3.120000 3.460000 0.513530 3.880000 0.233492 4.820000 -0.043733 6.500000 -0.028788
CRB  CA1P 3.120000 3.460000 0.513530 3.880000 0.233492 4.820000 -0.043733 6.500000 -0.028788
CRB  CA2  3.180000 3.390000 0.510146 3.705000 0.234649 4.550000 -0.081113 6.500000 -0.044434
CRB  CA2P 3.180000 3.390000 0.510146 3.705000 0.234649 4.550000 -0.081113 6.500000 -0.044434
CRB  CA3  3.220000 3.380000 0.493937 3.660000 0.254302 4.460000 -0.075961 5.230000 -0.059485 6.500000 -0.037228
CRB  CA   3.060000 3.540000 0.497255 4.055000 0.251951 5.110000 -0.030552 6.500000 -0.025519
CRB  CM1  3.080000 3.270000 0.507041 3.580000 0.241892 4.400000 -0.081868 6.500000 -0.039547
CRB  CM1P 3.080000 3.270000 0.507041 3.580000 0.241892 4.400000 -0.081868 6.500000 -0.039547
CRB  CR   3.270000 3.480000 0.512060 3.805000 0.236717 4.680000 -0.075389 6.500000 -0.044611
CRB  CRB  3.270000 3.480000 0.512060 3.805000 0.236717 4.680000 -0.075389 6.500000 -0.044611
CRB  CRNP 3.280000 3.480000 0.512030 3.830000 0.238732 4.700000 -0.062725 6.500000 -0.037508
CRB  NCK  3.040000 3.200000 0.505653 3.650000 0.177862 5.250000 0.024981 6.500000 0.053423
CRB  NCR  3.010000 3.150000 0.525387 3.525000 0.202284 4.200000 -0.046584 6.500000 0.008767
CRB  NR   3.000000 3.140000 0.513109 3.455000 0.229914 4.180000 -0.071584 6.500000 -0.026348
CRB  NZ   3.020000 3.170000 0.540154 3.605000 0.189060 4.300000 -0.019794
CRB  NZNP 2.990000 3.130000 0.503288 3.410000 0.243792 4.130000 -0.064758 4.860000 -0.052963 6.500000 -0.023189
CRB  NZNQ 3.020000 3.160000 0.523434 3.555000 0.204293 4.270000 -0.029270 6.500000 -0.006934
CRB  OC   2.990000 3.140000 0.541823 3.535000 0.196455 6.500000 0.011661
CRB  OW   2.950000 3.120000 0.546242 3.515000 0.203210 4.250000 -0.029392 6.500000 -0.008252
CRB  OZ   2.950000 3.120000 0.546242 3.515000 0.203210 4.250000 0.008252
CRB  OZH  2.960000 3.120000 0.549796 3.555000 0.196942 4.280000 -0.020522 6.500000 -0.004087
CRB  SG   2.860000 3.190000 0.538504 3.670000 0.216160 4.560000 -0.021384 6.500000 -0.009890
CRB  SGNP 2.880000 3.210000 0.554134 3.765000 0.188604 4.630000 -0.009245 6.500000 -0.003293
CA1  CA1  3.000000 3.580000 0.501260 4.190000 0.250319 5.300000 -0.020336 6.500000 -0.020147
CA1  CA1P 3.000000 3.580000 0.501260 4.190000 0.250319 5.300000 -0.020336 6.500000 -0.020147
CA1  CA2  3.220000 3.580000 0.511237 4.005000 0.240607 4.980000 -0.045318 6.500000 -0.034424
CA1  CA2P 3.220000 3.580000 0.511237 4.005000 0.240607 4.980000 -0.045318 6.500000 -0.034424
CA1  CA3  3.200000 3.470000 0.503168 3.805000 0.243199 4.700000 -0.074190 6.500000 -0.046222
CA1  CM1  2.890000 3.200000 0.512616 3.590000 0.232293 4.460000 -0.048725 6.500000 -0.024114
CA1  CM1P 2.890000 3.200000 0.512616 3.590000 0.232293 4.460000 -0.048725 6.500000 -0.024114
CA1  NCK  3.210000 3.470000 0.418916 3.960000 0.215487 5.890000 0.079129 6.500000 0.085475
CA1  NCR  3.110000 3.330000 0.519756 3.820000 0.189628 5.350000 0.021823 6.500000 0.040016
CA1  NR   3.080000 3.300000 0.551597 3.780000 0.189086 4.610000 -0.014567 6.500000 -0.006605
CA1  NZ   3.150000 3.380000 0.493240 3.890000 0.178631 4.470000 0.053793 6.500000 0.024935
CA1  NZNP 3.050000 3.270000 0.532354 3.640000 0.227022 4.470000 -0.048411 6.500000 -0.023916
CA1  NZNQ 3.130000 3.360000 0.512385 3.870000 0.174543 4.320000 0.045982 6.500000 0.020055
CA1  OC   3.080000 3.320000 0.527348 3.820000 0.188623 5.200000 0.025262 6.500000 0.042468
CA1  OW   3.030000 3.290000 0.522911 3.810000 0.176907 4.200000 0.038104 6.500000 0.013761
CA1  OZ   3.030000 3.290000 0.522911 3.810000 0.176907 4.200000 0.038104 6.500000 0.013761
CA1  OZH  3.040000 3.310000 0.516383 3.830000 0.176224 4.290000 0.046089 6.500000 0.019292
CA1P CA1P 3.000000 3.580000 0.501260 4.190000 0.250319 5.300000 -0.020336 6.500000 -0.020147
CA1P CA2  3.220000 3.580000 0.511237 4.005000 0.240607 4.980000 -0.045318 6.500000 -0.034424
CA1P CA2P 3.220000 3.580000 0.511237 4.005000 0.240607 4.980000 -0.045318 6.500000 -0.034424
CA1P CA3  3.200000 3.470000 0.503168 3.805000 0.243199 4.700000 -0.074190 6.500000 -0.046222
CA1P CM1  2.890000 3.200000 0.512616 3.590000 0.232293 4.460000 -0.048725 6.500000 -0.024114
CA1P CM1P 2.890000 3.200000 0.512616 3.590000 0.232293 4.460000 -0.048725 6.500000 -0.024114
CA1P NCK  3.210000 3.470000 0.418916 3.960000 0.215487 5.890000 0.079129 6.500000 0.085475
CA1P NCR  3.110000 3.330000 0.519756 3.820000 0.189628 5.350000 0.021823 6.500000 0.040016
CA1P NR   3.080000 3.300000 0.551597 3.780000 0.189086 4.610000 -0.014567 6.500000 -0.006605
CA1P NZ   3.150000 3.380000 0.493240 3.890000 0.178631 4.470000 0.053793 6.500000 0.024935
CA1P NZNP 3.050000 3.270000 0.532354 3.640000 0.227022 4.470000 -0.048411 6.500000 -0.023916
CA1P NZNQ 3.130000 3.360000 0.512385 3.870000 0.174543 4.320000 0.045982 6.500000 0.020055
CA1P OC   3.080000 3.320000 0.527348 3.820000 0.188623 5.200000 0.025262 6.500000 0.042468
CA1P OW   3.030000 3.290000 0.522911 3.810000 0.176907 4.200000 0.038104 6.500000 0.013761
CA1P OZ   3.030000 3.290000 0.522911 3.810000 0.176907 4.200000 0.038104 6.500000 0.013761
CA1P OZH  3.040000 3.310000 0.516383 3.830000 0.176224 4.290000 0.046089 6.500000 0.019292
CA1P SG   2.690000 3.250000 0.513571 3.890000 0.205172 4.260000 0.028722 6.500000 0.003463
CA1P SGNP 2.740000 3.290000 0.499609 3.920000 0.202383 4.380000 0.041374 6.500000 0.013687
CA1  SG   2.690000 3.250000 0.513571 3.890000 0.205172 4.260000 0.028722 6.500000 0.003463
CA1  SGNP 2.740000 3.290000 0.499609 3.920000 0.202383 4.380000 0.041374 6.500000 0.013687
CA2  CA2  3.180000 3.400000 0.511094 3.705000 0.241741 4.560000 -0.089832 6.500000 -0.050059
CA2  CA2P 3.180000 3.400000 0.511094 3.705000 0.241741 4.560000 -0.089832 6.500000 -0.050059
CA2  CA3  3.210000 3.380000 0.485232 3.635000 0.254767 4.430000 -0.088200 5.220000 -0.069624 6.500000 -0.043526
CA2  CM1  3.100000 3.300000 0.510443 3.605000 0.244002 4.440000 -0.086901 6.500000 -0.043784
CA2  CM1P 3.100000 3.300000 0.510443 3.605000 0.244002 4.440000 -0.070901 6.500000 -0.035784
CA2  NCK  3.180000 3.370000 0.454697 3.830000 0.163109 4.370000 0.067121 6.500000 0.105530
CA2  NCR  3.120000 3.270000 0.544771 3.730000 0.180610 5.930000 0.004141 6.500000 0.027116
CA2  NR   3.110000 3.260000 0.513280 3.605000 0.223526 4.370000 -0.051896 6.500000 -0.021583
CA2  NZ   3.150000 3.310000 0.513758 3.790000 0.172961 4.090000 0.028865 6.500000 0.012153
CA2  NZNP 3.100000 3.240000 0.497580 3.535000 0.244496 4.300000 -0.088365 6.500000 -0.038723
CA2  NZNQ 3.130000 3.290000 0.580455 3.895000 0.155114
CA2  OC   3.100000 3.260000 0.554614 3.730000 0.173721 5.990000 0.000851 6.500000 0.028226
CA2  OW   3.070000 3.240000 0.555211 3.745000 0.183005 4.500000 -0.009721 6.500000 -0.001656
```

