Supporting Information

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Table S1. Energy weights for FASPR energy terms.

Name	Value
w_{hb}	1
w_{ss}	6
$w_{rot}(ALA)$	0
$w_{rot}(CYS)$	5.5
$w_{rot}(ASP)$	2
$w_{rot}(GLU)$	1
$w_{rot}(PHE)$	1.5
$w_{rot}(GLY)$	0
$w_{rot}(HIS)$	3
$w_{rot}(ILE)$	1
$w_{rot}(LYS)$	2
$w_{rot}(LEU)$	2
$w_{rot}(MET)$	1.5
$w_{rot}(ASN)$	2
$w_{rot}(PRO)$	1.5
$w_{rot}(GLN)$	2.5
$w_{rot}(ARG)$	1.5
$w_{rot}(SER)$	1.5
$w_{rot}(THR)$	2
$w_{rot}(VAL)$	2
$w_{rot}(TRP)$	3.5
$w_{rot}(TYR)$	1.5

Table S2. The atomic parameters of 18 atom types defined in FASPR.

Atom types	Radius (σ)	Well-depth (ε)
Main-chain CA	1.78	0.25
Main-chain C	1.40	0.14
CH1	2.30	0.30
CH2	1.91	0.37
CH3	1.96	0.48
Aromatic C	1.73	0.38
Side-chain CO, COO,HCNN	1.43	0.07
Cys CB	1.99	0.38
Main-chain N	1.42	0.08
Side-chain -NH-, -NH2, -NH3	1.69	0.24
His NE2	1.56	0.46
Pro N	1.70	0.48
Main-chain O	1.48	0.22
OC	1.44	0.27
OOC	1.40	0.07
OH	1.43	0.12
Cys S	2.15	0.44
Met S	1.74	0.40

Table S3. Amino acid hydrogen bonding donor and acceptor atoms.

Donor (*D*)	Donor base (*DB*)	Acceptor (*A*)	Acceptor base (*AB*)
Backbone N	Backbone CA	Backbone O	Backbone C
His ND1	His CG	Asp OD1/OD2	Asp CG
Lys NZ	Lys CE	Glu OE1/OE2	Glu CD
Asn ND2	Asn CG	His NE2	His CD2
Gln NE2	Gln CD	Asn OD1	Asn CG
Arg NE	Arg CD	Gln OE1	Gln CD
Arg NH1/NH2	Arg CZ	Ser OG	Ser CB
Ser OG	Ser CB	Thr OG1	Thr CB
Thr OG1	Thr CB	Tyr OH	Tyr CZ
Trp NE1	Trp CD1		
Tyr OH	Tyr CZ		

Table S4. Hemisphere radii for 20 amino acids.

Amino acid	Radius of hemisphere (Å)
ALA	3.2
CYS	3.2
ASP	3.2
GLU	3.7
PHE	4.3
GLY	2.4
HIS	3.7
ILE	3.2
LYS	5.0
MET	4.3
ASN	3.2
PRO	3.2
GLN	3.7
ARG	6.2
SER	3.2
THR	3.2
VAL	3.2
TRP	5.3
TYR	5.7

Table S5. PDB IDs of 100 training proteins.

135L, 1A8Q, 1AGY, 1BJ7, 1BK7, 1BKR, 1BN6, 1C44, 1C5H, 1CHD, 1EDG, 1EW4, 1EYH, 1F32, 1G9O, 1GQZ, 1GYV, 1H75, 1HD5, 1I2H, 1I2T, 1IUK, 1JOS, 1JYH, 1K6A, 1KF5, 1KHI, 1KNG, 1KXO, 1L6P, 1LMI, 1LN4, 1LPL, 1LZL, 1MHN, 1NOA, 1O9Z, 1OA4, 1OI7, 1OMP, 1OW1, 1P3C, 1P7S, 1PGS, 1Q2U, 1Q42, 1Q5Z, 1QAD, 1QK8, 1QWK, 1R26, 1R62, 1R9W, 1RYN, 1SNO, 1T2I, 1T3Y, 1TG0, 1TSF, 1U53, 1UAI, 1UCH, 1UCS, 1UGN, 1UJ8, 1UOY, 1WLY, 1WPA, 1X6Q, 1X91, 1XAK, 1XTE, 1Y9U, 1YCK, 1YP5, 1YRW, 1Z3Y, 1ZD8, 1ZEQ, 1ZHV, 1ZPW, 1ZZK, 2A4V, 2AHE, 2AWG, 2B29, 2B49, 2BV9, 2ERF, 2ESK, 2FI9, 2FK9, 2FQ3, 2FR2, 2HVM, 2IGD, 2LIS, 2OVO, 3EZM, 4PTI

Table S6. PDB IDs of 379 test proteins.

1AHO, 1ATZ, 1B2P, 1B8Z, 1B9W, 1BGF, 1BYI, 1C02, 1C48, 1CEI, 1DPT, 1DQ0, 1DV7, 1DYS, 1E5M, 1E6F, 1EDQ, 1ELK, 1ERZ, 1ES5, 1ES9, 1F41, 1F60, 1F94, 1FCQ, 1FO9, 1FPO, 1FTR, 1FVK, 1G61, 1G8A, 1G8Q, 1GMU, 1GO3, 1GPP, 1GQN, 1GS9, 1GSO, 1GVP, 1GXN, 1H03, 1H4A, 1H4Y, 1HCL, 1HM5, 1HZ6, 1HZ9, 1I4J, 1IGQ, 1IJQ, 1IJY, 1ILK, 1IU8, 1J23, 1J2A, 1J7G, 1JB3, 1JCD, 1JKS, 1JY2, 1K33, 1KMT, 1KMZ, 1KN3, 1KOE, 1KPT, 1KU8, 1KVA, 1KVE, 1KYF, 1KZQ, 1L3K, 1LBV, 1LM5, 1LTU, 1M5T, 1M6J, 1MD6, 1MF7, 1MG7, 1MIX, 1MKK, 1MML, 1MOL, 1N1J, 1N93, 1NAR, 1NM8, 1NWA, 1NXM, 1OAI, 1OAQ, 1OGM, 1OK7, 1P1X, 1P9H, 1PCF, 1PDO, 1PE9, 1PGV, 1PM4, 1PXZ, 1QAH, 1QKD, 1R12, 1R29, 1R77, 1R8N, 1RFY, 1RGX, 1RL0, 1RWZ, 1RYL, 1RZ2, 1S7I, 1S7K, 1SAU, 1SH8, 1SMX, 1SNT, 1SQE, 1SRV, 1SUU, 1SWH, 1T1J, 1TJE, 1TKS, 1TP6, 1TUA, 1TUO, 1TY0, 1TZV, 1U07, 1U2H, 1U5X, 1UEB, 1UEK, 1UJN, 1UKF, 1ULN, 1ULR, 1UNP, 1USM, 1UXZ, 1UZ3, 1V05, 1V0S, 1V6T, 1V7Q, 1V8E, 1V8H, 1V8I, 1VDK, 1VE2, 1VGT, 1VH5, 1VJS, 1VPI, 1W5R, 1W7B, 1WBA, 1WD7, 1WKA, 1WKO, 1WLG, 1WLZ, 1WM3, 1WMH, 1WQJ, 1WTJ, 1WU9, 1WVH, 1WYC, 1WZ3, 1X1E, 1X2I, 1X6I, 1XDZ, 1XFK, 1XS0, 1XXO, 1Y2T, 1Y7Y, 1YAC, 1YHH, 1YN3, 1YPF, 1YT4, 1YTL, 1YU5, 1YW5, 1YXY, 1YZM, 1Z0C, 1Z0P, 1ZKR, 1ZO2, 1ZRS, 1ZUH, 1ZV1, 1ZVA, 1ZVT, 1ZXT, 2A35, 2A6W, 2A8F, 2AHF, 2AHN, 2B0A, 2B0J, 2B2F, 2BAY, 2BK8, 2BPD, 2BVP, 2CG7, 2CGH, 2CHC, 2CI3, 2CIU, 2COV, 2CWC, 2CWK, 2CWL, 2CWR, 2CYG, 2D4P, 2D68, 2D8E, 2DQW, 2DYU, 2E01, 2E10, 2E3Z, 2E64, 2E7A, 2E8F, 2E8G, 2E9Y, 2EBB, 2EBE, 2ECR, 2EGJ, 2EHG, 2EPI, 2ETX, 2EX0, 2F23, 2F5G, 2F6L, 2FBN, 2FBQ, 2FD5, 2FHZ, 2FJZ, 2FL4, 2FLU, 2FRG, 2FVH, 2FW7, 2G2U, 2G30, 2G40, 2G69, 2G7I, 2G7O, 2GAS, 2GDQ, 2GEC, 2GGV, 2GIY, 2GKG, 2GKV, 2GOM, 2GQV, 2GXG, 2H14, 2H2R, 2H2Z, 2H7W, 2H7Z, 2H8E, 2H8O, 2HC8, 2HLR, 2HLY, 2HOQ, 2HPL, 2HWW, 2HY5, 2HZF, 2I3F, 2I49, 2I5D, 2I6V, 2IBL, 2IC6, 2IC7, 2IIA, 2IJK, 2IP2, 2IPR, 2IRU, 2IUM, 2IXM, 2IY9, 2IZ6, 2J2J, 2J5Y, 2J6B, 2J71, 2J8B, 2J9W, 2JCP, 2NML, 2NNU, 2NPT, 2NRR, 2NV0, 2O0Q, 2O2K, 2O6S, 2O6X, 2OEB, 2OHW, 2OIX, 2OL7, 2OSA, 2OTU, 2P1G, 2P38, 2P4H, 2P52, 2P5D, 2P5K, 2P65, 2P84, 2PBP, 2PBQ, 2PEF, 2PET, 2PGE, 2PKF, 2PMR, 2PND, 2PST, 2PTV, 2PV2, 2Q8O, 2QIY, 2QOL, 2QPW, 2QR3, 2QT4, 2R6U, 2R77, 2R99, 2RCZ, 2RFA, 2RIK, 2RJD, 2RK5, 2VC8, 2YXF, 2YYV, 2YZ1, 2Z14, 2Z1E, 2Z37, 2ZFY, 3ADO, 3BB7, 3BN6, 3C4S, 3PHS, 3SSW, 4RWU, 5WOF, 6XIA

Table S7. The values of TM-score and RMSD between the 379 I-TASSER models and their native counterparts.

PDB ID	TM-score	RMSD (Å)	PDB ID	TM-score	RMSD (Å)
1AHO	0.9151	1.257	1YW5	0.9962	0.309
1ATZ	0.9603	1.276	1YXY	0.9972	0.300
1B2P	0.9936	0.329	1YZM	0.9435	0.697
1B8Z	0.9771	0.468	1Z0C	0.9876	0.616
1B9W	0.9786	0.550	1Z0P	0.9463	1.422
1BGF	0.9866	0.487	1ZKR	0.9937	0.551
1BYI	0.9907	0.611	1ZO2	0.9877	0.465
1C02	0.9866	0.687	1ZRS	0.9830	1.531
1C48	0.9899	0.298	1ZUH	0.9391	2.209
1CEI	0.8867	1.714	1ZV1	0.9429	0.653
1DPT	0.9932	0.333	1ZVA	0.8891	1.950
1DQ0	0.9961	0.362	1ZVT	0.9480	1.649
1DV7	0.9256	2.952	1ZXT	0.9318	0.952
1DYS	0.9970	0.375	2A35	0.9793	1.155
1E5M	0.9930	0.619	2A6W	0.9850	0.740
1E6F	0.9487	1.260	2A8F	0.9795	0.532
1EDQ	0.9964	0.498	2AHF	0.9978	0.329
1ELK	0.9975	0.232	2AHN	0.9970	0.305
1ERZ	0.9948	0.468	2B0A	0.9984	0.203
1ES5	0.9954	0.414	2B0J	0.8053	3.599
1ES9	0.9978	0.252	2B2F	0.9989	0.233
1F41	0.9793	0.756	2BAY	0.9003	1.091
1F60	0.9989	0.247	2BK8	0.8415	2.339
1F94	0.8957	1.061	2BPD	0.9491	1.210
1FCQ	0.9899	0.667	2BVP	0.9768	0.948
1FO9	0.9956	0.565	2CG7	0.9693	0.620
1FPO	0.9975	0.244	2CGH	0.9647	1.480
1FTR	0.9968	0.362	2CHC	0.9970	0.269
1FVK	0.9898	0.524	2CI3	0.9922	0.573
1G61	0.9974	0.286	2CIU	0.9898	0.425
1G8A	0.9703	1.204	2COV	0.9952	0.242
1G8Q	0.8745	2.021	2CWC	0.9941	0.655
1GMU	0.9611	0.901	2CWK	0.9891	0.491
1GO3	0.9870	0.689	2CWL	0.9862	0.879
1GPP	0.9633	1.199	2CWR	0.9394	0.986
1GQN	0.9775	1.311	2CYG	0.9964	0.390
1GS9	0.9566	1.202	2D4P	0.9787	0.644
1GSO	0.9773	1.194	2D68	0.9575	0.717
1GVP	0.9787	0.507	2D8E	0.9839	0.440
1GXN	0.9966	0.383	2DQW	0.9858	0.886
1H03	0.8604	1.762	2DYU	0.9976	0.329
1H4A	0.9889	0.539	2E01	0.9609	3.772

1H4Y	0.9813	0.623	2E10	0.9602	2.648
1HCL	0.8786	4.642	2E3Z	0.9930	0.674
1HM5	0.9956	0.560	2E64	0.9930	0.496
1HZ6	0.9228	1.327	2E7A	0.9687	0.938
1HZ9	0.9752	0.476	2E8F	0.9974	0.218
1I4J	0.7650	3.512	2E8G	0.9991	0.172
1IGQ	0.9268	1.103	2E9Y	0.9963	0.395
1IJQ	0.9801	0.981	2EBB	0.9851	0.442
1IJY	0.9943	0.312	2EBE	0.9463	1.035
1ILK	0.6074	14.385	2ECR	0.9840	0.735
1IU8	0.9959	0.342	2EGJ	0.9736	0.699
1J23	0.9966	0.248	2EHG	0.9976	0.225
1J2A	0.9400	1.839	2EPI	0.9696	1.294
1J7G	0.9933	0.367	2ETX	0.9877	0.588
1JB3	0.9828	0.640	2EX0	0.9869	0.845
1JCD	0.6822	1.931	2F23	0.9255	1.645
1JKS	0.9537	5.268	2F5G	0.9521	1.131
1JY2	0.6986	3.902	2F6L	0.9957	0.319
1K33	0.4746	4.666	2FBN	0.9974	0.237
1KMT	0.9474	1.109	2FBQ	0.9980	0.247
1KMZ	0.5162	12.617	2FD5	0.9983	0.209
1KN3	0.9898	0.626	2FHZ	0.9952	0.264
1KOE	0.9944	0.371	2FJZ	0.9277	0.976
1KPT	0.9975	0.188	2FL4	0.9940	0.352
1KU8	0.9907	0.419	2FLU	0.9927	0.580
1KVA	0.9597	1.110	2FRG	0.9115	1.375
1KVE	0.9086	1.203	2FVH	0.9689	0.684
1KYF	0.9943	0.445	2FW7	0.9805	0.795
1KZQ	0.9983	0.240	2G2U	0.9915	0.578
1L3K	0.9591	1.068	2G30	0.9947	0.420
1LBV	0.9847	0.779	2G40	0.9823	1.332
1LM5	0.9676	0.959	2G69	0.9400	1.126
1LTU	0.9980	0.275	2G7I	0.9309	1.146
1M5T	0.9722	0.716	2G7O	0.9670	0.541
1M6J	0.9986	0.219	2GAS	0.9934	0.535
1MD6	0.9915	0.432	2GDQ	0.9879	0.811
1MF7	0.9838	1.118	2GEC	0.9354	2.176
1MG7	0.9976	0.379	2GGV	0.5946	3.155
1MIX	0.9347	4.645	2GIY	0.9949	0.358
1MKK	0.8830	1.846	2GKG	0.9657	0.818
1MML	0.9374	2.225	2GKV	0.9924	0.455
1MOL	0.9682	0.737	2GOM	0.9798	0.385
1N1J	0.9855	0.412	2GQV	0.9489	0.713
1N93	0.9944	0.735	2GXG	0.8677	1.982
1NAR	0.9980	0.284	2H14	0.9926	0.554

1NM8	0.9889	0.997	2H2R	0.8127	3.792
1NWA	0.9968	0.276	2H2Z	0.9798	1.289
1NXM	0.9800	0.946	2H7W	0.9806	0.572
1OAI	0.7616	2.528	2H7Z	0.9372	1.016
1OAQ	0.9692	0.815	2H8E	0.9954	0.277
1OGM	0.9992	0.238	2H8O	0.9942	0.624
1OK7	0.9916	0.655	2HC8	0.9732	0.834
1P1X	0.9982	0.247	2HLR	0.7555	2.861
1P9H	0.9739	1.164	2HLY	0.9950	0.416
1PCF	0.9551	0.642	2HOQ	0.9958	0.372
1PDO	0.9932	0.351	2HPL	0.7633	2.273
1PE9	0.9961	0.468	2HWW	0.9536	1.409
1PGV	0.9893	0.515	2HY5	0.9954	0.288
1PM4	0.7034	4.687	2HZF	0.9520	1.162
1PXZ	0.9991	0.204	2I3F	0.9981	0.235
1QAH	0.9749	0.719	2I49	0.9984	0.287
1QKD	0.9500	0.705	2I5D	0.9950	0.448
1R12	0.9973	0.304	2I6V	0.8238	1.717
1R29	0.9645	0.861	2IBL	0.6856	5.386
1R77	0.9458	1.314	2IC6	0.8484	1.474
1R8N	0.9977	0.245	2IC7	0.9967	0.293
1RFY	0.9001	1.272	2IIA	0.9744	1.118
1RGX	0.9597	0.750	2IJK	0.9069	1.426
1RL0	0.9980	0.265	2IP2	0.9988	0.230
1RWZ	0.9882	0.663	2IPR	0.9366	1.349
1RYL	0.9871	0.712	2IRU	0.9901	0.668
1RZ2	0.9248	2.529	2IUM	0.9965	0.320
1S7I	0.9963	0.251	2IXM	0.9909	0.639
1S7K	0.9523	1.672	2IY9	0.9985	0.261
1SAU	0.9915	0.367	2IZ6	0.9759	0.895
1SH8	0.9953	0.318	2J2J	0.9963	0.309
1SMX	0.8982	1.873	2J5Y	0.9788	0.395
1SNT	0.9824	1.074	2J6B	0.9940	0.299
1SQE	0.8647	2.953	2J71	0.9866	0.465
1SRV	0.9895	0.471	2J8B	0.9169	1.377
1SUU	0.9904	0.667	2J9W	0.9935	0.315
1SWH	0.7224	8.168	2JCP	0.8155	2.639
1T1J	0.9827	0.565	2NML	0.8800	1.643
1TJE	0.9828	0.761	2NNU	0.9871	0.608
1TKS	0.9719	1.287	2NPT	0.8470	6.698
1TP6	0.9790	0.658	2NRR	0.9344	2.082
1TUA	0.9963	0.315	2NV0	0.9677	1.186
1TUO	0.9953	0.727	2O0Q	0.8821	1.837
1TY0	0.9964	0.324	2O2K	0.9935	0.660
1TZV	0.9786	0.720	2O6S	0.9941	0.415

1U07	0.9658	0.723	2O6X	0.9911	0.672
1U2H	0.9919	0.324	2OEB	0.9980	0.203
1U5X	0.9733	0.839	2OHW	0.9961	0.264
1UEB	0.9933	0.423	2OIX	0.9915	0.502
1UEK	0.9986	0.230	2OL7	0.5037	22.763
1UJN	0.9974	0.403	2OSA	0.9778	0.987
1UKF	0.9972	0.269	2OTU	0.9686	0.951
1ULN	0.8264	1.623	2P1G	0.9877	0.719
1ULR	0.9910	0.324	2P38	0.9966	0.271
1UNP	0.9011	1.822	2P4H	0.9926	0.910
1USM	0.9445	1.177	2P52	0.9705	1.264
1UXZ	0.9905	0.422	2P5D	0.9742	0.876
1UZ3	0.8462	9.326	2P5K	0.9432	0.794
1V05	0.9832	0.473	2P65	0.9707	0.928
1V0S	0.9753	1.828	2P84	0.9926	0.388
1V6T	0.9978	0.283	2PBP	0.9849	0.746
1V7Q	0.9845	0.625	2PBQ	0.9917	0.483
1V8E	0.9956	0.379	2PEF	0.9081	7.248
1V8H	0.9929	0.322	2PET	0.9978	0.263
1V8I	0.9755	0.988	2PGE	0.9888	0.809
1VDK	0.9964	0.471	2PKF	0.9867	0.814
1VE2	0.9873	0.840	2PMR	0.9918	0.288
1VGT	0.9517	1.378	2PND	0.9235	1.288
1VH5	0.9933	0.362	2PST	0.9264	0.832
1VJS	0.9832	1.864	2PTV	0.9423	1.177
1VPI	0.9467	1.029	2PV2	0.9844	0.476
1W5R	0.9939	0.510	2Q8O	0.9489	1.496
1W7B	0.9916	0.691	2QIY	0.9805	0.839
1WBA	0.9929	0.414	2QOL	0.9665	2.186
1WD7	0.9910	0.604	2QPW	0.7638	6.193
1WKA	0.9768	0.704	2QR3	0.8905	1.663
1WKO	0.9966	0.281	2QT4	0.9828	0.482
1WLG	0.9001	2.199	2R6U	0.9577	1.954
1WLZ	0.6017	3.892	2R77	0.8908	3.033
1WM3	0.9150	0.974	2R99	0.9956	0.319
1WMH	0.9246	0.987	2RCZ	0.6719	17.625
1WQJ	0.9462	1.000	2RFA	0.9958	0.359
1WTJ	0.9875	0.769	2RIK	0.8661	2.611
1WU9	0.9418	0.915	2RJD	0.9826	1.241
1WVH	0.9352	1.339	2RK5	0.9872	0.389
1WYC	0.9910	0.759	2VC8	0.9748	0.489
1WZ3	0.5252	14.226	2YXF	0.8779	3.079
1X1E	0.9912	0.548	2YYV	0.9970	0.307
1X2I	0.9730	0.513	2YZ1	0.7111	7.582
1X6I	0.9925	0.307	2Z14	0.9745	1.323

1XDZ	0.9960	0.364	2Z1E	0.9804	1.587
1XFK	0.9996	0.136	2Z37	0.9936	0.478
1XS0	0.9810	0.727	2ZFY	0.9967	0.325
1XXO	0.9303	1.962	3ADO	0.9968	0.364
1Y2T	0.9948	0.323	3BB7	0.9981	0.314
1Y7Y	0.9821	0.403	3BN6	0.9828	0.717
1YAC	0.9980	0.237	3C4S	0.9220	0.844
1YHH	0.9913	0.565	3PHS	0.9984	0.231
1YN3	0.9887	0.391	3SSW	0.6000	4.822
1YPF	0.9731	1.625	4RWU	0.9915	0.301
1YT4	0.9967	0.346	5WOF	0.7912	2.951
1YTL	0.9979	0.214	6XIA	0.9977	0.364
1YU5	0.9752	0.578			

Table S8. The lower bounds, upper bounds and increments for optimizing parameters.

Parameter name	Lower bound	Upper bound	Increments
w_{hb}	0	10	0.5
w_{ss}	0	10	0.5
$w_{rot}(CYS)$	0	10	0.5
$w_{rot}(ASP)$	0	10	0.5
$w_{rot}(GLU)$	0	10	0.5
$w_{rot}(PHE)$	0	10	0.5
$w_{rot}(HIS)$	0	10	0.5
$w_{rot}(ILE)$	0	10	0.5
$w_{rot}(LYS)$	0	10	0.5
$w_{rot}(LEU)$	0	10	0.5
$w_{rot}(MET)$	0	10	0.5
$w_{rot}(ASN)$	0	10	0.5
$w_{rot}(PRO)$	0	10	0.5
$w_{rot}(GLN)$	0	10	0.5
$w_{rot}(ARG)$	0	10	0.5
$w_{rot}(SER)$	0	10	0.5
$w_{rot}(THR)$	0	10	0.5
$w_{rot}(VAL)$	0	10	0.5
$w_{rot}(TRP)$	0	10	0.5
$w_{rot}(TYR)$	0	10	0.5
Self-energy threshold	10	30	5
Main-chain CA radius	1.3	2.4	0.01
Main-chain C radius	1.3	2.4	0.01
CH1 radius	1.3	2.4	0.01
CH2 radius	1.3	2.4	0.01
CH3 radius	1.3	2.4	0.01
Aromatic C radius	1.3	2.4	0.01
Side-chain CO, COO,HCNN radius	1.3	2.4	0.01
Cys CB radius	1.3	2.4	0.01
Main-chain N radius	1.3	2.4	0.01
Side-chain -NH-, -NH2, -NH3 radius	1.3	2.4	0.01
His NE2 radius	1.3	2.4	0.01
Pro N radius	1.3	2.4	0.01
Main-chain O radius	1.3	2.4	0.01
OC radius	1.3	2.4	0.01
OOC radius	1.3	2.4	0.01
OH radius	1.3	2.4	0.01
Cys S radius	1.4	2.5	0.01
Met S radius	1.4	2.5	0.01
Main-chain CA well-depth	0.05	0.5	0.01
Main-chain C well-depth	0.05	0.5	0.01
CH1 well-depth	0.05	0.5	0.01

CH2 well-depth	0.05	0.5	0.01
CH3 well-depth	0.05	0.5	0.01
Aromatic C well-depth	0.05	0.5	0.01
Side-chain CO, COO,HCNN well-depth	0.05	0.5	0.01
Cys CB well-depth	0.05	0.5	0.01
Main-chain N well-depth	0.05	0.5	0.01
Side-chain -NH-, -NH2, -NH3 well-depth	0.05	0.5	0.01
His NE2 well-depth	0.05	0.5	0.01
Pro N well-depth	0.05	0.5	0.01
Main-chain O well-depth	0.05	0.5	0.01
OC well-depth	0.05	0.5	0.01
OOC well-depth	0.05	0.5	0.01
OH well-depth	0.05	0.5	0.01
Cys S well-depth	0.05	0.5	0.01
Met S well-depth	0.05	0.5	0.01

Table S9. Protein side-chain packing results for 18 amino acid types in terms of χ_{1-4} recovery rate on 379 native backbones for the residues in three categories.

Residue	χ_{1-4} recovery rate (%)						
	FASPR	CISRR	RASP	SCATD	SCWRL4	SCWRL4v	ABACUS2
All residues							
CYS	85.5	90.8	91.0	76.5	89.1	89.5	90.9
ASP	59.6	58.6	59.2	51.8	62.5	59.6	61.9
GLU	29.7	26.5	27.8	20.3	29.9	27.3	30.9
PHE	83.8	83.1	79.4	71.5	80.8	77.3	87.2
HIS	60.1	63.2	55.7	54.9	59.7	56.2	65.6
ILE	84.4	85.4	83.4	80.7	84.6	83.4	87.1
LYS	33.5	33.5	32.2	25.7	31.2	29.5	33.6
LEU	85.8	86.4	84.3	80.2	84.7	83.4	87.3
MET	52.7	54.1	50.6	38.8	49.8	47.0	54.2
ASN	59.3	56.2	57.3	46.3	57.8	57.1	60.7
PRO	80.4	79.3	81.7	78.7	80.6	79.7	79.0
GLN	32.9	27.6	30.2	20.0	32.5	30.4	32.1
ARG	27.5	26.7	25.0	13.6	29.3	24.0	29.6
SER	70.0	69.1	70.2	66.1	71.5	70.5	72.9
THR	91.6	90.9	91.4	88.7	91.6	91.1	92.6
VAL	93.8	93.9	94.0	92.5	94.3	93.7	95.1
TRP	77.6	79.2	72.4	47.6	71.9	67.1	86.3
TYR	80.2	78.6	76.8	68.0	78.1	75.6	86.0
Total	69.1	68.6	67.8	61.7	68.8	67.0	71.1
Core residues							
CYS	88.1	92.6	91.3	83.0	90.2	90.4	90.5
ASP	59.3	65.2	59.9	54.0	68.2	62.3	66.8
GLU	43.2	38.7	39.3	30.3	45.9	40.8	44.4
PHE	85.6	86.7	80.3	75.2	84.0	80.9	90.0
HIS	59.6	65.6	58.0	58.8	66.7	60.4	70.5
ILE	87.3	88.9	85.9	84.6	87.4	85.8	90.3
LYS	42.3	42.0	39.4	31.9	37.1	37.1	40.4
LEU	87.3	89.0	85.9	83.5	87.1	85.8	89.2
MET	59.5	63.1	59.5	50.1	63.3	59.8	66.2
ASN	65.7	67.3	62.6	52.0	62.4	61.7	69.7
PRO	84.2	82.6	85.1	83.9	83.3	83.3	83.7
GLN	44.1	38.2	39.8	30.6	44.1	41.4	40.5
ARG	34.1	38.0	32.5	26.5	41.5	32.9	44.9
SER	75.6	72.7	73.5	70.6	76.0	74.1	79.9
THR	92.9	93.3	93.3	91.4	93.1	92.9	95.7
VAL	95.4	95.7	95.5	94.0	95.7	95.2	96.9
TRP	82.4	86.4	78.4	57.8	77.7	75.2	92.3
TYR	82.0	82.5	80.0	72.7	81.1	79.8	89.7
Total	80.3	81.4	78.9	74.7	80.7	78.9	83.8
Surface residues							
CYS	80.0	80.0	87.7	49.2	81.5	83.1	84.6
ASP	57.9	56.3	56.7	49.5	58.6	56.2	57.6
GLU	23.6	21.3	22.6	15.8	21.2	20.8	23.5
PHE	76.1	67.6	70.0	55.6	65.9	60.8	75.1
HIS	58.0	55.2	50.5	46.7	50.8	48.0	53.9
ILE	73.7	73.9	73.9	68.3	74.7	75.6	76.0
LYS	29.2	28.2	27.0	21.5	26.0	25.4	27.5
LEU	79.8	77.6	79.4	70.7	78.8	77.7	80.2

MET	35.4	35.9	35.4	21.5	26.2	25.6	34.4
ASN	54.0	48.2	53.0	41.3	53.6	52.5	55.5
PRO	77.2	75.5	78.4	76.2	77.3	76.6	74.7
GLN	25.4	21.9	20.8	13.7	23.3	21.3	23.0
ARG	22.6	20.4	19.8	8.0	21.4	16.9	19.6
SER	67.8	67.6	68.3	62.5	68.9	68.3	67.3
THR	91.3	90.1	90.1	86.9	90.5	90.5	90.2
VAL	88.6	88.7	88.9	87.8	89.8	89.3	89.0
TRP	70.3	62.5	61.7	27.3	57.8	53.9	69.5
TYR	68.2	66.2	67.6	57.2	67.2	61.2	69.2
Total	56.8	54.8	55.5	48.4	55.5	54.1	56.0

Note: the total number of clashes in the 379 structures repacked by ABACUS2 on native main chains is 35.

Table S10. The computational time for side-chain modeling on 379 native main chains.