```
CA2  OZ   3.070000 3.240000 0.555211 3.745000 0.183005 4.500000 0.009721 6.500000 0.001656
CA2  OZH  3.070000 3.250000 0.551723 3.740000 0.174597 4.000000 0.018990 6.500000 0.003762
CA2P CA2P 3.180000 3.400000 0.511094 3.705000 0.241741 4.560000 -0.089832 6.500000 -0.050059
CA2P CA3  3.210000 3.380000 0.485232 3.635000 0.254767 4.430000 -0.088200 5.220000 -0.069624 6.500000 -0.043526
CA2P CM1  3.100000 3.300000 0.510443 3.605000 0.244002 4.440000 -0.086901 6.500000 -0.043784
CA2P CM1P 3.100000 3.300000 0.510443 3.605000 0.244002 4.440000 -0.070901 6.500000 -0.035784
CA2P NCK  3.180000 3.370000 0.454697 3.830000 0.163109 4.370000 0.067121 6.500000 0.105530
CA2P NCR  3.120000 3.270000 0.544771 3.730000 0.180610 5.930000 0.004141 6.500000 0.027116
CA2P NR   3.110000 3.260000 0.513280 3.605000 0.223526 4.370000 -0.051896 6.500000 -0.021583
CA2P NZ   3.150000 3.310000 0.513758 3.790000 0.172961 4.090000 0.028865 6.500000 0.012153
CA2P NZNP 3.100000 3.240000 0.497580 3.535000 0.244496 4.300000 -0.088365 6.500000 -0.038723
CA2P NZNQ 3.130000 3.290000 0.580455 3.895000 0.155114
CA2P OC   3.100000 3.260000 0.554614 3.730000 0.173721 5.990000 0.000851 6.500000 0.028226
CA2P OW   3.070000 3.240000 0.555211 3.745000 0.183005 4.500000 -0.009721 6.500000 -0.001656
CA2P OZ   3.070000 3.240000 0.555211 3.745000 0.183005 4.500000 0.009721 6.500000 0.001656
CA2P OZH  3.070000 3.250000 0.551723 3.740000 0.174597 4.000000 0.018990 6.500000 0.003762
CA2P SG   2.950000 3.300000 0.535873 3.810000 0.209499 4.740000 -0.017158 6.500000 -0.009832
CA2P SGNP 2.970000 3.320000 0.594448 4.095000 0.152966
CA2  SG   2.950000 3.300000 0.535873 3.810000 0.209499 4.740000 -0.017158 6.500000 -0.009832
CA2  SGNP 2.970000 3.320000 0.594448 4.095000 0.152966
CA3  CA3  3.240000 3.380000 0.466401 3.595000 0.276916 4.380000 -0.128730 5.170000 -0.100396 6.500000 -0.061140
CA3  CM1  3.180000 3.340000 0.496573 3.610000 0.259949 4.390000 -0.080221 5.180000 -0.064569 6.500000 -0.038346
CA3  CM1P 3.180000 3.340000 0.496573 3.610000 0.259949 4.390000 -0.064221 5.180000 -0.052569 6.500000 -0.032346
CA3  NCK  3.200000 3.410000 0.413269 3.850000 0.173070 5.060000 0.087320 6.500000 0.125652
CA3  NCR  3.120000 3.260000 0.539003 3.710000 0.161709 5.930000 0.000535 6.500000 0.038952
CA3  NR   3.110000 3.250000 0.501900 3.575000 0.221176 4.300000 -0.060159 6.500000 -0.022312
CA3  NZ   3.160000 3.330000 0.487620 3.790000 0.161516 4.130000 0.042772 6.500000 0.024925
CA3  NZNP 3.100000 3.230000 0.475113 3.500000 0.243844 4.220000 -0.070468 4.940000 -0.056815 6.500000 -0.026571
CA3  NZNQ 3.140000 3.290000 0.523719 3.760000 0.168341 4.000000 0.019870 6.500000 0.009200
CA3  OC   3.110000 3.250000 0.533362 3.700000 0.172031 5.820000 0.005028 6.500000 0.041130
CA3  OW   3.080000 3.230000 0.562704 3.760000 0.168244
CA3  OZ   3.080000 3.230000 0.562704 3.760000 0.168244
CA3  OZH  3.090000 3.250000 0.530959 3.730000 0.169634 3.990000 0.023776 6.500000 0.010028
CA3  SG   3.030000 3.310000 0.536800 3.740000 0.212763 4.620000 -0.028477 6.500000 -0.015398
CA3  SGNP 3.060000 3.330000 0.601518 4.065000 0.149197
CA   CA1  2.650000 3.460000 0.488265 4.240000 0.259974 5.410000 -0.015886 6.500000 -0.017499
CA   CA1P 2.650000 3.460000 0.488265 4.240000 0.259974 5.410000 -0.015886 6.500000 -0.017499
CA   CA2  3.120000 3.630000 0.493250 4.160000 0.254993 5.230000 -0.030879 6.500000 -0.028953
CA   CA2P 3.120000 3.630000 0.493250 4.160000 0.254993 5.230000 -0.030879 6.500000 -0.028953
CA   CA3  3.270000 3.670000 0.495306 4.100000 0.259638 5.130000 -0.045357 6.500000 -0.038967
CA   CA   2.110000 3.240000 0.484326 4.295000 0.266943 5.530000 -0.011802 6.500000 -0.014398
CA   CM1  3.060000 3.540000 0.497223 4.055000 0.251330 5.110000 -0.031082 6.500000 -0.025818