PDB ID	Time (seconds)						
	FASPR	CISRR	RASP	SCATD	SCWRL4	SCWRL4v	ABACUS2
1AHO	0.02	0.88	0.03	0.16	0.63	0.13	2.55
1ATZ	0.05	3.16	0.08	0.33	1.30	0.27	9.70
1B2P	0.03	1.78	0.05	0.22	0.92	0.19	5.54
1B8Z	0.02	0.90	0.04	0.23	0.76	0.12	2.23
1B9W	0.02	1.17	0.04	0.22	0.77	0.17	3.23
1BGF	0.09	3.19	0.12	0.34	2.41	0.42	6.60
1BYI	0.07	3.82	0.11	0.34	1.93	0.34	11.70
1C02	0.09	5.04	0.12	0.41	3.03	0.48	9.43
1C48	0.02	1.01	0.03	0.18	0.62	0.12	2.83
1CEI	0.03	1.44	0.05	0.22	1.13	0.18	3.70
1DPT	0.04	1.80	0.06	0.24	1.04	0.2	5.19
1DQ0	0.09	4.49	0.10	0.36	1.77	0.35	13.07
1DV7	0.13	5.12	0.13	0.51	3.09	0.46	11.60
1DYS	0.16	9.42	0.21	0.64	4.21	0.79	21.95
1E5M	0.16	11.32	0.20	0.69	3.82	0.75	26.37
1E6F	0.03	1.75	0.06	0.26	1.02	0.22	5.71
1EDQ	0.27	17.25	0.32	0.99	5.23	1.17	35.57
1ELK	0.07	2.66	0.09	0.34	1.69	0.27	7.96
1ERZ	0.19	8.58	0.20	0.71	5.19	0.73	19.13
1ES5	0.09	5.50	0.10	0.45	1.90	0.37	14.59
1ES9	0.11	5.03	0.13	0.47	3.20	0.57	12.27
1F41	0.04	1.73	0.05	0.26	1.03	0.19	5.15
1F60	0.20	13.23	0.27	0.93	5.26	1	26.16
1F94	0.02	1.15	0.03	0.18	0.57	0.11	2.65
1FCQ	0.26	10.91	0.28	0.80	5.75	0.89	22.22
1FO9	0.24	12.65	0.24	0.79	5.44	2.45	22.54
1FPO	0.14	3.68	0.14	0.49	3.07	14.53	9.10
1FTR	0.11	7.04	0.15	0.55	2.49	0.52	15.50
1FVK	0.08	3.56	0.12	0.37	2.21	0.39	10.03
1G61	0.06	3.98	0.09	0.36	1.43	0.31	11.88
1G8A	0.13	5.85	0.16	0.54	3.69	0.51	13.75
1G8Q	0.02	1.17	0.04	0.21	0.79	0.15	3.83
1GMU	0.06	2.24	0.07	0.31	1.31	0.22	6.30
1GO3	0.08	3.25	0.09	0.38	2.03	0.31	8.45
1GPP	0.13	5.52	0.13	0.48	2.85	0.49	11.67
1GQN	0.13	5.35	0.14	0.48	5.62	0.68	15.26
1GS9	0.13	5.40	0.27	0.47	3.97	1.11	7.97
1GSO	0.18	10.36	0.23	0.78	4.35	0.83	23.74
1GVP	0.02	1.13	0.04	0.21	0.98	0.16	3.38
1GXN	0.14	9.52	0.17	0.64	3.41	0.6	21.25
1H03	0.04	1.50	0.05	0.24	0.78	0.17	4.83
1H4A	0.12	5.98	0.13	0.45	3.38	0.45	12.18
1H4Y	0.06	2.36	0.07	0.31	1.56	0.25	5.72
1HCL	0.14	7.31	0.18	0.58	3.44	0.61	17.79
1HM5	0.31	19.87	0.36	1.00	8.75	1.65	38.34
1HZ6	0.01	0.77	0.03	0.17	0.49	0.09	2.68
1HZ9	0.02	1.14	0.04	0.20	0.73	0.12	2.54
1I4J	0.05	1.90	0.06	0.32	1.59	0.21	4.68
1IGQ	0.02	0.76	0.04	0.19	0.70	0.1	2.14
1IJQ	0.12	7.94	0.16	0.53	2.87	0.56	20.07

1IJY	0.06	2.22	0.07	0.31	1.52	0.25	6.60
1ILK	0.07	2.65	0.10	0.39	2.06	0.31	6.05
1IU8	0.08	4.29	0.12	0.39	1.99	0.35	11.93
1J23	0.06	2.44	0.07	0.33	1.60	0.24	6.32
1J2A	0.06	3.08	0.09	0.30	1.48	0.3	8.23
1J7G	0.06	2.59	0.08	0.29	1.38	0.26	7.04
1JB3	0.09	2.79	0.08	0.31	1.71	0.29	6.35
1JCD	0.01	0.32	0.02	0.14	0.48	0.08	1.18
1JKS	0.15	8.62	0.19	0.61	4.20	0.66	16.97
1JY2	0.01	0.33	0.02	0.15	0.28	0.07	1.32
1K33	0.03	0.81	0.05	0.19	1.00	0.15	2.49
1KMT	0.06	2.80	0.09	0.34	1.96	0.34	6.58
1KMZ	0.05	1.92	0.06	0.25	0.96	0.18	5.71
1KN3	0.09	4.30	0.10	0.39	2.25	0.36	10.52
1KOE	0.08	3.87	0.10	0.41	2.39	0.35	8.90
1KPT	0.03	1.98	0.05	0.24	0.96	0.17	4.38
1KU8	0.04	2.08	0.05	0.24	0.90	0.18	6.07
1KVA	0.13	3.18	0.11	0.39	2.35	0.35	7.72
1KVE	0.01	0.44	0.02	0.16	0.45	0.08	1.32
1KYF	0.12	5.84	0.16	0.49	3.54	0.61	14.73
1KZQ	0.06	3.69	0.10	0.35	1.59	0.35	11.70
1L3K	0.09	3.45	0.11	0.42	2.37	0.38	8.44
1LBV	0.14	7.02	0.15	0.57	13.22	0.5	15.43
1LM5	0.10	4.50	0.12	0.48	2.84	0.73	10.35
1LTU	0.14	8.31	0.16	0.52	3.36	0.57	18.63
1M5T	0.05	2.42	0.07	0.32	1.64	0.24	6.54
1M6J	0.11	6.50	0.14	0.52	2.75	0.47	14.69
1MD6	0.06	2.48	0.07	0.29	1.33	0.23	7.18
1MF7	0.13	6.21	0.15	0.52	3.51	6.62	11.84
1MG7	0.18	11.12	0.22	0.69	4.62	0.84	22.78
1MIX	0.15	5.08	0.15	0.57	4.00	3.98	11.82
1MKK	0.05	1.67	0.06	0.23	1.43	0.22	3.79
1MML	0.11	6.25	0.16	0.48	3.20	0.56	14.28
1MOL	0.06	2.09	0.07	0.28	1.55	0.28	4.49
1N1J	0.03	1.17	0.05	0.22	0.88	0.15	3.26
1N93	0.14	7.94	0.18	0.62	3.66	0.67	17.17
1NAR	0.17	7.46	0.18	0.62	4.25	1.25	18.99
1NM8	0.42	24.15	0.52	1.26	9.25	21.93	44.47
1NWA	0.09	4.32	0.11	0.49	2.80	0.4	9.39
1NXM	0.11	3.93	0.11	0.38	2.45	1.64	10.21
1OAI	0.02	1.00	0.04	0.17	0.81	0.13	2.85
1OAQ	0.07	2.25	0.07	0.29	1.71	0.24	6.26
1OGM	0.31	18.33	0.36	0.90	5.51	2.22	42.85
1OK7	0.21	12.44	0.24	0.81	7.91	1.09	24.43
1P1X	0.13	5.36	0.14	0.53	2.82	9.41	15.19
1P9H	0.04	1.48	0.06	0.25	1.05	0.25	6.39
1PCF	0.02	1.12	0.04	0.22	1.14	0.16	2.60
1PDO	0.04	1.78	0.06	0.26	1.03	0.19	6.04
1PE9	0.13	8.52	0.17	0.54	3.70	0.68	22.84
1PGV	0.13	4.66	0.12	0.52	3.18	0.4	10.05
1PM4	0.08	2.35	0.06	0.28	1.54	0.23	5.98
1PXZ	0.18	8.72	0.17	0.68	4.23	7.33	22.66
1QAH	0.03	1.74	0.06	0.25	1.09	0.21	5.67

1QKD	0.02	1.02	0.03	0.20	0.75	0.12	2.37
1R12	0.12	6.41	0.14	0.52	3.00	0.5	14.15
1R29	0.05	2.01	0.07	0.27	1.23	0.26	5.74
1R77	0.04	2.15	0.05	0.26	0.92	0.18	4.86
1R8N	0.08	3.91	0.11	0.37	2.12	0.35	8.71
1RFY	0.03	1.12	0.05	0.22	1.09	0.17	3.55
1RGX	0.02	0.81	0.04	0.20	0.59	0.13	2.78
1RL0	0.08	7.22	0.16	0.58	4.81	6.01	15.33
1RWZ	0.13	6.60	0.14	0.59	2.94	0.49	13.86
1RYL	0.08	3.79	0.11	0.41	2.32	0.31	8.07
1RZ2	0.14	6.03	0.17	0.51	6.10	0.73	13.77
1S7I	0.03	1.51	0.07	0.25	1.37	0.23	4.60
1S7K	0.10	3.48	0.10	0.34	2.54	0.36	8.03
1SAU	0.06	2.66	0.08	0.29	1.95	0.27	6.10
1SH8	0.23	4.25	0.13	0.49	3.20	0.57	7.41
1SMX	0.03	1.34	0.05	0.23	1.18	0.18	3.43
1SNT	0.19	10.05	0.23	0.79	5.52	0.93	23.73
1SQE	0.06	2.11	0.07	0.29	1.78	0.26	5.00
1SRV	0.06	2.99	0.08	0.37	1.79	0.25	7.01
1SUU	0.13	8.84	0.15	0.65	3.20	0.58	18.73
1SWH	0.03	1.46	0.05	0.21	0.88	0.15	4.91
1T1J	0.06	2.37	0.08	0.31	1.78	0.24	6.35
1TJE	0.13	5.70	0.15	0.45	3.97	0.67	13.40
1TKS	0.09	4.61	0.11	0.43	2.19	0.37	11.70
1TP6	0.07	2.63	0.07	0.35	2.34	12.19	5.83
1TUA	0.11	4.62	0.14	0.55	3.66	0.43	9.54
1TUO	0.37	13.66	0.23	0.88	6.05	1.08	27.39
1TY0	0.11	5.43	0.13	0.48	2.68	37.45	15.28
1TZV	0.14	3.84	0.13	0.54	15.89	13.85	8.68
1U07	0.04	1.48	0.08	0.28	1.35	0.19	3.85
1U2H	0.06	2.22	0.07	0.31	2.03	0.23	4.53
1U5X	0.07	2.79	0.08	0.29	1.52	0.24	6.88
1UEB	0.07	3.43	0.11	0.38	1.99	0.39	8.97
1UEK	0.16	6.48	0.15	0.54	3.57	0.46	13.34
1UJN	0.16	8.01	0.18	0.58	3.27	0.55	17.70
1UKF	0.15	4.37	0.10	0.49	4.47	5.33	10.72
1ULN	0.03	1.14	0.04	0.22	0.88	0.16	2.93
1ULR	0.04	1.77	0.05	0.24	1.08	0.15	3.81
1UNP	0.20	3.18	0.11	0.46	42.66	11.86	6.17
1USM	0.05	1.94	0.06	0.29	1.37	0.19	4.06
1UXZ	0.05	2.45	0.07	0.27	1.78	13.4	6.53
1UZ3	0.04	1.61	0.06	0.31	1.28	0.22	4.21
1V05	0.02	1.24	0.04	0.20	0.61	0.15	4.12
1V0S	0.24	18.72	0.26	0.98	6.20	8.32	34.62
1V6T	0.13	6.70	0.15	0.55	2.90	0.6	15.52
1V7Q	0.10	4.21	0.11	0.44	2.39	0.34	9.35
1V8E	0.10	5.25	0.11	0.45	2.26	0.39	12.09
1V8H	0.04	2.37	0.06	0.28	1.37	0.22	4.40
1V8I	0.10	3.02	0.09	0.40	2.08	0.3	7.30
1VDK	0.21	13.42	0.28	0.92	5.51	1.05	28.55
1VE2	0.13	3.44	0.09	0.45	1.63	0.3	10.01
1VGT	0.07	3.46	0.10	0.38	1.84	0.34	10.59
1VH5	0.06	2.68	0.08	0.36	1.62	0.25	6.75

1VJS	0.29	20.78	0.31	1.00	22.44	1.83	34.79
1VPI	0.04	2.01	0.06	0.28	1.35	0.23	5.05
1W5R	0.13	7.10	0.15	0.54	3.40	0.54	16.25
1W7B	0.21	10.40	0.22	0.80	4.74	6.27	22.45
1WBA	0.08	3.55	0.09	0.37	1.91	0.35	9.47
1WD7	0.12	5.10	0.15	0.57	2.83	0.48	13.06
1WKA	0.08	3.63	0.09	0.40	2.25	0.37	7.38
1WKO	0.08	2.98	0.09	0.35	1.84	0.34	9.89
1WLG	0.09	5.44	0.13	0.39	1.88	0.55	16.23
1WLZ	0.05	1.75	0.06	0.27	1.37	0.21	4.77
1WM3	0.03	1.36	0.06	0.22	1.05	0.18	3.44
1WMH	0.03	1.74	0.05	0.22	0.84	0.16	4.30
1WQJ	0.01	0.80	0.03	0.17	0.51	0.11	2.15
1WTJ	0.13	7.59	0.17	0.64	3.39	0.65	19.16
1WU9	0.02	0.60	0.04	0.17	0.57	0.14	1.96
1WVH	0.05	1.80	0.06	0.26	1.27	0.23	6.25
1WYC	0.20	11.61	0.23	0.80	18.15	27.37	23.73
1WZ3	0.02	0.86	0.04	0.20	0.64	0.14	2.44
1X1E	0.11	4.25	0.12	0.52	2.64	0.42	11.90
1X2I	0.02	1.15	0.04	0.22	1.00	0.13	2.55
1X6I	0.06	2.30	0.07	0.31	1.72	0.25	4.71
1XDZ	0.11	6.00	0.14	0.50	2.81	9.74	15.10
1XFK	0.17	10.52	0.21	0.63	4.32	0.86	21.31
1XS0	0.04	2.31	0.06	0.27	1.15	0.25	6.06
1XXO	0.06	2.59	0.08	0.36	1.94	0.29	6.26
1Y2T	0.08	3.21	0.08	0.35	1.98	0.28	7.69
1Y7Y	0.04	1.68	0.04	0.25	1.11	0.17	2.84
1YAC	0.07	3.92	0.09	0.37	1.71	0.33	10.68
1YHH	0.13	4.76	0.14	0.48	3.71	0.57	13.85
1YN3	0.03	1.47	0.05	0.26	0.89	0.18	4.49
1YPF	0.12	6.26	0.16	0.60	3.33	0.69	16.60
1YT4	0.12	8.03	0.14	0.60	3.52	0.79	16.08
1YTL	0.07	3.27	0.09	0.36	1.78	0.35	8.94
1YU5	0.02	1.06	0.04	0.21	0.84	0.14	2.92
1YW5	0.08	3.82	0.10	0.39	2.12	0.36	9.48
1YXY	0.08	4.34	0.11	0.47	2.52	0.46	12.03
1YZM	0.02	0.64	0.04	0.19	0.89	0.12	1.91
1Z0C	0.07	3.64	0.10	0.44	2.00	0.32	10.66
1Z0P	0.03	1.29	0.06	0.24	1.08	0.17	3.04
1ZKR	0.05	2.58	0.08	0.30	1.38	0.23	7.61
1ZO2	0.07	1.87	0.08	0.27	1.79	5.61	6.50
1ZRS	0.15	7.78	0.15	0.58	3.64	0.64	15.87
1ZUH	0.09	2.90	0.10	0.34	1.82	0.37	7.54
1ZV1	0.03	0.85	0.05	0.18	0.98	0.15	2.63
1ZVA	0.02	0.81	0.03	0.17	0.59	0.13	2.43
1ZVT	0.09	5.81	0.12	0.46	2.31	0.47	12.27
1ZXT	0.02	1.12	0.05	0.20	1.04	0.14	2.74
2A35	0.10	4.63	0.11	0.42	2.43	0.35	10.74
2A6W	0.12	6.14	0.15	0.51	2.62	0.5	13.64
2A8F	0.02	1.01	0.03	0.18	0.47	0.13	3.86
2AHF	0.29	13.80	0.26	0.91	6.92	14.86	28.59
2AHN	0.06	3.13	0.09	0.31	1.29	0.33	10.65
2B0A	0.07	3.54	0.09	0.35	1.76	0.33	9.75

2B0J	0.12	6.57	0.15	0.57	2.90	0.6	18.72
2B2F	0.11	7.62	0.13	0.51	2.21	0.47	22.75
2BAY	0.02	0.89	0.03	0.18	0.69	0.12	2.40
2BK8	0.03	1.41	0.05	0.25	1.10	0.19	4.64
2BPD	0.06	2.96	0.07	0.30	1.54	0.28	7.00
2BVP	0.46	7.79	0.22	0.71	9.25	2.76	16.90
2CG7	0.03	1.99	0.05	0.26	1.27	0.18	3.20
2CGH	0.09	5.45	0.12	0.48	2.30	0.41	12.03
2CHC	0.24	4.11	0.12	0.40	2.69	0.35	8.05
2CI3	0.13	6.75	0.17	0.60	3.28	0.67	16.68
2CIU	0.07	3.09	0.09	0.37	2.52	0.35	5.97
2COV	0.05	1.82	0.06	0.23	1.08	0.21	4.27
2CWC	0.17	8.85	0.19	0.71	4.17	0.58	16.62
2CWK	0.08	3.74	0.10	0.45	2.30	0.32	7.55
2CWL	0.16	7.08	0.19	0.59	3.44	1.64	17.60
2CWR	0.02	1.02	0.04	0.20	0.64	0.19	3.96
2CYG	0.12	7.18	0.16	0.56	3.08	0.66	18.41
2D4P	0.06	2.63	0.07	0.33	1.78	0.24	5.38
2D68	0.02	0.98	0.04	0.21	0.81	0.13	2.64
2D8E	0.05	1.65	0.07	0.30	1.70	0.21	3.62
2DQW	0.14	7.01	0.16	0.59	3.29	0.51	14.41
2DYU	0.15	8.38	0.19	0.57	3.70	0.77	20.38
2E01	0.28	17.05	0.50	0.95	5.81	1.18	30.03
2E10	0.08	4.46	0.11	0.50	1.84	0.33	11.74
2E3Z	0.32	17.38	0.31	0.99	17.62	1.31	36.51
2E64	0.09	4.58	0.11	0.45	2.08	0.34	12.74
2E7A	0.06	2.43	0.07	0.28	1.41	0.26	7.03
2E8F	0.06	2.58	0.08	0.31	1.89	0.28	6.06
2E8G	0.12	6.71	0.15	0.58	3.13	0.49	13.59
2E9Y	0.15	6.88	0.16	0.56	3.35	0.59	16.73
2EBB	0.07	2.00	0.08	0.27	1.52	0.33	5.13
2EBE	0.04	1.62	0.05	0.26	0.89	0.21	4.59
2ECR	0.06	3.10	0.07	0.33	1.56	0.28	6.17
2EGJ	0.10	2.81	0.09	0.33	2.25	0.39	7.12
2EHG	0.07	2.94	0.09	0.34	1.88	0.31	8.06
2EPI	0.04	1.54	0.06	0.25	1.28	0.2	4.43
2ETX	0.08	3.68	0.10	0.43	1.98	0.35	9.41
2EX0	0.21	11.69	0.29	0.80	5.51	1.18	27.06
2F23	0.09	3.28	0.12	0.40	2.75	21.08	6.99
2F5G	0.07	2.36	0.09	0.33	1.88	0.32	6.24
2F6L	0.08	3.35	0.11	0.38	2.40	0.33	8.30
2FBN	0.08	3.09	0.09	0.37	1.72	0.3	8.75
2FBQ	0.12	5.38	0.13	0.48	2.98	2.12	10.17
2FD5	0.07	2.93	0.10	0.40	2.02	1.38	7.70
2FHZ	0.04	1.88	0.05	0.25	0.79	0.19	4.97
2FJZ	0.02	0.74	0.03	0.17	0.62	0.15	2.32
2FL4	0.10	2.90	0.11	0.38	2.57	0.37	6.95
2FLU	0.13	7.60	0.14	0.56	2.92	0.59	17.10
2FRG	0.05	1.73	0.07	0.24	1.50	0.4	4.48
2FVH	0.04	1.74	0.07	0.29	1.32	0.26	4.17
2FW7	0.04	2.10	0.06	0.28	0.94	0.21	6.57
2G2U	0.12	7.73	0.17	0.63	3.40	0.56	15.44
2G30	0.11	5.24	0.14	0.45	2.56	0.57	13.74

2G40	0.06	2.72	0.08	0.33	1.57	0.31	7.50
2G69	0.04	1.45	0.05	0.23	0.85	0.21	4.00
2G7I	0.05	2.31	0.07	0.32	1.40	0.26	5.46
2G7O	0.02	0.62	0.03	0.19	0.54	0.12	2.01
2GAS	0.16	7.47	0.18	0.59	3.72	0.79	18.43
2GDQ	0.24	13.22	0.36	0.74	16.04	10.74	25.72
2GEC	0.06	2.68	0.08	0.37	2.05	0.33	6.54
2GGV	0.01	0.47	0.02	0.14	0.43	0.14	1.32
2GIY	0.07	3.03	0.08	0.33	1.59	0.36	8.85
2GKG	0.04	2.36	0.07	0.32	1.48	0.35	5.99
2GKV	0.04	2.66	0.06	0.28	0.94	0.21	8.24
2GOM	0.03	1.08	0.05	0.24	1.16	0.16	2.88
2GQV	0.02	0.93	0.03	0.18	0.75	0.11	2.38
2GXG	0.06	2.17	0.09	0.38	2.11	0.28	6.26
2H14	0.12	6.73	0.13	0.52	2.45	0.53	21.49
2H2R	0.07	3.09	0.08	0.32	1.68	0.27	7.53
2H2Z	0.13	6.66	0.17	0.51	3.04	0.65	18.95
2H7W	0.04	1.53	0.06	0.22	1.17	0.23	5.04
2H7Z	0.02	1.21	0.03	0.22	0.70	0.14	2.87
2H8E	0.07	3.15	0.08	0.35	1.79	0.28	5.98
2H8O	0.12	8.29	0.16	0.58	3.40	0.59	14.98
2HC8	0.02	1.40	0.05	0.24	0.72	0.21	4.46
2HLR	0.01	0.86	0.03	0.16	0.44	0.12	2.35
2HLY	0.09	4.22	0.11	0.42	2.16	0.45	10.60
2HOQ	0.15	5.93	0.16	0.55	3.23	0.55	14.80
2HPL	0.05	1.92	0.06	0.24	1.19	0.18	4.88
2HWW	0.07	2.88	0.10	0.39	1.68	0.29	8.44
2HY5	0.08	3.10	0.09	0.36	2.09	0.35	6.97
2HZF	0.05	2.08	0.07	0.27	1.48	0.24	5.28
2I3F	0.10	5.48	0.14	0.50	2.93	0.47	13.17
2I49	0.22	14.11	0.25	0.76	5.26	1.1	28.46
2I5D	0.09	3.51	0.13	0.38	2.69	0.38	10.20
2I6V	0.04	1.52	0.06	0.23	1.14	0.2	3.80
2IBL	0.02	1.08	0.05	0.22	0.76	0.15	3.14
2IC6	0.03	1.18	0.05	0.23	0.90	0.14	2.72
2IC7	0.09	3.63	0.10	0.39	2.23	0.36	9.11
2IIA	0.02	1.18	0.04	0.20	0.70	0.14	3.66
2IJK	0.02	0.84	0.03	0.17	0.59	0.15	2.19
2IP2	0.18	7.86	0.20	0.67	3.79	0.63	16.87
2IPR	0.05	2.52	0.07	0.28	1.22	0.26	6.94
2IRU	0.13	7.51	0.15	0.64	3.29	0.74	16.33
2IUM	0.05	3.04	0.09	0.30	1.46	0.3	10.40
2IXM	0.16	8.24	0.19	0.70	5.20	1.08	19.72
2IY9	0.12	7.01	0.13	0.54	2.78	0.67	17.98
2IZ6	0.03	1.91	0.05	0.26	0.82	0.2	6.59
2J2J	0.07	3.56	0.08	0.34	1.59	0.3	9.96
2J5Y	0.01	0.78	0.03	0.19	0.43	0.14	2.02
2J6B	0.03	1.90	0.06	0.27	1.08	0.24	4.97
2J71	0.10	2.29	0.07	0.28	1.52	0.91	5.06
2J8B	0.03	1.29	0.04	0.22	0.70	0.19	3.52
2J9W	0.06	2.27	0.07	0.31	1.37	0.37	5.36
2JCP	0.06	2.68	0.07	0.36	1.27	0.33	7.65
2NML	0.05	2.19	0.07	0.26	1.65	0.43	4.80

2NNU	0.09	4.06	0.13	0.37	2.50	0.53	11.94
2NPT	0.04	2.04	0.06	0.27	1.31	0.23	4.36
2NRR	0.12	2.68	0.10	0.43	2.35	0.39	7.33
2NV0	0.08	3.93	0.10	0.39	2.33	0.48	10.25
2O0Q	0.05	1.68	0.07	0.26	1.36	0.27	5.22
2O2K	0.22	10.65	0.22	0.86	5.35	1.21	21.26
2O6S	0.08	3.92	0.09	0.36	2.21	0.43	11.04
2O6X	0.17	8.45	0.20	0.65	4.59	0.96	20.88
2OEB	0.06	3.14	0.08	0.32	1.74	0.28	8.75
2OHW	0.06	2.39	0.09	0.32	1.91	0.28	6.94
2OIX	0.11	3.82	0.11	0.44	4.89	5.21	9.50
2OL7	0.07	4.79	0.10	0.45	1.96	0.49	11.30
2OSA	0.10	4.61	0.11	0.40	2.03	0.4	12.36
2OTU	0.04	1.46	0.06	0.22	1.10	0.22	5.10
2P1G	0.12	5.27	1.32	0.56	3.36	6.98	13.38
2P38	0.10	3.15	0.11	0.37	2.58	0.37	8.13
2P4H	0.12	7.32	0.15	0.60	2.69	0.62	18.05
2P52	0.11	5.85	0.12	0.50	3.49	0.52	11.70
2P5D	0.10	3.98	0.10	0.43	2.61	0.48	8.56
2P5K	0.03	1.02	0.04	0.21	1.18	0.19	2.84
2P65	0.08	3.72	0.11	0.41	2.07	0.34	9.16
2P84	0.08	2.96	0.09	0.33	2.57	1.49	6.69
2PBP	0.15	6.05	0.17	0.55	3.44	0.55	13.14
2PBQ	0.06	2.61	0.08	0.32	1.55	0.3	8.37
2PEF	0.17	10.75	0.21	0.63	3.50	0.91	29.02
2PET	0.12	5.17	0.14	0.48	2.89	0.54	11.27
2PGE	0.22	10.38	0.24	0.69	6.16	22.85	22.26
2PKF	0.16	8.55	0.17	0.59	3.89	1.32	17.46
2PMR	0.04	1.39	0.05	0.22	0.95	0.16	3.82
2PND	0.07	2.41	0.08	0.34	2.11	0.29	6.11
2PST	0.03	1.13	0.04	0.21	0.79	0.14	2.66
2PTV	0.06	2.54	0.07	0.33	1.92	0.25	4.96
2PV2	0.05	1.51	0.06	0.26	1.09	0.22	4.12
2Q8O	0.05	1.78	0.06	0.24	1.22	0.23	5.76
2QIY	0.07	2.72	0.08	0.33	1.60	0.66	7.17
2QOL	0.12	7.54	0.15	0.60	3.16	0.54	16.39
2QPW	0.07	3.14	0.08	0.31	1.50	0.27	7.27
2QR3	0.04	1.82	0.06	0.28	1.12	0.22	6.11
2QT4	0.02	1.15	0.04	0.21	0.61	0.12	3.02
2R6U	0.04	1.72	0.05	0.28	0.87	0.18	4.95
2R77	0.08	4.56	0.11	0.39	1.86	0.36	11.77
2R99	0.07	3.33	0.10	0.32	1.84	0.35	8.86
2RCZ	0.02	0.77	0.04	0.24	0.67	0.13	2.39
2RFA	0.09	4.71	0.12	0.40	2.42	0.44	12.20
2RIK	0.12	6.36	0.17	0.50	3.50	0.61	14.91
2RJD	0.16	9.61	0.18	0.65	3.95	0.69	19.70
2RK5	0.03	1.36	0.05	0.22	0.86	0.16	4.43
2VC8	0.02	0.72	0.03	0.17	0.45	0.15	2.85
2YXF	0.05	1.68	0.06	0.25	1.35	0.24	5.04
2YYV	0.09	4.54	0.11	0.43	2.42	0.39	12.87
2YZ1	0.04	1.39	0.05	0.26	0.83	0.18	4.81
2Z14	0.06	2.36	0.07	0.29	1.58	0.25	5.86
2Z1E	0.12	6.80	0.14	0.54	2.52	0.48	16.31

2Z37	0.13	5.62	0.12	0.52	2.08	0.42	14.67
2ZFY	0.14	6.12	0.17	0.52	3.91	0.57	14.90
3ADO	0.15	6.61	0.19	0.69	3.80	0.63	18.18
3BB7	0.12	6.78	0.14	0.54	2.57	0.6	19.50
3BN6	0.28	3.99	0.09	0.35	2.01	0.36	9.13
3C4S	0.01	0.86	0.03	0.16	0.60	0.1	2.29
3PHS	0.10	5.74	0.13	0.52	2.95	0.53	12.46
3SSW	0.05	1.41	0.07	0.27	1.37	0.21	4.27
4RWU	0.03	1.22	0.05	0.25	1.00	0.16	3.37
5WOF	0.03	1.47	0.05	0.22	1.05	0.21	3.88
6XIA	0.23	12.92	0.24	0.81	5.38	0.85	23.21
Total	34.30	1638.65	42.20	153.16	984.96	453.51	3871.18

Table S11. Protein side-chain packing results for 18 amino acid types in terms of χ_{1-4} recovery rate on 379 I-TASSER modeled backbones for the residues in three categories.

Residue	χ_{1-4} success rate (%)							
	FASPR	CISRR	RASP	SCATD	SCWRL4	SCWRL4v	ABACUS2	I-TASSER
All residues								
CYS	75.1	79.6	76.6	68.0	77.0	75.7	80.0	74.5
ASP	47.7	47.4	47.0	43.4	49.2	46.5	50.3	44.6
GLU	21.2	21.0	21.1	17.8	23.3	20.9	23.1	25.1
PHE	72.3	71.9	69.4	63.5	68.9	64.1	73.9	73.1
HIS	49.9	50.7	46.9	45.3	49.7	46.7	52.8	62.2
ILE	72.2	70.9	68.9	68.2	71.3	69.9	74.0	58.0
LYS	27.0	27.9	23.8	22.2	24.6	23.4	25.5	16.0
LEU	78.1	75.4	72.9	72.2	74.9	72.6	76.6	67.3
MET	36.3	37.6	33.0	29.3	35.2	32.1	38.8	39.8
ASN	45.3	42.3	44.2	36.9	44.0	42.8	45.4	44.5
PRO	63.6	62.0	64.9	64.0	63.2	63.3	65.1	61.8
GLN	23.2	21.2	22.2	15.8	25.3	22.6	24.6	28.5
ARG	19.8	19.1	17.4	10.5	20.4	16.2	19.2	20.3
SER	56.5	56.7	56.9	54.2	58.6	57.1	58.7	54.6
THR	78.4	75.9	75.9	73.1	77.2	75.9	77.7	59.6
VAL	84.2	82.7	82.2	82.4	83.9	82.7	85.2	74.1
TRP	62.6	63.8	56.4	41.0	57.4	52.4	69.2	72.1
TYR	67.4	66.9	64.3	59.5	65.3	63.3	70.1	67.9
Total	58.0	57.1	55.9	52.7	57.4	55.3	59.1	53.3
Core residues								
CYS	80.0	81.9	80.7	75.6	80.3	78.8	81.7	77.9
ASP	51.3	52.5	50.5	48.7	55.8	50.3	52.5	60.9
GLU	29.4	30.6	29.4	28.5	36.9	32.4	33.9	45.3
PHE	76.2	77.7	72.5	69.6	74.7	70.1	81.4	76.9
HIS	51.8	54.7	51.2	50.7	55.8	51.8	56.4	73.2
ILE	76.6	75.7	73.7	73.5	76.5	74.9	78.9	64.5
LYS	35.8	39.1	30.0	30.3	33.2	30.0	32.2	33.6
LEU	80.8	78.8	76.2	77.2	79.2	77.0	79.2	75.1
MET	43.4	45.1	39.4	39.6	46.3	41.3	48.6	51.2
ASN	52.0	52.4	51.3	45.8	48.0	46.7	55.5	65.9
PRO	72.4	71.9	72.0	70.8	70.3	71.7	72.9	71.0
GLN	32.2	33.6	27.6	27.0	35.5	35.2	34.2	52.0
ARG	28.3	27.9	26.0	20.3	34.3	27.4	31.1	38.7
SER	62.3	60.8	61.7	58.5	65.2	61.7	66.4	63.5
THR	83.6	82.9	83.2	79.3	84.6	83.1	86.3	69.3
VAL	87.8	87.0	86.3	86.0	87.8	86.3	89.6	80.1
TRP	68.7	73.9	63.0	50.9	65.3	60.3	79.2	77.7
TYR	71.8	71.9	70.2	64.6	70.3	68.6	76.5	71.9
Total	70.9	70.7	68.4	66.7	71.0	68.5	73.1	69.1
Surface residues								
CYS	60.0	64.6	63.1	44.6	66.2	61.5	64.6	63.1
ASP	44.3	43.7	44.7	39.4	44.7	42.3	46.9	34.7
GLU	17.7	17.3	17.5	13.7	17.7	17.2	17.6	16.1
PHE	59.4	53.2	56.3	45.1	50.5	47.1	55.6	61.8
HIS	42.3	41.4	39.2	35.4	40.4	39.5	42.3	45.8
ILE	59.5	58.5	55.3	54.5	58.2	56.8	59.9	39.9
LYS	22.0	23.2	19.9	17.6	20.3	20.1	20.9	9.8
LEU	67.6	65.0	64.8	58.7	62.1	59.8	66.0	46.1

MET	17.9	20.0	20.5	13.3	13.8	14.9	20.5	19.0
ASN	41.1	34.5	39.4	31.2	39.2	39.6	38.1	33.0
PRO	58.0	55.4	60.0	58.7	58.5	57.7	59.2	55.4
GLN	15.9	15.5	15.8	10.0	18.8	15.3	17.4	14.8
ARG	16.0	15.4	14.5	6.2	12.7	11.8	11.8	11.3
SER	53.5	54.5	53.7	50.6	55.2	54.2	51.7	46.6
THR	73.7	69.5	70.1	67.7	71.0	70.8	69.0	50.3
VAL	73.9	72.2	71.1	73.3	73.3	72.0	73.1	58.3
TRP	50.8	38.3	43.8	19.5	39.1	33.6	50.0	61.7
TYR	47.8	48.5	45.2	42.8	48.5	45.2	47.5	51.5
Total	44.0	42.5	42.8	38.5	42.9	41.7	43.1	35.5

Note: the total number of clashes in 379 I-TASSER and ABACUS2 structures is 0 and 132, respectively.