CA   CM1P 3.060000 3.540000 0.497223 4.055000 0.251330 5.110000 -0.031082 6.500000 -0.025818
CA   NCK  3.100000 3.410000 0.488521 3.920000 0.171802 4.470000 0.057016 6.500000 0.068947
CA   NCR  3.020000 3.320000 0.544383 3.850000 0.181201 4.130000 0.018975 6.500000 0.019882
CA   NR   3.000000 3.310000 0.540566 3.790000 0.209812 4.700000 -0.019316 6.500000 -0.011236
CA   NZ   3.050000 3.360000 0.530339 3.890000 0.178258 4.270000 0.033302 6.500000 0.008227
CA   NZNP 2.990000 3.290000 0.518927 3.710000 0.228782 4.590000 -0.038020 6.500000 -0.021296
CA   NZNQ 3.040000 3.340000 0.676238 5.110000 0.073305 6.500000 -0.000091
CA   OC   2.980000 3.310000 0.541686 3.840000 0.180076 4.140000 0.021713 6.500000 0.022041
CA   OW   2.890000 3.270000 0.605362 4.150000 0.142014 6.500000 -0.000705
CA   OZ   2.890000 3.270000 0.605362 4.150000 0.142014 6.500000 -0.000705
CA   OZH  2.900000 3.280000 0.531622 3.830000 0.187466 4.190000 0.029219 6.500000 0.004450
CA   SG   2.340000 3.110000 0.526109 4.030000 0.217163
CA   SGNP 2.370000 3.150000 0.493907 3.930000 0.220770 4.320000 0.030812 6.500000 0.003389
CM1  CM1  3.110000 3.310000 0.511690 3.620000 0.238909 4.440000 -0.081978 6.500000 -0.041414
CM1  CM1P 3.110000 3.310000 0.511690 3.620000 0.238909 4.440000 -0.065978 6.500000 -0.033414
CM1  NCK  3.060000 3.240000 0.472437 3.690000 0.172220 4.790000 0.049299 6.500000 0.080063
CM1  NCR  3.010000 3.160000 0.557411 3.615000 0.173002 4.230000 -0.03012 6.500000 0.022239
CM1  NR   3.000000 3.150000 0.519249 3.475000 0.220593 4.210000 -0.060367 6.500000 -0.021032
CM1  NZ   3.030000 3.190000 0.532889 3.650000 0.167914 3.890000 0.019127 6.500000 0.008818
CM1  NZNP 2.990000 3.130000 0.510424 3.415000 0.241579 4.130000 -0.061345 4.860000 -0.050630 6.500000 -0.021950
CM1  NZNQ 3.020000 3.170000 0.561716 3.660000 0.171902
CM1  OC   3.000000 3.150000 0.544844 3.600000 0.167292 6.500000 0.021617
CM1  OW   2.960000 3.130000 0.555512 3.585000 0.185509 4.300000 -0.016432
CM1  OZ   2.960000 3.130000 0.555512 3.585000 0.185509 4.300000 0.016432
CM1  OZH  2.970000 3.140000 0.575299 3.715000 0.152087
CM1P CM1P 3.110000 3.310000 0.511690 3.620000 0.238909 4.440000 -0.065978 6.500000 -0.033414
CM1P NCK  3.060000 3.240000 0.472437 3.690000 0.172220 4.790000 0.049299 6.500000 0.080063
CM1P NCR  3.010000 3.160000 0.557411 3.615000 0.173002 4.230000 -0.03012 6.500000 0.022239
CM1P NR   3.000000 3.150000 0.519249 3.475000 0.220593 4.210000 -0.060367 6.500000 -0.021032
CM1P NZ   3.030000 3.190000 0.532889 3.650000 0.167914 3.890000 0.019127 6.500000 0.008818
CM1P NZNP 2.990000 3.130000 0.510424 3.415000 0.241579 4.130000 -0.061345 4.860000 -0.050630 6.500000 -0.021950
CM1P NZNQ 3.020000 3.170000 0.561716 3.660000 0.171902
CM1P OC   3.000000 3.150000 0.544844 3.600000 0.167292 6.500000 0.021617
CM1P OW   2.960000 3.130000 0.555512 3.585000 0.185509 4.300000 -0.016432
CM1P OZ   2.960000 3.130000 0.555512 3.585000 0.185509 4.300000 0.016432
CM1P OZH  2.970000 3.140000 0.575299 3.715000 0.152087
CM1P SG   2.870000 3.200000 0.543728 3.705000 0.202910 4.580000 -0.016346 6.500000 -0.007280
CM1P SGNP 2.880000 3.210000 0.595545 3.930000 0.159813
CM1  SG   2.870000 3.200000 0.543728 3.705000 0.202910 4.580000 -0.016346 6.500000 -0.007280
CM1  SGNP 2.880000 3.210000 0.595545 3.930000 0.159813
CR   CA1  3.120000 3.460000 0.513530 3.880000 0.233492 4.820000 -0.043733 6.500000 -0.028788
CR   CA1P 3.120000 3.460000 0.513530 3.880000 0.233492 4.820000 -0.043733 6.500000 -0.028788
CR   CA2  3.180000 3.390000 0.510146 3.705000 0.234649 4.550000 -0.081113 6.500000 -0.044434
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CR   CA2P 3.180000 3.390000 0.510146 3.705000 0.234649 4.550000 -0.081113 6.500000 -0.044434
CR   CA3  3.220000 3.380000 0.493937 3.660000 0.254302 4.460000 -0.075961 5.230000 -0.059485 6.500000 -0.037228