Table S12. Protein side-chain packing results for 18 amino acid types in terms of χ_{1-4} recovery rate on 379 perturbed backbones (RMSD = 0.21 Å) for the residues in three categories.

Residue	χ_{1-4} recovery rate (%)						
	FASPR	CISRR	RASP	SCATD	SCWRL4	SCWRL4v	ABACUS2
All residues							
CYS	85.4	90.5	90.7	76.4	88.9	89.5	91.4
ASP	59.0	57.3	58.3	52.1	61.4	58.5	60.5
GLU	28.7	26.5	27.0	20.7	29.9	27.2	30.4
PHE	83.2	81.6	78.5	70.8	79.8	76.1	86.0
HIS	60.1	61.2	55.6	53.2	60.4	54.9	64.3
ILE	83.5	84.8	82.4	79.8	83.9	82.6	86.2
LYS	32.6	33.3	31.3	25.6	30.9	28.9	32.7
LEU	85.1	85.6	82.9	79.1	83.9	82.8	86.5
MET	50.3	53.1	48.5	37.7	48.3	44.5	52.8
ASN	57.8	55.2	56.0	45.0	57.3	55.1	59.3
PRO	79.8	78.9	80.7	78.2	80.1	78.7	78.7
GLN	31.6	27.6	29.8	19.7	32.2	30.3	32.3
ARG	26.3	26.0	23.7	13.4	28.8	23.8	27.9
SER	69.7	68.7	69.0	65.8	70.7	69.7	71.6
THR	91.2	90.6	91.1	88.3	91.4	91.2	92.0
VAL	93.6	93.8	93.4	92.2	93.9	93.1	94.7
TRP	77.1	78.6	71.7	47.4	70.8	65.7	84.3
TYR	79.2	78.5	75.7	67.5	77.8	74.9	84.7
Total	68.4	68.0	66.9	61.2	68.3	66.3	70.2
Core residues							
CYS	87.9	92.2	90.7	82.4	89.2	90.0	90.9
ASP	56.4	60.1	57.2	54.4	65.2	59.7	66.2
GLU	38.1	39.6	37.2	31.5	45.6	40.5	42.3
PHE	84.9	84.0	79.5	74.4	83.0	79.0	89.2
HIS	60.7	64.5	56.9	56.6	66.1	59.3	66.9
ILE	86.5	88.6	84.8	83.5	86.5	85.3	89.4
LYS	40.1	41.7	38.1	31.6	36.5	32.9	38.1
LEU	86.6	88.3	84.6	82.5	86.2	85.1	88.4
MET	56.4	63.9	56.2	48.0	62.5	57.2	64.1
ASN	61.5	65.3	59.3	49.6	61.5	56.6	67.0
PRO	83.2	81.9	84.2	81.6	83.5	80.7	83.9
GLN	40.8	39.8	38.5	29.3	41.4	42.8	41.4
ARG	33.9	37.6	31.1	24.7	40.3	32.5	41.0
SER	74.5	71.9	71.6	70.2	74.6	71.9	78.2
THR	92.4	93.5	91.9	90.9	92.2	92.7	95.1
VAL	95.3	95.4	94.9	94.0	95.2	94.4	96.3
TRP	81.1	84.4	77.7	56.3	77.7	74.9	90.3
TYR	80.7	82.1	78.6	71.7	81.0	78.9	87.6
Total	79.3	80.6	77.6	73.9	79.9	77.7	82.7
Surface residues							
CYS	78.5	80.0	84.6	50.8	81.5	83.1	87.7
ASP	58.2	55.8	56.4	49.6	58.2	55.9	56.5
GLU	23.1	21.0	22.5	16.1	21.3	21.2	23.2
PHE	74.1	67.2	69.6	55.3	66.6	61.4	71.7
HIS	58.0	55.2	51.7	44.8	51.1	46.7	54.2
ILE	72.7	73.1	73.1	68.5	74.7	73.7	74.7
LYS	28.5	27.7	26.1	21.5	26.0	25.3	27.1

LEU	78.9	76.2	78.0	69.8	77.7	77.0	79.6
MET	33.3	33.3	32.8	21.0	24.1	24.1	34.4
ASN	54.4	47.9	52.3	40.8	53.0	51.5	54.2
PRO	76.9	75.7	77.4	76.5	76.9	76.4	74.7
GLN	24.5	20.9	21.3	14.2	23.8	21.5	23.3
ARG	22.1	19.9	19.9	7.9	22.0	16.9	19.9
SER	68.3	67.4	67.7	62.8	69.0	68.7	67.3
THR	91.3	89.7	90.2	86.7	90.9	90.5	89.7
VAL	87.9	88.3	88.1	87.0	89.3	89.5	88.7
TRP	71.1	64.8	59.4	26.6	54.7	51.6	64.8
TYR	69.2	65.2	66.6	57.5	65.6	60.2	71.6
Total	56.5	54.3	55.0	48.3	55.3	53.9	55.6

Table S13. Protein side-chain packing results for 18 amino acid types in terms of χ_{1-4} recovery rate on 379 perturbed backbones (RMSD = 0.57 Å) for the residues in three categories.

Residue	χ_{1-4} recovery rate (%)						
	FASPR	CISRR	RASP	SCATD	SCWRL4	SCWRL4v	ABACUS2
All residues							
CYS	82.7	86.3	86.6	73.8	86.0	86.7	86.3
ASP	57.2	54.8	56.1	50.4	58.7	56.6	56.8
GLU	25.9	24.3	24.8	19.4	26.0	23.9	26.3
PHE	79.3	77.6	74.9	68.4	75.1	71.3	79.5
HIS	55.9	57.7	52.8	50.7	54.1	50.1	58.0
ILE	80.5	79.6	77.8	76.0	79.4	78.5	80.5
LYS	30.5	30.9	28.5	24.2	29.2	27.2	29.8
LEU	82.1	79.6	77.8	76.6	79.3	77.2	80.8
MET	45.7	45.9	42.8	33.7	42.5	39.6	43.4
ASN	54.3	51.6	52.3	42.8	53.9	52.2	54.3
PRO	78.2	76.2	78.3	75.5	77.6	75.8	76.1
GLN	28.6	23.3	25.5	17.3	29.0	26.7	27.6
ARG	24.1	23.3	21.8	12.7	26.0	21.6	24.6
SER	67.0	66.3	66.6	63.0	68.2	67.6	67.0
THR	89.7	87.0	88.7	86.8	89.2	88.7	89.3
VAL	92.4	91.6	91.8	91.2	92.1	91.2	92.0
TRP	71.9	69.4	63.9	44.8	63.9	60.2	76.1
TYR	76.3	74.4	71.5	65.5	73.9	70.5	79.0
Total	65.8	64.2	63.6	59.0	64.9	62.9	65.6
Core residues							
CYS	85.1	87.5	86.6	78.4	87.3	87.5	87.0
ASP	53.8	54.0	54.4	50.5	58.5	54.8	54.0
GLU	32.7	33.0	30.6	27.9	33.9	31.8	30.3
PHE	79.4	80.6	76.1	71.4	77.9	72.9	82.4
HIS	53.4	58.8	49.9	52.8	57.7	50.9	59.6
ILE	82.5	81.9	78.9	79.0	81.5	80.3	82.0
LYS	36.2	39.7	35.8	28.7	34.2	30.3	35.5
LEU	83.5	80.8	78.3	78.5	81.0	78.3	81.3
MET	51.8	53.3	49.7	42.3	53.9	50.1	52.0
ASN	57.3	57.7	54.4	47.6	58.0	52.2	58.0
PRO	80.2	76.9	79.5	78.6	79.0	76.9	78.5
GLN	36.2	30.9	31.6	24.0	37.8	36.2	33.9
ARG	27.9	31.1	26.0	23.7	34.8	26.5	36.4
SER	66.4	64.7	64.0	62.6	67.3	66.4	66.7
THR	90.5	87.6	89.5	87.8	89.4	89.1	90.1
VAL	93.7	93.3	92.8	92.3	93.4	92.3	93.3
TRP	74.7	73.2	66.7	51.6	68.7	67.2	82.6
TYR	78.0	77.0	73.5	69.2	76.4	74.1	80.3
Total	75.5	74.8	72.7	70.3	75.1	72.7	75.9
Surface residues							
CYS	75.4	75.4	83.1	53.8	80.0	81.5	78.5
ASP	57.0	55.0	55.1	49.2	57.0	55.3	55.3
GLU	21.8	20.1	21.3	15.6	20.4	19.6	21.4
PHE	74.4	64.8	65.9	54.9	62.5	61.1	67.6
HIS	54.9	53.3	53.6	43.9	48.6	45.5	50.2
ILE	71.8	72.2	71.2	66.4	71.8	72.2	72.2
LYS	27.0	26.4	24.4	20.9	24.8	24.3	25.6

LEU	76.5	73.3	75.1	68.4	74.3	72.6	75.3
MET	31.3	32.3	32.8	22.6	24.6	24.1	30.3
ASN	51.4	47.5	50.5	39.3	50.2	49.8	51.5
PRO	76.7	75.0	76.8	75.2	76.7	74.8	74.7
GLN	24.4	19.4	20.9	13.2	21.8	20.9	21.1
ARG	22.0	17.9	18.8	7.8	19.6	17.3	19.5
SER	67.8	67.0	67.1	61.3	68.5	68.5	65.6
THR	90.7	88.9	89.5	87.5	89.6	89.2	89.2
VAL	87.9	87.6	87.8	87.0	88.1	87.6	87.6
TRP	66.4	59.4	59.4	29.7	54.7	49.2	63.3
TYR	65.2	63.2	64.2	55.9	64.2	58.5	68.9
Total	55.3	53.1	53.8	47.7	53.8	52.7	53.8

Table S14. Protein side-chain packing results for 18 amino acid types in terms of χ_{1-4} recovery rate on 379 perturbed backbones (RMSD = 0.93 Å) for the residues in three categories.

Residue	χ_{1-4} recovery rate (%)						
	FASPR	CISRR	RASP	SCATD	SCWRL4	SCWRL4v	ABACUS2
All residues							
CYS	81.1	82.0	84.0	72.9	82.5	82.7	79.6
ASP	54.8	53.1	54.0	49.1	56.6	54.2	53.6
GLU	25.1	22.0	22.4	18.1	25.4	22.6	24.3
PHE	73.7	71.0	68.7	64.8	67.9	64.5	71.8
HIS	54.0	53.5	49.2	48.4	52.1	47.9	53.8
ILE	75.8	72.4	72.2	72.2	74.4	72.5	74.2
LYS	29.2	28.7	26.1	22.6	26.7	25.3	26.6
LEU	78.9	72.9	73.1	73.9	74.6	73.0	75.6
MET	39.4	38.9	37.2	30.4	36.9	34.2	39.7
ASN	51.6	48.8	48.8	41.7	49.4	47.8	49.8
PRO	76.1	74.2	75.5	73.5	74.6	72.3	74.0
GLN	24.8	22.1	23.0	16.9	25.9	23.9	25.0
ARG	21.8	21.3	19.8	11.9	23.2	18.6	21.5
SER	64.7	63.7	63.8	61.2	65.4	65.3	64.7
THR	88.4	84.4	87.3	85.2	88.0	87.1	85.8
VAL	91.1	88.6	89.3	89.6	89.6	89.0	88.7
TRP	67.3	64.8	60.0	41.2	59.4	55.2	67.6
TYR	71.1	70.4	67.7	62.2	68.6	66.2	73.6
Total	63.0	60.4	60.3	57.0	61.5	59.5	61.5
Core residues							
CYS	83.0	83.4	84.3	78.3	83.7	83.4	80.2
ASP	48.9	51.3	50.7	48.5	55.4	52.5	50.5
GLU	34.5	28.2	25.5	27.0	31.8	26.1	29.7
PHE	73.7	72.2	68.8	67.6	68.7	65.3	72.1
HIS	51.8	55.0	49.3	47.7	53.9	49.9	56.9
ILE	76.7	73.0	72.9	74.0	75.2	73.0	74.4
LYS	30.3	31.6	25.7	22.8	27.0	24.8	24.1
LEU	79.1	71.9	72.9	76.0	75.2	73.6	75.0
MET	44.4	44.7	42.1	36.9	45.7	42.4	48.6
ASN	47.8	49.3	45.8	42.3	46.7	43.6	50.2
PRO	76.0	72.6	74.3	73.4	72.9	69.1	75.0
GLN	29.9	26.3	25.0	21.7	29.9	26.6	28.6
ARG	24.7	28.1	23.3	21.9	30.6	23.7	27.6
SER	62.4	60.6	60.9	59.8	62.8	62.9	64.9
THR	89.2	85.0	87.4	86.3	87.8	87.1	88.1
VAL	92.2	89.4	89.8	90.5	89.9	89.7	89.7
TRP	71.2	69.7	64.0	46.9	67.0	61.3	73.2
TYR	72.2	73.4	69.7	65.1	70.9	68.5	74.6
Total	71.4	68.8	68.0	67.1	69.8	67.7	70.2
Surface residues							
CYS	72.3	80.0	78.5	55.4	76.9	76.9	81.5
ASP	55.3	53.2	54.0	48.1	55.7	53.5	52.9
GLU	21.3	18.8	20.0	14.8	20.4	18.7	20.8
PHE	69.6	61.1	65.2	53.9	59.0	56.3	64.5
HIS	52.7	51.1	47.3	45.5	46.4	43.6	46.1
ILE	68.9	68.9	67.2	65.8	69.5	69.3	69.7
LYS	26.0	25.4	23.7	21.3	24.0	23.6	25.4

LEU	74.4	72.1	72.3	65.8	72.9	72.0	74.4
MET	28.7	26.7	28.7	20.5	22.6	23.1	27.7
ASN	51.6	46.2	48.8	39.5	48.3	48.1	49.3
PRO	74.2	73.4	75.9	73.7	74.0	72.7	73.4
GLN	20.4	19.5	20.2	13.2	21.2	20.4	20.8
ARG	21.6	17.2	18.6	8.2	18.7	15.2	18.0
SER	66.9	66.3	66.2	61.0	67.1	67.6	64.7
THR	90.1	87.3	88.5	85.8	89.0	88.6	87.3
VAL	87.2	85.6	85.5	85.8	87.6	86.1	86.2
TRP	64.1	58.6	57.0	28.1	52.3	50.8	54.7
TYR	63.2	60.9	61.2	54.2	59.2	54.2	66.9
Total	53.9	51.7	52.3	46.9	52.5	51.3	52.3

Table S15. Protein side-chain packing results for 18 amino acid types in terms of χ_{1-4} recovery rate on 379 perturbed backbones (RMSD = 1.48 Å) for the residues in three categories.