CR   CA   3.060000 3.540000 0.497255 4.055000 0.251951 5.110000 -0.030552 6.500000 -0.025519
CR   CM1  3.080000 3.270000 0.507041 3.580000 0.241892 4.400000 -0.081868 6.500000 -0.039547
CR   CM1P 3.080000 3.270000 0.507041 3.580000 0.241892 4.400000 -0.065868 6.500000 -0.032547
CR   CR   3.270000 3.480000 0.512060 3.805000 0.236717 4.680000 -0.075389 6.500000 -0.044611
CR   CRNP 3.280000 3.480000 0.512030 3.830000 0.238732 4.700000 -0.062725 6.500000 -0.037508
CR   NCK  3.040000 3.200000 0.505653 3.650000 0.177862 5.250000 0.024981 6.500000 0.053423
CR   NCR  3.010000 3.150000 0.525387 3.525000 0.202284 4.200000 -0.046584 6.500000 0.008767
CRNP CA1  3.130000 3.470000 0.527788 3.935000 0.221083 4.900000 -0.027470 6.500000 -0.018558
CRNP CA1P 3.130000 3.470000 0.527788 3.935000 0.221083 4.900000 -0.027470 6.500000 -0.018558
CRNP CA2  3.190000 3.390000 0.517098 3.745000 0.231420 4.600000 -0.057882 6.500000 -0.031282
CRNP CA2P 3.190000 3.390000 0.517098 3.745000 0.231420 4.600000 -0.057882 6.500000 -0.031282
CRNP CA3  3.230000 3.390000 0.504935 3.715000 0.237132 4.530000 -0.076254 6.500000 -0.039235
CRNP CA   3.070000 3.550000 0.506148 4.100000 0.244601 5.170000 -0.022281 6.500000 -0.019697
CRNP CM1  3.080000 3.280000 0.522104 3.620000 0.226383 4.440000 -0.061830 6.500000 -0.028802
CRNP CM1P 3.080000 3.280000 0.522104 3.620000 0.226383 4.440000 -0.061830 6.500000 -0.028802
CRNP CRNP 3.280000 3.480000 0.512374 3.830000 0.240248 4.710000 -0.061288 6.500000 -0.036438
CRNP NCK  3.010000 3.160000 0.575854 3.665000 0.162002 4.240000 -0.024541 6.500000 0.022670
CRNP NCR  3.000000 3.140000 0.523730 3.475000 0.221589 4.180000 -0.063659 6.500000 -0.008474
CRNP NR   3.000000 3.140000 0.491940 3.430000 0.233816 4.160000 -0.086885 6.500000 -0.032734
CRNP NZ   3.010000 3.150000 0.507610 3.485000 0.220317 4.210000 -0.054270 6.500000 -0.018200
CRNP NZNP 2.990000 3.130000 0.501017 3.400000 0.237660 4.120000 -0.070282 4.860000 -0.057489 6.500000 -0.025333
CRNP NZNQ 3.010000 3.150000 0.507779 3.490000 0.220829 4.220000 -0.053152 6.500000 -0.017013
CRNP OC   2.990000 3.130000 0.517959 3.475000 0.218164 4.180000 -0.062713
CRNP OW   2.950000 3.110000 0.526147 3.470000 0.216817 4.210000 -0.044660 6.500000 -0.014468
CRNP OZ   2.950000 3.110000 0.526147 3.470000 0.216817 4.210000 -0.044660 6.500000 -0.014468
CRNP OZH  2.950000 3.110000 0.536834 3.485000 0.212919 4.220000 -0.039223 6.500000 -0.012047
CRNP SG   2.870000 3.200000 0.550713 3.730000 0.200391 4.590000 -0.012675 6.500000 -0.004699
CRNP SGNP 2.870000 3.200000 0.554106 3.740000 0.198886 4.610000 -0.011720 6.500000 -0.004319
CR   NR   3.000000 3.140000 0.513109 3.455000 0.229914 4.180000 -0.071584 6.500000 -0.026348
CR   NZ   3.020000 3.170000 0.540154 3.605000 0.189060 4.300000 -0.019794
CR   NZNP 2.990000 3.130000 0.503288 3.410000 0.243792 4.130000 -0.064758 4.860000 -0.052963 6.500000 -0.023189
CR   NZNQ 3.020000 3.160000 0.523434 3.555000 0.204293 4.270000 -0.029270 6.500000 -0.006934
CR   OC   2.990000 3.140000 0.541823 3.535000 0.196455 6.500000 0.011661
CR   OW   2.950000 3.120000 0.546242 3.515000 0.203210 4.250000 -0.029392 6.500000 -0.008252
CR   OZ   2.950000 3.120000 0.546242 3.515000 0.203210 4.250000 0.008252
CR   OZH  2.960000 3.120000 0.549796 3.555000 0.196942 4.280000 -0.020522 6.500000 -0.004087
CR   SG   2.860000 3.190000 0.538504 3.670000 0.216160 4.560000 -0.021384 6.500000 -0.009890
CR   SGNP 2.880000 3.210000 0.554134 3.765000 0.188604 4.630000 -0.009245 6.500000 -0.003293
NCK  NCK  2.760000 2.950000 0.375654 3.320000 0.152362 4.400000 0.118815 6.500000 0.129016
NCK  NCR  2.710000 2.860000 0.472701 3.250000 0.155717 4.440000 0.062920 6.500000 0.089777
NCK  NR   2.450000 2.560000 0.562741 2.950000 0.164577 3.370000 -0.033149 6.500000 0.029683