Residue	χ_{1-4} recovery rate (%)						
	FASPR	CISRR	RASP	SCATD	SCWRL4	SCWRL4v	ABACUS2
All residues							
CYS	75.8	77.9	77.5	67.2	78.2	78.3	72.4
ASP	52.7	50.1	52.1	47.1	53.2	53.8	50.6
GLU	22.3	20.7	20.6	17.2	23.3	23.7	20.2
PHE	65.2	62.9	62.6	60.1	59.8	60.3	61.7
HIS	50.0	48.6	43.1	44.5	46.4	46.6	46.0
ILE	69.6	64.9	65.4	66.1	66.8	66.8	66.7
LYS	25.3	25.7	23.8	20.7	24.3	24.5	24.5
LEU	73.9	64.5	65.3	69.3	67.3	67.5	67.0
MET	32.6	31.6	30.7	25.2	30.1	30.3	27.8
ASN	47.3	44.6	45.4	39.2	47.4	48.1	46.1
PRO	74.1	68.5	72.4	71.6	71.8	71.8	69.6
GLN	23.4	19.5	19.8	15.0	23.6	23.9	22.4
ARG	18.1	16.9	17.0	10.3	19.4	19.6	16.8
SER	63.2	61.1	61.4	59.4	62.5	62.6	61.2
THR	86.3	79.6	83.5	83.1	83.9	84.0	80.7
VAL	87.3	81.0	85.0	85.8	84.3	84.3	82.0
TRP	56.1	52.7	48.2	35.4	50.5	51.1	55.1
TYR	66.2	63.3	59.4	58.5	61.1	62.0	64.3
Total	58.9	54.9	55.6	53.8	56.6	56.9	55.5
Core residues							
CYS	77.1	80.0	79.0	71.3	78.1	78.1	72.4
ASP	43.8	44.6	45.2	44.2	47.3	48.3	41.5
GLU	25.8	23.7	23.4	22.2	30.3	30.3	21.6
PHE	64.7	62.3	60.6	60.7	59.3	59.9	60.7
HIS	47.2	44.4	39.8	43.4	47.7	47.7	46.1
ILE	69.5	64.5	64.8	65.6	66.6	66.7	66.2
LYS	27.0	28.3	27.0	21.5	26.4	26.7	27.0
LEU	72.9	62.2	63.5	70.4	65.8	66.1	64.8
MET	34.6	32.3	34.2	28.7	34.8	35.0	31.5
ASN	42.3	43.4	42.0	38.5	44.2	44.9	41.8
PRO	73.3	63.5	68.1	70.7	69.4	69.4	64.9
GLN	24.3	18.1	19.4	17.4	23.0	23.4	19.7
ARG	18.2	19.6	18.9	15.9	21.7	21.9	20.5
SER	59.2	54.3	55.1	56.1	57.1	57.2	56.3
THR	84.9	76.1	80.6	79.7	81.1	81.1	76.4
VAL	87.5	80.6	84.6	86.0	84.1	84.1	81.1
TRP	56.6	57.6	51.1	38.7	53.8	55.1	58.6
TYR	67.4	63.6	59.8	59.8	62.1	63.1	66.0
Total	65.3	60.2	60.9	61.5	62.3	62.6	60.8
Surface residues							
CYS	67.7	63.1	72.3	50.8	76.9	78.5	64.6
ASP	55.2	52.1	54.2	47.7	54.1	54.5	52.4
GLU	20.2	19.1	19.0	14.8	18.9	19.2	17.9
PHE	67.6	61.1	64.8	52.2	57.0	57.3	60.1
HIS	49.2	48.9	46.7	40.8	43.6	43.6	40.8
ILE	67.8	66.6	67.0	66.0	66.8	66.8	66.0
LYS	24.4	23.9	23.1	18.1	22.7	23.1	23.2

LEU	74.9	69.5	69.6	66.7	71.5	71.5	70.4
MET	25.6	27.2	28.7	20.0	23.1	23.6	25.1
ASN	48.8	43.8	47.0	38.5	48.1	48.7	48.4
PRO	74.1	71.8	74.3	72.7	72.6	72.8	71.2
GLN	20.9	17.7	19.1	12.1	21.1	21.3	19.7
ARG	18.0	15.2	17.1	7.6	17.6	17.6	16.6
SER	66.7	66.0	65.4	61.0	65.6	65.7	64.3
THR	88.4	84.8	86.4	85.8	87.1	87.2	84.4
VAL	85.0	82.5	85.2	84.5	84.7	84.7	82.8
TRP	55.5	44.5	42.2	24.2	46.9	46.9	50.0
TYR	58.9	56.9	53.5	53.5	52.2	52.5	56.9
Total	52.5	50.0	51.0	46.1	50.9	51.1	50.0

Table S16. Protein side-chain packing results for 18 amino acid types in terms of χ_{1-4} recovery rate on 379 perturbed backbones (RMSD = 1.88 Å) for the residues in three categories.

Residue	χ_{1-4} recovery rate (%)						
	FASPR	CISRR	RASP	SCATD	SCWRL4	SCWRL4v	ABACUS2
All residues							
CYS	74.5	72.9	75.1	66.9	76.5	75.1	69.4
ASP	52.1	48.4	50.3	47.5	52.5	50.5	49.5
GLU	20.7	19.0	19.8	16.1	20.0	19.1	20.1
PHE	62.9	58.6	59.9	57.2	54.5	51.9	57.9
HIS	48.1	45.9	43.9	43.7	45.1	41.9	45.0
ILE	67.4	60.8	62.6	64.0	63.8	63.0	63.2
LYS	25.0	24.5	22.6	21.5	23.8	22.1	22.8
LEU	71.6	59.6	63.0	67.2	64.0	63.9	63.1
MET	30.9	30.4	30.0	25.0	27.4	25.7	27.6
ASN	45.4	41.6	43.2	37.2	44.0	42.0	42.7
PRO	73.1	68.7	72.6	71.4	70.6	70.4	68.3
GLN	21.8	17.3	18.9	13.7	21.5	19.2	19.3
ARG	16.0	14.8	14.9	9.1	16.9	13.8	14.5
SER	61.7	59.3	61.2	57.8	62.5	62.5	59.9
THR	84.3	77.0	82.4	80.9	82.9	82.4	78.0
VAL	87.2	80.4	84.4	85.3	83.4	82.8	79.9
TRP	54.0	49.5	45.2	33.3	44.8	43.0	48.7
TYR	60.0	57.6	55.6	54.3	56.8	54.1	57.8
Total	57.2	52.3	54.1	52.4	54.4	53.2	52.9
Core residues							
CYS	75.6	73.2	75.8	71.3	77.3	75.2	69.6
ASP	42.6	41.5	39.9	44.8	45.8	42.8	41.1
GLU	21.6	18.6	20.1	18.3	21.6	18.3	21.0
PHE	61.4	55.9	58.3	57.3	52.7	50.7	56.9
HIS	43.9	44.7	43.4	40.4	42.8	41.5	42.3
ILE	67.3	59.6	61.5	64.3	63.1	62.3	62.8
LYS	25.7	24.1	22.8	22.5	20.2	21.8	22.5
LEU	70.3	56.0	60.2	67.6	61.4	61.8	60.3
MET	31.4	32.7	31.4	28.1	30.0	27.7	28.9
ASN	40.7	38.7	38.3	35.8	40.7	38.7	36.7
PRO	73.6	66.7	72.0	71.7	69.6	69.4	66.8
GLN	21.7	16.1	19.4	14.1	22.0	19.7	20.1
ARG	15.9	17.5	14.3	13.8	17.7	15.0	17.1
SER	58.6	53.1	56.7	56.0	58.6	59.3	57.4
THR	80.2	70.6	77.6	78.2	79.1	78.0	72.2
VAL	87.5	79.3	83.9	85.6	83.0	82.0	78.8
TRP	54.8	51.1	47.4	38.0	48.9	48.6	52.4
TYR	58.3	55.2	53.9	53.9	54.8	52.3	58.2
Total	63.0	56.2	58.6	59.8	59.0	58.0	57.6
Surface residues							
CYS	67.7	70.8	73.8	58.5	67.7	70.8	69.2
ASP	54.4	51.6	52.5	48.2	54.1	52.4	51.0
GLU	19.1	18.7	18.8	14.6	17.7	17.4	18.5
PHE	65.5	58.7	60.1	49.5	54.6	51.9	56.3
HIS	50.5	47.6	48.3	44.2	46.4	45.1	42.0
ILE	63.7	62.0	61.4	61.4	65.8	63.7	62.8
LYS	23.7	23.5	21.0	19.4	23.2	21.3	21.5

LEU	71.9	68.2	69.1	64.1	68.6	67.8	67.4
MET	27.7	28.2	26.7	20.0	21.5	22.1	23.6
ASN	48.3	42.1	46.1	38.5	46.4	44.4	45.6
PRO	72.1	69.1	73.1	71.9	71.0	70.6	69.1
GLN	20.8	17.6	18.5	12.0	19.9	17.6	17.4
ARG	16.4	14.4	16.0	7.3	15.5	13.3	13.5
SER	64.3	63.8	63.1	59.3	64.4	64.2	61.6
THR	88.1	83.2	85.7	84.1	85.8	85.5	82.7
VAL	85.9	81.3	83.9	83.8	83.9	83.3	82.4
TRP	60.9	49.2	44.5	23.4	43.8	35.2	46.1
TYR	57.5	53.2	52.5	52.8	55.2	52.2	52.8
Total	51.4	48.7	49.7	45.5	49.8	48.6	48.1

Table S17. Protein side-chain packing results for 18 amino acid types in terms of χ_{1-4} recovery rate on 379 perturbed backbones (RMSD = 2.38 Å) for the residues in three categories.

Residue	χ_{1-4} recovery rate (%)						
	FASPR	CISRR	RASP	SCATD	SCWRL4	SCWRL4v	ABACUS2
All residues							
CYS	71.4	69.5	70.6	63.9	72.5	72.1	64.1
ASP	50.1	47.2	48.2	45.2	49.7	47.8	46.6
GLU	20.3	19.5	18.9	15.7	20.4	19.3	19.6
PHE	58.5	56.1	54.9	54.2	51.6	47.9	53.5
HIS	46.0	44.6	39.6	40.1	42.8	39.2	41.4
ILE	63.2	57.3	58.6	60.6	60.2	58.7	59.0
LYS	22.8	22.6	20.5	20.0	21.5	20.6	21.3
LEU	68.1	55.6	59.5	64.9	61.0	60.8	59.3
MET	27.2	24.6	23.7	21.6	22.7	22.3	23.8
ASN	45.9	40.6	42.7	36.5	41.8	41.3	41.6
PRO	72.8	67.2	71.8	69.7	69.8	69.9	68.5
GLN	20.3	15.9	19.6	13.5	20.7	18.3	18.0
ARG	15.9	13.8	14.4	9.8	15.3	13.7	14.1
SER	59.9	57.8	59.0	57.4	60.1	60.8	57.3
THR	84.0	73.8	80.4	81.1	81.3	80.4	75.8
VAL	84.0	76.3	81.8	82.4	81.3	80.6	76.1
TRP	47.9	44.5	40.1	32.7	41.3	37.2	43.7
TYR	57.9	54.7	52.6	52.6	53.4	51.8	54.0
Total	55.0	49.8	51.6	50.7	52.1	51.0	50.2
Core residues							
CYS	72.4	66.7	68.4	66.2	70.3	69.9	61.2
ASP	42.6	40.7	40.9	40.9	44.2	41.8	37.9
GLU	18.3	15.3	16.5	15.6	19.8	17.4	14.4
PHE	57.4	55.2	51.9	54.3	49.0	45.9	52.4
HIS	42.3	42.3	36.3	34.7	42.8	38.5	38.2
ILE	60.7	54.0	55.8	59.3	57.4	55.7	56.2
LYS	17.6	18.2	15.3	20.5	17.9	17.9	17.9
LEU	66.8	52.1	56.6	64.9	58.4	58.3	55.9
MET	28.7	25.0	25.6	23.7	25.4	24.7	26.4
ASN	39.8	36.5	39.6	36.5	36.3	37.2	36.1
PRO	72.6	64.2	69.6	67.7	67.7	67.4	65.8
GLN	20.4	16.4	20.4	18.1	20.4	17.8	15.1
ARG	17.3	13.4	14.3	13.8	16.6	14.5	13.6
SER	56.4	52.1	54.1	55.7	55.7	55.4	52.5
THR	80.1	67.4	77.1	78.4	78.4	76.7	69.5
VAL	83.8	74.9	81.2	81.2	80.6	79.8	74.8
TRP	44.9	41.7	37.7	36.0	38.2	35.5	44.9
TYR	56.1	54.8	51.8	51.8	51.5	51.3	53.3
Total	59.7	52.6	55.0	56.9	55.7	54.5	53.1
Surface residues							
CYS	64.6	72.3	72.3	53.8	69.2	70.8	66.2
ASP	53.3	50.5	51.7	46.6	52.3	50.9	49.1
GLU	19.6	19.0	17.9	13.9	18.1	17.1	17.8
PHE	58.7	56.3	56.7	47.8	54.6	49.5	56.0
HIS	48.9	49.2	44.5	42.9	43.9	40.8	42.6
ILE	66.4	63.5	63.0	62.6	65.3	64.3	64.1
LYS	22.1	21.9	20.2	18.4	21.3	20.8	21.1

LEU	69.5	63.6	66.3	64.9	66.5	65.3	64.4
MET	20.5	23.1	20.5	19.0	19.0	18.5	23.6
ASN	48.4	41.2	46.8	37.7	45.0	44.5	45.8
PRO	72.5	68.9	72.6	71.4	71.2	70.9	69.3
GLN	20.4	17.0	19.8	11.2	19.2	16.3	18.1
ARG	15.9	13.8	14.4	8.2	14.2	13.3	13.8
SER	63.3	62.5	62.6	58.8	64.1	65.3	61.8
THR	87.9	81.4	84.5	85.6	85.3	84.9	82.6
VAL	85.6	80.8	82.5	83.2	83.6	83.5	80.7
TRP	53.9	47.7	43.8	28.1	46.1	38.3	43.0
TYR	55.5	52.8	49.8	48.8	53.8	49.8	53.5
Total	50.6	47.7	48.7	45.1	49.0	48.0	47.7

Table S18. Protein side-chain packing results for 18 amino acid types in terms of χ_{1-4} recovery rate on 379 perturbed backbones (RMSD = 2.55 Å) for the residues in three categories.