NCK  NZ   2.690000 2.810000 0.525426 3.210000 0.164171 4.730000 0.020653 6.500000 0.031425
NCK  NZNP 2.650000 2.760000 0.478896 2.970000 0.251267 3.570000 -0.097667 4.230000 -0.084840 6.500000 -0.022287
NCK  NZNQ 2.730000 2.890000 0.436486 3.280000 0.162133 4.610000 0.077763 6.500000 0.072762
NCK  OC   2.490000 2.670000 0.397575 3.040000 0.159287 4.280000 0.106364 6.500000 0.101492
NCK  OW   2.480000 2.680000 0.371078 3.060000 0.142101 3.740000 0.124071 6.500000 0.100916
NCK  OZ   2.480000 2.680000 0.371078 3.060000 0.142101 3.740000 0.124071 6.500000 0.100916
NCK  OZH  2.490000 2.700000 0.355094 3.080000 0.212148 5.380000 0.107248 6.500000 0.058902
NCK  SG   2.890000 3.200000 0.341682 3.660000 0.250176 6.180000 0.110973 6.500000 0.080418
NCK  SGNP 2.830000 3.080000 0.395383 3.530000 0.217187 5.570000 0.093704 6.500000 0.068322
NCR  NCR  2.680000 2.800000 0.534762 3.190000 0.145983 5.040000 0.011937 6.500000 0.046332
NCR  NR   2.450000 2.550000 0.514011 2.830000 0.214701 3.340000 -0.046620 3.820000 -0.031858 6.500000 0.011918
NCR  NZ   2.680000 2.790000 0.557863 3.215000 0.165034 3.680000 -0.022955 6.500000 0.019716
NCR  NZNP 2.650000 2.760000 0.478896 2.970000 0.251267 3.570000 -0.097667 4.230000 -0.084840 6.500000 -0.022287
NCR  NZNQ 2.690000 2.820000 0.515966 3.210000 0.157552 4.730000 0.022762 6.500000 0.035841
NCR  OC   2.460000 2.580000 0.491326 2.960000 0.157423 4.390000 0.039882 6.500000 0.061201
NCR  OW   2.440000 2.570000 0.487853 2.970000 0.165959 4.090000 0.050739 6.500000 0.048288
NCR  OZ   2.440000 2.570000 0.487853 2.970000 0.165959 4.090000 0.050739 6.500000 0.048288
NCR  OZH  2.450000 2.590000 0.451971 2.980000 0.160530 3.970000 0.061490 6.500000 0.053766
NCR  SG   2.770000 2.990000 0.459954 3.440000 0.163775 4.160000 0.072614 6.500000 0.071318
NCR  SGNP 2.750000 2.960000 0.483718 3.410000 0.158706 3.830000 0.060298 6.500000 0.057405
NR   NR   2.660000 2.760000 0.474700 2.990000 0.249271 3.580000 -0.083345 4.230000 -0.070950 6.500000 -0.016570
NR   NZNP 2.650000 2.760000 0.475074 2.965000 0.243674 3.550000 -0.105817 4.240000 -0.093861 6.500000 -0.025448
NR   NZNQ 2.450000 2.550000 0.526402 2.850000 0.211022 3.360000 -0.054288
NR   OC   2.650000 2.770000 0.506452 3.040000 0.216899 3.610000 -0.050834 4.180000 -0.039115 6.500000 0.003259
NR   OW   2.420000 2.530000 0.524508 2.850000 0.193192 3.370000 -0.040814 6.500000 0.005861
NR   OZ   2.630000 2.750000 0.513916 3.045000 0.209952 3.640000 -0.066128
NR   OZH  2.420000 2.530000 0.534318 2.865000 0.186669 3.370000 -0.034815 6.500000 0.007947
NR   SG   2.710000 2.910000 0.541651 3.380000 0.186477 4.610000 0.019025 6.500000 0.010843
NR   SGNP 2.690000 2.890000 0.563781 3.360000 0.172158 3.580000 0.015146 6.500000 0.006438
NZNP NZNP 2.650000 2.750000 0.474648 2.955000 0.258434 3.550000 -0.111812 4.240000 -0.098969 6.500000 -0.027620
NZNP NZNQ 2.650000 2.760000 0.478896 2.970000 0.251267 3.570000 -0.097667 4.230000 -0.084840 6.500000 -0.022287
NZNP OC   2.640000 2.750000 0.484535 2.970000 0.247309 3.570000 -0.091283 4.230000 -0.079295 6.500000 -0.020774
NZNP OW   2.620000 2.730000 0.487731 2.965000 0.237678 3.570000 -0.077597 4.230000 -0.067413 6.500000 -0.017387
NZNP OZ   2.620000 2.730000 0.487731 2.965000 0.237678 3.570000 -0.077597 4.230000 -0.067413 6.500000 -0.017387
NZNP OZH  2.620000 2.730000 0.487731 2.965000 0.237678 3.570000 -0.077597 4.230000 -0.067413 6.500000 -0.017387
NZNP SG   2.670000 2.870000 0.540425 3.230000 0.210075 3.950000 -0.041484 6.500000 -0.011448
NZNP SGNP 2.660000 2.870000 0.536950 3.210000 0.215217 3.930000 -0.051921 6.500000 -0.015724
NZNQ NZNQ 2.700000 2.840000 0.502797 3.240000 0.162627 4.430000 0.036398 6.500000 0.025912
NZNQ OC   2.470000 2.610000 0.456276 2.990000 0.158970 4.060000 0.059709 6.500000 0.054553