Residue	χ_{1-4} recovery rate (%)						
	FASPR	CISRR	RASP	SCATD	SCWRL4	SCWRL4v	ABACUS2
All residues							
CYS	70.9	66.1	68.5	62.4	71.0	70.2	62.9
ASP	49.0	45.2	47.1	44.6	49.0	47.1	45.0
GLU	18.1	17.6	17.4	14.9	19.5	17.3	18.6
PHE	56.1	54.0	54.1	52.2	50.2	47.4	49.0
HIS	43.5	43.5	36.6	39.4	40.1	36.2	40.7
ILE	62.9	55.0	57.4	59.3	58.4	57.4	57.8
LYS	22.4	21.2	21.1	20.1	21.5	20.1	20.1
LEU	67.4	54.4	58.7	63.7	58.9	58.9	59.7
MET	22.3	22.6	23.5	18.6	22.0	19.0	20.5
ASN	43.0	39.2	40.0	35.1	42.0	40.2	40.6
PRO	72.2	66.1	70.0	68.5	68.2	67.8	66.0
GLN	20.0	15.3	17.2	13.4	19.3	18.1	16.9
ARG	14.5	14.0	14.1	9.5	14.8	12.9	12.6
SER	58.9	57.7	57.9	57.3	59.9	60.4	56.0
THR	82.8	72.9	79.1	80.2	80.2	79.9	74.1
VAL	84.8	76.4	81.7	82.9	81.3	80.6	76.8
TRP	45.6	39.1	39.8	31.0	38.1	36.1	41.8
TYR	56.3	51.3	50.8	51.4	51.5	49.0	51.5
Total	53.9	48.5	50.5	49.9	51.0	49.8	49.0
Core residues							
CYS	71.8	65.0	67.1	66.0	70.7	69.4	61.1
ASP	40.3	37.7	35.4	38.1	40.1	38.1	34.6
GLU	17.4	17.7	15.6	17.4	19.8	18.3	20.1
PHE	54.5	52.0	51.0	52.1	48.7	45.6	49.2
HIS	38.8	37.4	31.2	34.7	35.5	33.3	36.0
ILE	60.4	51.6	54.9	58.2	55.7	55.0	55.3
LYS	17.6	16.6	16.6	16.6	16.9	17.9	16.0
LEU	64.5	48.7	54.5	61.7	55.0	54.9	53.8
MET	22.0	21.8	23.7	19.9	23.7	19.9	21.4
ASN	37.8	34.3	32.3	32.3	33.2	30.8	33.0
PRO	71.9	63.2	66.1	65.8	63.7	64.2	62.8
GLN	16.1	11.5	15.1	15.1	14.8	15.8	13.5
ARG	14.7	12.7	11.5	12.7	14.1	13.8	14.3
SER	52.1	49.8	50.3	53.6	51.4	52.8	49.5
THR	79.1	64.5	72.9	74.4	74.4	74.1	66.9
VAL	84.7	74.5	80.5	81.6	80.1	79.0	74.7
TRP	46.2	39.5	38.5	32.8	39.0	39.5	42.2
TYR	55.7	50.5	49.3	50.1	48.5	48.4	51.0
Total	58.2	50.2	52.8	55.0	53.4	52.6	51.4
Surface residues							
CYS	70.8	69.2	78.5	52.3	75.4	75.4	66.2
ASP	51.9	48.6	50.0	46.1	51.4	49.5	48.3
GLU	18.1	17.1	17.6	13.2	17.6	16.5	17.3
PHE	58.7	57.0	58.0	47.8	51.2	49.1	50.9
HIS	47.3	47.3	41.4	41.4	40.8	38.9	41.1
ILE	65.6	62.8	62.2	61.2	63.5	62.8	63.5
LYS	22.1	21.0	20.8	18.5	21.0	19.8	21.3

LEU	72.6	67.7	69.1	67.0	68.7	67.2	69.7
MET	21.5	22.6	24.6	17.4	18.5	17.4	19.5
ASN	46.9	42.1	44.5	38.0	45.3	43.9	45.0
PRO	72.9	68.7	72.2	70.7	71.1	69.9	69.1
GLN	20.4	17.3	17.4	13.1	17.9	18.1	15.8
ARG	14.9	13.9	15.1	7.4	13.9	12.8	12.1
SER	64.2	63.6	62.5	60.3	65.6	66.2	59.6
THR	87.3	81.8	84.4	85.7	86.2	85.8	81.1
VAL	83.8	80.4	82.2	84.5	82.4	82.2	80.4
TRP	50.8	45.3	43.8	23.4	41.4	32.0	45.3
TYR	53.8	53.5	49.2	52.8	52.2	46.8	49.5
Total	50.2	47.6	48.4	45.3	48.7	47.7	46.9

Table S19. Protein side-chain packing results for 18 amino acid types in terms of χ_{1-4} recovery rate on 379 perturbed backbones (RMSD = 2.74 Å) for the residues in three categories.

Residue	χ_{1-4} recovery rate (%)						
	FASPR	CISRR	RASP	SCATD	SCWRL4	SCWRL4v	ABACUS2
All residues							
CYS	71.4	63.7	66.9	64.0	69.3	68.6	60.0
ASP	48.8	46.5	47.3	44.0	49.5	46.9	45.3
GLU	18.5	17.3	17.7	14.9	18.7	17.3	17.5
PHE	52.8	50.4	52.4	51.2	47.0	45.0	48.4
HIS	44.0	42.4	39.3	38.4	39.9	36.1	39.6
ILE	59.5	53.4	55.2	57.7	56.9	55.9	56.0
LYS	20.8	20.2	18.5	18.5	19.5	18.5	19.5
LEU	65.7	51.2	56.2	61.7	57.3	56.4	56.8
MET	22.2	21.6	21.8	21.2	21.7	19.9	18.8
ASN	43.5	38.4	40.8	35.5	40.7	39.2	39.6
PRO	72.1	67.0	71.3	69.3	69.2	69.2	67.3
GLN	18.1	15.9	17.5	12.7	19.0	17.2	17.2
ARG	13.8	13.1	13.7	8.1	14.4	12.4	12.6
SER	60.4	57.8	58.5	56.9	60.6	61.0	59.0
THR	82.6	72.6	78.8	79.0	79.7	79.6	74.1
VAL	83.8	73.9	80.4	81.6	79.1	78.6	74.4
TRP	43.8	39.4	38.1	31.2	38.7	36.6	38.0
TYR	53.7	53.7	50.2	51.0	50.3	48.9	52.1
Total	52.9	47.5	49.7	49.1	50.1	49.0	48.2
Core residues							
CYS	72.2	63.3	67.3	65.8	68.1	67.7	59.4
ASP	38.7	37.5	37.3	38.9	42.2	38.3	34.6
GLU	15.9	14.7	16.5	16.2	18.6	16.2	16.2
PHE	50.8	48.6	48.8	50.1	45.0	43.2	47.3
HIS	37.1	36.9	35.2	34.1	36.9	31.4	33.3
ILE	56.5	49.8	52.5	55.8	53.8	53.4	53.4
LYS	14.7	15.6	14.7	15.6	17.6	16.6	18.6
LEU	63.3	45.7	52.2	60.3	53.2	52.8	52.6
MET	22.0	19.5	19.9	21.6	22.9	22.2	19.5
ASN	36.3	32.1	34.5	31.2	34.1	33.6	31.9
PRO	72.6	63.9	71.2	68.1	68.4	68.9	63.9
GLN	15.1	11.5	15.1	12.8	16.4	15.1	13.5
ARG	12.9	13.1	13.4	11.3	15.4	12.2	14.1
SER	56.1	49.5	52.3	52.3	55.4	55.6	52.3
THR	78.1	64.9	72.7	75.4	73.3	73.4	66.7
VAL	83.5	71.0	79.4	80.2	78.5	77.6	71.9
TRP	44.4	37.0	37.7	31.3	37.2	36.0	37.2
TYR	50.7	50.4	46.5	49.0	46.0	46.6	49.2
Total	56.6	48.3	52.0	54.0	52.5	51.7	50.1
Surface residues							
CYS	70.8	63.1	64.6	61.5	64.6	66.2	67.7
ASP	52.4	49.9	50.4	44.7	51.1	48.9	48.1
GLU	17.8	17.6	17.2	14.1	16.6	16.8	16.6
PHE	59.4	57.7	60.1	47.8	50.9	46.4	53.2
HIS	47.3	46.1	42.9	39.8	39.8	38.9	40.1
ILE	63.9	62.4	60.3	60.5	63.5	61.8	59.1
LYS	21.5	20.4	19.7	18.0	19.1	18.4	20.6

LEU	69.1	64.0	66.2	63.4	66.5	65.0	64.2
MET	19.5	21.5	22.6	21.0	17.9	15.9	15.4
ASN	46.6	41.8	43.9	37.3	44.2	43.0	44.5
PRO	73.1	70.6	72.7	72.0	71.9	71.3	70.8
GLN	19.2	17.7	19.1	12.0	19.4	17.9	18.0
ARG	16.0	13.3	15.6	6.8	13.3	11.9	12.0
SER	61.9	61.7	61.4	57.7	63.5	64.0	60.6
THR	87.2	80.9	83.5	83.8	86.4	85.7	81.6
VAL	83.8	80.1	82.7	83.0	81.5	81.6	79.8
TRP	45.3	42.2	41.4	26.6	41.4	41.4	39.8
TYR	55.5	56.5	51.8	51.2	53.2	47.2	52.2
Total	49.7	47.3	48.1	44.5	48.0	47.0	46.6

Table S20. Protein side-chain packing results for 18 amino acid types in terms of χ_{1-4} recovery rate on 379 perturbed backbones (RMSD = 2.95 Å) for the residues in three categories.

Residue	χ_{1-4} recovery rate (%)						
	FASPR	CISRR	RASP	SCATD	SCWRL4	SCWRL4v	ABACUS2
All residues							
CYS	69.2	63.1	66.0	60.0	70.0	68.9	60.6
ASP	48.6	44.6	47.0	43.6	48.1	47.5	44.8
GLU	18.5	17.0	16.1	15.5	17.9	16.7	16.7
PHE	55.8	51.3	53.5	52.0	48.9	45.9	48.4
HIS	42.4	40.9	38.5	38.1	39.9	34.5	38.4
ILE	60.2	53.3	55.0	57.3	57.0	55.5	55.2
LYS	22.4	22.2	19.5	19.6	21.0	19.7	20.0
LEU	65.6	51.0	56.3	62.8	56.9	57.0	56.3
MET	23.0	20.3	22.3	18.7	20.5	20.3	18.3
ASN	42.8	36.5	39.8	34.1	39.0	38.5	39.1
PRO	72.9	65.3	71.0	68.6	69.5	68.6	66.6
GLN	19.7	15.0	16.3	11.6	18.7	16.3	16.2
ARG	14.7	12.2	13.2	9.5	14.3	13.0	13.3
SER	58.2	56.2	57.4	56.3	59.5	60.0	55.4
THR	82.6	71.7	78.9	80.2	79.8	79.4	74.0
VAL	83.2	73.8	79.5	80.8	78.4	78.7	74.4
TRP	42.5	37.8	35.4	27.1	35.3	34.7	37.4
TYR	52.8	49.0	48.5	49.4	48.1	45.5	48.9
Total	53.0	46.7	49.3	48.9	49.7	48.8	47.5
Core residues							
CYS	69.6	63.3	66.9	63.7	68.6	69.0	60.1
ASP	37.5	33.6	36.5	36.0	38.3	39.9	32.0
GLU	16.2	14.1	14.7	15.0	14.4	14.7	10.5
PHE	52.8	47.6	49.3	49.9	46.3	43.2	45.7
HIS	36.9	35.0	33.9	33.1	36.6	29.5	31.7
ILE	57.4	49.4	51.9	56.1	54.8	52.6	52.5
LYS	20.5	17.6	16.9	18.2	18.2	17.3	17.9
LEU	64.0	46.1	53.3	62.1	54.0	54.4	53.3
MET	22.8	17.4	22.9	18.7	21.6	20.7	19.5
ASN	36.3	31.9	31.4	31.0	33.8	30.5	32.1
PRO	69.3	58.3	64.1	61.8	61.5	60.8	62.0
GLN	20.1	10.9	14.5	11.8	17.4	14.5	11.8
ARG	15.7	12.9	12.9	13.6	15.2	14.1	15.4
SER	52.4	46.9	51.5	51.7	53.6	55.2	48.1
THR	78.2	64.3	73.8	75.9	74.5	74.7	67.1
VAL	82.6	71.5	78.7	79.3	77.6	77.4	72.3
TRP	41.2	36.5	34.7	31.3	35.2	36.2	36.0
TYR	50.7	47.3	47.4	48.4	45.2	44.9	47.4
Total	56.6	47.5	51.8	53.7	52.1	51.4	49.4
Surface residues							
CYS	69.2	64.6	64.6	52.3	70.8	66.2	63.1
ASP	51.9	49.0	49.9	46.1	51.4	50.2	49.0
GLU	18.3	17.7	16.4	14.2	16.8	15.4	17.0
PHE	59.0	51.2	57.0	48.1	49.8	46.8	52.2
HIS	47.3	47.0	42.6	40.1	41.1	37.0	43.9
ILE	64.5	60.8	58.9	62.4	61.2	61.6	59.7
LYS	23.2	21.5	19.9	19.6	20.6	20.0	20.8

LEU	68.7	60.9	61.3	64.1	63.7	62.1	63.4
MET	20.0	23.6	19.5	17.4	16.9	18.5	17.4
ASN	46.9	39.7	43.6	37.0	41.6	41.8	44.4
PRO	75.5	68.5	74.1	72.9	73.3	71.8	71.0
GLN	19.4	16.5	15.6	11.3	18.0	15.9	15.9
ARG	15.3	12.4	14.0	7.8	14.4	12.8	14.4
SER	62.6	63.0	62.1	58.6	63.3	63.7	60.3
THR	88.0	82.2	85.2	85.3	86.6	86.6	82.7
VAL	83.3	78.4	81.5	82.1	80.7	80.4	79.1
TRP	46.1	43.8	40.6	18.0	40.6	39.1	41.4
TYR	54.5	49.5	49.8	48.2	50.5	45.8	48.2
Total	50.1	46.5	47.4	44.9	47.8	46.8	46.8

Table S21. Protein side-chain packing results for 18 amino acid types in terms of χ_{1-4} recovery rate on 379 perturbed backbones (RMSD = 3.68 Å) for the residues in three categories.

Residue	χ_{1-4} recovery rate (%)						
	FASPR	CISRR	RASP	SCATD	SCWRL4	SCWRL4v	ABACUS2
All residues							
CYS	68.1	63.7	66.4	60.4	68.8	66.7	56.4
ASP	47.7	43.7	46.1	42.2	47.8	46.1	44.0
GLU	17.1	16.7	16.7	15.3	17.1	16.6	16.3
PHE	50.0	45.9	48.7	48.9	44.4	41.7	43.4
HIS	43.2	40.0	37.7	35.9	38.2	35.7	37.0
ILE	56.5	49.6	50.5	53.7	52.9	51.6	51.9
LYS	21.1	21.0	19.0	19.0	20.5	19.7	18.7
LEU	63.1	47.4	53.6	59.8	54.4	54.3	52.8
MET	21.6	19.6	18.7	17.5	19.0	18.0	17.2
ASN	41.0	36.3	38.7	33.5	38.4	36.9	37.3
PRO	71.1	63.9	68.4	67.2	68.1	66.7	66.2
GLN	17.7	14.3	15.9	11.7	19.2	17.2	15.7
ARG	12.5	10.5	11.9	7.3	12.5	10.6	10.9
SER	58.3	55.7	56.4	56.1	59.0	59.3	55.8
THR	79.8	69.9	77.0	78.8	77.9	78.0	71.4
VAL	82.5	71.5	78.2	78.7	77.3	76.9	71.8
TRP	39.2	35.3	32.4	25.1	33.8	30.0	33.5
TYR	50.0	49.0	44.4	46.8	45.0	42.1	46.2
Total	51.0	44.9	47.3	47.2	48.0	46.9	45.4
Core residues							
CYS	67.7	63.3	64.8	62.2	67.3	65.8	54.4
ASP	37.9	35.0	35.6	33.4	39.3	37.5	33.2
GLU	14.4	12.3	15.9	14.7	14.4	13.8	13.2
PHE	48.0	42.4	46.7	48.1	42.3	39.3	41.6
HIS	35.8	32.5	33.1	29.3	33.9	31.2	32.0
ILE	53.6	45.9	47.7	50.5	49.6	48.3	47.9
LYS	19.2	17.9	16.9	17.9	17.9	17.6	14.3
LEU	59.7	40.7	48.3	57.0	49.5	49.8	47.3
MET	19.9	17.0	18.5	18.9	20.7	18.7	17.0
ASN	34.3	30.1	29.4	29.0	27.4	26.8	27.7
PRO	68.9	58.7	64.2	63.9	63.7	63.4	61.8
GLN	16.1	11.2	14.1	9.9	16.1	13.8	13.2
ARG	12.4	9.9	10.8	9.2	11.1	9.9	10.6
SER	53.8	48.3	50.7	50.1	53.1	54.9	50.2
THR	71.4	58.1	68.7	72.6	67.6	69.8	61.2
VAL	81.6	69.0	77.2	77.3	75.9	75.8	69.3
TRP	37.2	31.0	30.0	23.3	32.3	29.3	31.3
TYR	46.6	44.4	40.7	41.9	40.7	38.5	42.1
Total	53.8	44.6	48.7	50.4	49.0	48.3	45.9
Surface residues							
CYS	64.6	66.2	61.5	52.3	63.1	63.1	56.9
ASP	51.4	47.9	50.4	45.0	51.4	49.4	48.0
GLU	17.9	16.8	16.1	14.4	16.4	15.6	16.7
PHE	59.4	51.9	55.3	47.4	49.1	46.8	51.5
HIS	46.4	46.4	41.7	38.6	41.4	39.2	36.1
ILE	62.4	59.1	57.6	60.3	61.2	60.8	63.0
LYS	20.9	21.3	19.8	18.6	20.4	19.9	20.3

LEU	67.0	61.5	65.1	63.7	64.8	63.2	64.0
MET	22.1	20.0	20.0	17.4	14.4	15.4	17.4
ASN	45.4	39.1	43.8	35.7	43.9	42.5	42.9
PRO	73.1	68.7	71.1	70.9	71.7	69.3	69.0
GLN	16.5	15.9	13.9	10.3	17.0	15.2	14.9
ARG	13.9	10.7	13.6	6.2	13.5	12.0	12.6
SER	62.1	61.9	61.5	59.2	63.3	63.6	59.3
THR	85.5	80.4	83.3	84.9	84.6	84.4	79.7
VAL	83.5	76.5	79.9	80.7	79.9	79.4	76.2
TRP	46.1	43.0	34.4	21.1	37.5	34.4	38.3
TYR	52.5	51.2	44.8	48.8	45.8	42.5	48.5
Total	48.8	45.7	46.7	44.2	47.3	46.2	45.5

Table S22. The total number of clashes in the repacked structures based on perturbed backbones.