NZNQ OW   2.460000 2.600000 0.436412 3.010000 0.158046 3.660000 0.075781 6.500000 0.045130
NZNQ OZ   2.460000 2.600000 0.436412 3.010000 0.158046 3.660000 0.075781 6.500000 0.045130
NZNQ OZH  2.460000 2.620000 0.425787 3.020000 0.164594 3.990000 0.084349 6.500000 0.042142
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NZNQ SG   2.810000 3.040000 0.432006 3.520000 0.198064 4.950000 0.079250 6.500000 0.030465
NZNQ SGNP 2.770000 2.990000 0.472593 3.460000 0.177405 4.340000 0.068782 6.500000 0.032998
NZ   NR   2.450000 2.550000 0.501008 2.805000 0.218441 3.330000 -0.057988 3.860000 -0.044978 6.500000 -0.001332
NZ   NZ   2.670000 2.780000 0.488896 3.045000 0.219862 3.620000 -0.050141 4.190000 -0.038520 6.500000 -0.003058
NZ   NZNP 2.650000 2.760000 0.475074 2.965000 0.243674 3.550000 -0.105817 4.240000 -0.093861 6.500000 -0.025448
NZ   NZNQ 2.680000 2.800000 0.546222 3.200000 0.157583 4.890000 0.005391 6.500000 0.011738
NZ   OC   2.460000 2.570000 0.505975 2.970000 0.161890 4.320000 0.029425 6.500000 0.029573
NZ   OW   2.440000 2.570000 0.487407 2.970000 0.163084 4.080000 0.042117 6.500000 0.026910
NZ   OZ   2.440000 2.570000 0.487407 2.970000 0.163084 4.080000 0.042117 6.500000 0.026910
NZ   OZH  2.440000 2.570000 0.488204 2.970000 0.167317 4.030000 0.046450 6.500000 0.028918
NZ   SG   2.810000 3.050000 0.431769 3.530000 0.197984 4.990000 0.080101 6.500000 0.030069
NZ   SGNP 2.760000 2.980000 0.479141 3.440000 0.166478 4.060000 0.064128 6.500000 0.032400
OC   OC   2.660000 2.780000 0.534743 3.180000 0.161330 4.910000 0.018521 6.500000 0.047329
OC   OW   2.440000 2.570000 0.458999 2.970000 0.161636 4.020000 0.054075 6.500000 0.049568
OC   OZ   2.640000 2.780000 0.517125 3.180000 0.165380 4.620000 0.025642 6.500000 0.034427
OC   OZH  2.440000 2.580000 0.454657 2.980000 0.161919 3.900000 0.064814 6.500000 0.055128
OC   SG   2.750000 2.980000 0.463321 3.440000 0.169672 4.300000 0.073449 6.500000 0.069287
OC   SGNP 2.730000 2.950000 0.484734 3.410000 0.159452 3.860000 0.062083 6.500000 0.057767
OW   OW   2.420000 2.560000 0.454142 2.980000 0.150144 3.330000 0.073228 6.500000 0.044704
OW   OZH  2.420000 2.570000 0.449897 2.990000 0.168694 3.870000 0.077856 6.500000 0.038782
OW   SG   2.710000 2.970000 0.460779 3.440000 0.183263 4.510000 0.071785 6.500000 0.030485
OW   SGNP 2.680000 2.930000 0.490539 3.410000 0.171476 4.040000 0.064018 6.500000 0.031591
OZH  OZH  2.430000 2.590000 0.421729 3.010000 0.185071 4.510000 0.079724 6.500000 0.029940
OZH  SG   2.730000 2.990000 0.448174 3.470000 0.196705 4.800000 0.077694 6.500000 0.029958
OZH  SGNP 2.690000 2.950000 0.481918 3.430000 0.176948 4.290000 0.068297 6.500000 0.031646
OZ   OW   2.420000 2.560000 0.454142 2.980000 0.150144 3.330000 0.073228 6.500000 0.044704
OZ   OZ   2.620000 2.770000 0.511054 3.190000 0.169160 4.270000 0.034400 6.500000 0.021677
OZ   OZH  2.420000 2.570000 0.449897 2.990000 0.168694 3.870000 0.077856 6.500000 0.038782
OZ   SG   2.710000 2.970000 0.460779 3.440000 0.183263 4.510000 0.071785 6.500000 0.030485
OZ   SGNP 2.680000 2.930000 0.490539 3.410000 0.171476 4.040000 0.064018 6.500000 0.031591
SGNP SGNP 2.480000 3.010000 0.468905 3.560000 0.193689 4.420000 0.066455 6.500000 0.029602
SG   SG   1.960000 2.990000 0.474522 3.560000 0.194552 4.340000 0.064358 6.500000 0.029167
SG   SGNP 2.500000 3.020000 0.464638 3.580000 0.196007 4.530000 0.068012 6.500000 0.030047
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Table S3. The Parameters for Hydrogen Bond Interactions
The details of the DMD algorithm for the hydrogen bond can be found in Ref (2). The hydrogen bond strengths for the backbone-backbone, backbone-sidechain, and sidechain-sidechain are 1.80 kcal/mol, 1.80 kcal/mol, and 1.50 kcal/mol, respectively.

A. The interaction parameters for hydrogen bonds

Backbone-Backbone hydrogen bonds between N_i H_i and C_j O_j.

Atom pair	d_{min}	d_0	d_1	d_{max}
Hi Oj	1.75 Å	2.15 Å	2.34 Å	2.50 Å
Ni Oj	2.76 Å	3.10 Å	3.20 Å	3.50 Å
Hi Cj	2.90 Å	3.27 Å	3.40 Å	3.75 Å

Sidechain (C_iO_i, where O_i is sp2 hybridized; such as ASP, GLU) and Backbone (N_jH_j).

Atom pair	d_{min}	d_0	d_1	d_{max}
Oi Hj	1.76 Å	2.25 Å	2.50 Å	3.00 Å
Ci Hj	2.56 Å	3.28 Å	3.46 Å	4.25 Å
Oi Nj	2.75 Å	3.15 Å	3.30 Å	4.00 Å

Sidechain (C_iO_i, where O_i is sp3 hybridized; such as SER, THR, and TYR) and Backbone (N_jH_j).

Atom pair	d_{min}	d_0	d_1	d_{max}
Oi Hj	1.80 Å	2.30 Å	2.53 Å	3.00 Å
Ci Hj	2.82 Å	3.44 Å	3.56 Å	4.50 Å
Oi Nj	2.77 Å	3.30 Å	3.50 Å	4.00 Å

Sidechain (C_iN_i, where N_i is in an aromatic ring; such as HIS) and Backbone (N_jH_j).

Atom pair	d_{min}	d_0	d_1	d_{max}
Ni Hj	1.76 Å	2.20 Å	2.50 Å	3.00 Å
Ci Hj	2.75 Å	3.28 Å	3.40 Å	4.25 Å
Ni Nj	2.65 Å	3.10 Å	3.35 Å	4.00 Å

Sidechain (NiHi or OiHi) and Backbone (CjOj)

Atom pair	d_{min}	d_0	d_1	d_{max}
Hi Oj	1.75 Å	2.20 Å	2.50 Å	3.00 Å
Ni Oj	2.68 Å	3.20 Å	3.41 Å	4.00 Å
Oi Oj	2.62 Å	3.14 Å	3.37 Å	4.00 Å
Hi Cj	2.74 Å	3.37 Å	3.67 Å	4.25 Å

Sidechain (C_iO_i, where O_i is sp2 hybridized; such as ASP, GLU) and Sidechain (NjHj or OjHj)

Atom pair	d_{min}	d_0	d_1	d_{max}
Oi Hj	1.68 Å	2.20 Å	2.46 Å	3.00 Å
Oi Nj	2.62 Å	3.15 Å	3.37 Å	4.00 Å
Oi Oj	2.62 Å	3.15 Å	3.37 Å	4.00 Å
Hi Cj	2.48 Å	3.28 Å	3.60 Å	4.25 Å

Sidechain (C_iO_i, where O_i is sp3 hybridized; such as SER, THR, and TYR) and Sidechain (NjHj or OjHj)

Atom pair	d_{min}	d_0	d_1	d_{max}
Oi Hj	1.73 Å	2.35 Å	2.75 Å	3.00 Å
Oi Nj	2.63 Å	3.27 Å	3.54 Å	4.00 Å
Oi Oj	2.67 Å	3.27 Å	3.54 Å	4.00 Å
Hi Cj	2.65 Å	3.71 Å	4.00 Å	4.50 Å

Sidechain (C_iN_i, where N_i is in an aromatic ring; such as HIS) and Sidechain (NjHj or OjHj)

Atom pair	d_{min}	d_0	d_1	d_{max}
Ni Hj	1.76 Å	2.20 Å	2.50 Å	3.00 Å
Ci Hj	2.75 Å	3.28 Å	3.45 Å	4.25 Å
Ni Nj	2.65 Å	3.10 Å	3.35 Å	4.00 Å
Ni Oj	2.64 Å	3.10 Å	3.35 Å	4.00 Å

B. The non-bonded interactions between hydrogen bonded backbone oxygen(OZB') and other atoms.

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OZB'  CA1     3.030000 3.250000 0.576702 3.350000 0.169029
OZB'  CA1P    3.030000 3.250000 0.576702 3.350000 0.169029
OZB'  CA2     3.070000 3.220000 0.535540 3.320000 0.216452 4.390000 -0.036738 6.500000 -0.015083
OZB'  CA2P    3.070000 3.220000 0.535540 3.320000 0.216452 4.390000 -0.036738 6.500000 -0.015083
OZB'  CA3     3.080000 3.210000 0.524178 3.300000 0.217982 4.310000 -0.045635 6.500000 -0.017160
OZB'  CA      2.890000 3.250000 0.544410 3.400000 0.201960 4.730000 -0.011692 6.500000 -0.006991
OZB'  CM1     2.960000 3.110000 0.532197 3.230000 0.216297 4.220000 -0.041431 6.500000 -0.013801
OZB'  CM1P    2.960000 3.110000 0.532197 3.230000 0.216297 4.220000 -0.041431 6.500000 -0.013801
OZB'  CRNP    2.950000 3.100000 0.530756 3.440000 0.227619 4.180000 -0.057713 6.500000 -0.020396
OZB'  CR      2.950000 3.110000 0.515084 3.450000 0.220726 4.200000 -0.051767 6.500000 -0.018366
OZB'  NCK     2.480000 2.630000 0.400406 3.020000 0.165299 4.150000 0.096090 6.500000 0.080254
OZB'  NCR     2.440000 2.550000 0.521903 2.950000 0.157499 4.380000 0.027397 6.500000 0.037278
OZB'  NZ      2.440000 2.560000 0.492802 2.960000 0.162251 4.190000 0.032509 6.500000 0.022603
OZB'  NR      2.630000 2.740000 0.514423 3.030000 0.218013 3.630000 -0.071255 6.500000 -0.010539
OZB'  NZNP    2.620000 2.730000 0.487731 2.965000 0.237678 3.570000 -0.077597 4.230000 -0.067413 6.500000 -0.017387
OZB'  NZNQ    2.460000 2.570000 0.491921 2.980000 0.166256 4.010000 0.048220 6.500000 0.029844
OZB'  OC      2.640000 2.750000 0.548167 3.160000 0.166380 4.930000 0.009648 6.500000 0.026865
OZB'  OZ      2.620000 2.740000 0.503986 3.160000 0.152531 4.650000 0.012851 6.500000 0.011016
OZB'  OW      2.420000 2.530000 0.512697 2.950000 0.168746 4.000000 0.041074 6.500000 0.024763
OZB'  OZH     2.420000 2.540000 0.485712 2.960000 0.168460 3.230000 0.100000 3.850000 0.052334 6.500000 0.030287
OZB'  SG      2.710000 2.910000 0.504109 3.380000 0.165152 3.810000 0.053629 6.500000 0.026705
OZB'  SGNP    2.680000 2.900000 0.511938 3.370000 0.162880 3.740000 0.047030 6.500000 0.023894
OZB'  OZB     2.620000 2.740000 0.503986 3.160000 0.152531 4.650000 0.012851 6.500000 0.011016
OZB'  NZB     2.440000 2.570000 0.487407 2.650000 0.152635
OZB'  CRB     2.300000 2.637000 1.500000 2.780000 0.500000 4.250000 -0.043904 6.500000 -0.011375
OZB'  CRN     2.950000 3.110000 0.532149 3.475000 0.216186 4.250000 -0.043904 6.500000 -0.011375
OZB'  OZB'    2.620000 2.730000 0.552767 3.150000 0.158011
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Supplemental References

1. Ding, F., Buldyrev, S. V. & Dokholyan, N. V. (2005) *Biophys. J.* **88**, 147-155.

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