RMSD (Å)	#Clash in 379 structures repacked by different methods						
	FASPR	CISRR	RASP	SCATD	SCWRL4	SCWRL4v	ABACUS2
0.21	174	74	872	1532	581	235	50
0.57	537	231	1974	2834	1273	1019	211
0.93	1126	739	3419	5126	2366	2369	753
1.48	4538	2447	7750	9988	5747	6006	2508
1.88	5899	3353	9269	12120	7450	7657	3474
2.38	7922	4934	12602	15751	9870	10386	4933
2.55	9126	5562	14241	17661	11519	11983	5798
2.74	9864	6492	15383	18895	12547	13000	6711
2.95	10180	6272	15269	19106	12588	13189	6562
3.68	13426	8828	20418	24071	16868	17586	9239

Table S23. The number and the ratio of rotamers eliminated in different searching steps.

PDB ID	#rotamer	Self-energy check		Goldstein DEE		Split DEE		Tree Decomposition	
		Number	Ratio (%)	Number	Ratio (%)	Number	Ratio (%)	Number	Ratio (%)
1AHO	505	19	3.76	440	87.13	0	0.00	46	9.11
1ATZ	1269	157	12.37	1006	79.28	8	0.63	98	7.72
1B2P	893	93	10.41	699	78.28	56	6.27	45	5.04
1B8Z	603	25	4.15	462	76.62	52	8.62	64	10.61
1B9W	787	74	9.40	686	87.17	0	0.00	27	3.43
1BGF	1299	85	6.54	934	71.90	171	13.16	109	8.39
1BYI	1522	198	13.01	1208	79.37	1	0.07	115	7.56
1C02	1556	100	6.43	1195	76.80	144	9.25	117	7.52
1C48	539	54	10.02	402	74.58	53	9.83	30	5.57
1CEI	794	81	10.20	638	80.35	7	0.88	68	8.56
1DPT	846	52	6.15	669	79.08	63	7.45	62	7.33
1DQ0	1660	185	11.14	1315	79.22	45	2.71	115	6.93
1DV7	1758	178	10.13	1196	68.03	125	7.11	259	14.73
1DYS	2738	375	13.70	1999	73.01	102	3.73	262	9.57
1E5M	2847	346	12.15	2100	73.76	91	3.20	310	10.89
1E6F	910	129	14.18	724	79.56	0	0.00	57	6.26
1EDQ	4072	604	14.83	2996	73.58	168	4.13	304	7.47
1ELK	1276	120	9.40	1085	85.03	24	1.88	47	3.68
1ERZ	2573	307	11.93	1862	72.37	186	7.23	218	8.47
1ES5	1649	291	17.65	1276	77.38	21	1.27	61	3.70
1ES9	1880	224	11.91	1468	78.09	55	2.93	133	7.07
1F41	818	93	11.37	618	75.55	79	9.66	28	3.42
1F60	3605	435	12.07	2757	76.48	99	2.75	314	8.71
1F94	514	84	16.34	351	68.29	1	0.19	78	15.18
1FCQ	3076	455	14.79	2040	66.32	177	5.75	404	13.13
1FO9	2970	504	16.97	1878	63.23	280	9.43	308	10.37
1FPO	1803	181	10.04	1311	72.71	112	6.21	199	11.04
1FTR	2304	313	13.59	1750	75.95	85	3.69	156	6.77
1FVK	1603	124	7.74	1268	79.10	118	7.36	93	5.80
1G61	1590	172	10.82	1278	80.38	32	2.01	108	6.79
1G8A	2040	228	11.18	1494	73.24	83	4.07	235	11.52
1G8Q	735	59	8.03	647	88.03	3	0.41	26	3.54
1GMU	1088	101	9.28	877	80.61	20	1.84	90	8.27
1GO3	1501	118	7.86	1176	78.35	23	1.53	184	12.26
1GPP	1935	231	11.94	1341	69.30	188	9.72	175	9.04
1GQN	1948	192	9.86	1442	74.02	134	6.88	180	9.24
1GS9	1602	174	10.86	1065	66.48	211	13.17	152	9.49
1GSO	3067	382	12.46	2341	76.33	122	3.98	222	7.24
1GVP	701	51	7.28	575	82.03	17	2.43	58	8.27
1GXN	2457	449	18.27	1780	72.45	59	2.40	169	6.88
1H03	910	81	8.90	763	83.85	4	0.44	62	6.81
1H4A	1680	235	13.99	1251	74.46	57	3.39	137	8.15
1H4Y	982	78	7.94	741	75.46	91	9.27	72	7.33
1HCL	2441	323	13.23	1838	75.30	78	3.20	202	8.28
1HM5	4711	619	13.14	3488	74.04	189	4.01	415	8.81
1HZ6	517	36	6.96	481	93.04	0	0.00	0	0.00
1HZ9	586	57	9.73	465	79.35	0	0.00	64	10.92
1I4J	963	59	6.13	791	82.14	39	4.05	74	7.68

1IGQ	517	39	7.54	434	83.95	6	1.16	38	7.35
1IJQ	2334	302	12.94	1853	79.39	58	2.49	121	5.18
1IJY	1112	128	11.51	832	74.82	24	2.16	128	11.51
1ILK	1549	80	5.16	1237	79.86	90	5.81	142	9.17
1IU8	1591	163	10.25	1261	79.26	57	3.58	110	6.91
1J23	1115	78	7.00	881	79.01	61	5.47	95	8.52
1J2A	1314	135	10.27	1064	80.97	28	2.13	87	6.62
1J7G	1257	139	11.06	1028	81.78	1	0.08	89	7.08
1JB3	1189	133	11.19	870	73.17	47	3.95	139	11.69
1JCD	408	1	0.25	380	93.14	0	0.00	27	6.62
1JKS	2569	305	11.87	1913	74.46	154	5.99	197	7.67
1JY2	400	9	2.25	373	93.25	0	0.00	18	4.50
1K33	687	30	4.37	561	81.66	4	0.58	92	13.39
1KMT	1137	137	12.05	831	73.09	44	3.87	125	10.99
1KMZ	961	120	12.49	753	78.36	25	2.60	63	6.56
1KN3	1524	245	16.08	1097	71.98	70	4.59	112	7.35
1KOE	1351	180	13.32	980	72.54	49	3.63	142	10.51
1KPT	822	143	17.40	635	77.25	5	0.61	39	4.74
1KU8	894	119	13.31	732	81.88	5	0.56	38	4.25
1KVA	1405	129	9.18	1037	73.81	55	3.91	184	13.10
1KVE	383	29	7.57	320	83.55	0	0.00	34	8.88
1KYF	2198	178	8.10	1626	73.98	196	8.92	198	9.01
1KZQ	1641	206	12.55	1371	83.55	4	0.24	60	3.66
1L3K	1567	193	12.32	1188	75.81	47	3.00	139	8.87
1LBV	2085	260	12.47	1412	67.72	104	4.99	309	14.82
1LM5	1585	210	13.25	1093	68.96	93	5.87	189	11.92
1LTU	2256	327	14.49	1634	72.43	119	5.27	176	7.80
1M5T	1104	76	6.88	923	83.61	0	0.00	105	9.51
1M6J	2037	297	14.58	1547	75.95	11	0.54	182	8.93
1MD6	1144	94	8.22	991	86.63	15	1.31	44	3.85
1MF7	1855	179	9.65	1304	70.30	218	11.75	154	8.30
1MG7	3087	356	11.53	2335	75.64	164	5.31	232	7.52
1MIX	2013	188	9.34	1518	75.41	128	6.36	179	8.89
1MKK	905	47	5.19	647	71.49	51	5.64	160	17.68
1MML	2092	274	13.10	1580	75.53	80	3.82	158	7.55
1MOL	919	62	6.75	705	76.71	56	6.09	96	10.45
1N1J	787	56	7.12	639	81.19	4	0.51	88	11.18
1N93	2637	303	11.49	2085	79.07	42	1.59	207	7.85
1NAR	2535	273	10.77	1911	75.38	125	4.93	226	8.92
1NM8	4984	541	10.85	3660	73.43	216	4.33	567	11.38
1NWA	1471	212	14.41	1000	67.98	125	8.50	134	9.11
1NXM	1747	197	11.28	1290	73.84	145	8.30	115	6.58
1OAI	604	48	7.95	502	83.11	32	5.30	22	3.64
1OAQ	931	102	10.96	586	62.94	127	13.64	116	12.46
1OGM	4076	618	15.16	2848	69.87	243	5.96	367	9.00
1OK7	3139	313	9.97	2177	69.35	273	8.70	376	11.98
1P1X	1862	209	11.22	1477	79.32	52	2.79	124	6.66
1P9H	1022	89	8.71	871	85.23	1	0.10	61	5.97
1PCF	693	46	6.64	612	88.31	0	0.00	35	5.05
1PDO	993	84	8.46	838	84.39	49	4.93	22	2.22
1PE9	2565	302	11.77	2072	80.78	70	2.73	121	4.72
1PGV	1642	150	9.14	1219	74.24	27	1.64	246	14.98
1PM4	949	64	6.74	665	70.07	57	6.01	163	17.18

1PXZ	2656	356	13.40	1941	73.08	191	7.19	168	6.33
1QAH	848	114	13.44	689	81.25	1	0.12	44	5.19
1QKD	533	83	15.57	406	76.17	1	0.19	43	8.07
1R12	2084	178	8.54	1732	83.11	11	0.53	163	7.82
1R29	1046	90	8.60	883	84.42	12	1.15	61	5.83
1R77	830	127	15.30	629	75.78	13	1.57	61	7.35
1R8N	1433	175	12.21	1035	72.23	67	4.68	156	10.89
1RFY	739	56	7.58	642	86.87	0	0.00	41	5.55
1RGX	655	57	8.70	528	80.61	30	4.58	40	6.11
1RL0	2155	253	11.74	1513	70.21	103	4.78	286	13.27
1RWZ	2017	200	9.92	1589	78.78	80	3.97	148	7.34
1RYL	1444	167	11.57	1090	75.48	68	4.71	119	8.24
1RZ2	2144	248	11.57	1584	73.88	131	6.11	181	8.44
1S7I	985	48	4.87	835	84.77	2	0.20	100	10.15
1S7K	1456	119	8.17	1112	76.37	77	5.29	148	10.16
1SAU	1094	98	8.96	853	77.97	63	5.76	80	7.31
1SH8	1369	118	8.62	885	64.65	93	6.79	273	19.94
1SMX	771	49	6.36	644	83.53	9	1.17	69	8.95
1SNT	2818	421	14.94	1988	70.55	127	4.51	282	10.01
1SQE	1098	86	7.83	859	78.23	66	6.01	87	7.92
1SRV	1139	122	10.71	839	73.66	10	0.88	168	14.75
1SUU	2450	369	15.06	1864	76.08	69	2.82	148	6.04
1SWH	723	78	10.79	572	79.11	22	3.04	51	7.05
1T1J	1077	122	11.33	783	72.70	50	4.64	122	11.33
1TJE	2013	200	9.94	1440	71.54	193	9.59	180	8.94
1TKS	1650	209	12.67	1247	75.58	55	3.33	139	8.42
1TP6	1031	142	13.77	730	70.81	49	4.75	110	10.67
1TUA	1859	209	11.24	1394	74.99	98	5.27	158	8.50
1TUO	3230	478	14.80	2123	65.73	259	8.02	370	11.46
1TY0	1858	199	10.71	1410	75.89	60	3.23	189	10.17
1TZV	1502	121	8.06	1036	68.97	173	11.52	172	11.45
1U07	843	45	5.34	653	77.46	10	1.19	135	16.01
1U2H	943	68	7.21	649	68.82	112	11.88	114	12.09
1U5X	1023	109	10.65	709	69.31	56	5.47	149	14.57
1UEB	1482	158	10.66	1174	79.22	52	3.51	98	6.61
1UEK	1920	185	9.64	1362	70.94	107	5.57	266	13.85
1UJN	2347	261	11.12	1802	76.78	100	4.26	184	7.84
1UKF	1547	212	13.70	1034	66.84	95	6.14	206	13.32
1ULN	675	93	13.78	513	76.00	8	1.19	61	9.04
1ULR	765	107	13.99	575	75.16	1	0.13	82	10.72
1UNP	1280	111	8.67	848	66.25	132	10.31	189	14.77
1USM	779	78	10.01	590	75.74	30	3.85	81	10.40
1UXZ	944	115	12.18	717	75.95	22	2.33	90	9.53
1UZ3	940	98	10.43	744	79.15	32	3.40	66	7.02
1V05	674	62	9.20	583	86.50	0	0.00	29	4.30
1V0S	3576	666	18.62	2446	68.40	172	4.81	292	8.17
1V6T	2134	259	12.14	1576	73.85	63	2.95	236	11.06
1V7Q	1376	223	16.21	924	67.15	89	6.47	140	10.17
1V8E	1663	218	13.11	1297	77.99	14	0.84	134	8.06
1V8H	870	46	5.29	704	80.92	22	2.53	98	11.26
1V8I	1304	122	9.36	990	75.92	42	3.22	150	11.50
1VDK	3756	529	14.08	2938	78.22	88	2.34	201	5.35
1VE2	1434	197	13.74	1074	74.90	3	0.21	160	11.16

1VGT	1571	200	12.73	1251	79.63	20	1.27	100	6.37
1VH5	1103	112	10.15	853	77.33	39	3.54	99	8.98
1VJS	4038	665	16.47	2891	71.59	182	4.51	300	7.43
1VPI	1022	149	14.58	826	80.82	0	0.00	47	4.60
1W5R	2067	309	14.95	1538	74.41	38	1.84	182	8.81
1W7B	2856	340	11.90	2148	75.21	122	4.27	246	8.61
1WBA	1431	183	12.79	1041	72.75	98	6.85	109	7.62
1WD7	1991	235	11.80	1479	74.28	75	3.77	202	10.15
1WKA	1311	161	12.28	967	73.76	49	3.74	134	10.22
1WKO	1348	158	11.72	1028	76.26	43	3.19	119	8.83
1WLG	2073	215	10.37	1722	83.07	0	0.00	136	6.56
1WLZ	859	100	11.64	648	75.44	61	7.10	50	5.82
1WM3	745	43	5.77	596	80.00	47	6.31	59	7.92
1WMH	820	98	11.95	622	75.85	37	4.51	63	7.68
1WQJ	573	35	6.11	494	86.21	10	1.75	34	5.93
1WTJ	2375	335	14.11	1814	76.38	44	1.85	182	7.66
1WU9	613	32	5.22	509	83.03	0	0.00	72	11.75
1WVH	985	109	11.07	860	87.31	0	0.00	16	1.62
1WYC	2877	480	16.68	1986	69.03	119	4.14	292	10.15
1WZ3	659	33	5.01	604	91.65	0	0.00	22	3.34
1X1E	1757	235	13.38	1329	75.64	83	4.72	110	6.26
1X2I	586	71	12.12	468	79.86	0	0.00	47	8.02
1X6I	944	87	9.22	617	65.36	110	11.65	130	13.77
1XDZ	2117	257	12.14	1612	76.15	57	2.69	191	9.02
1XFK	2703	348	12.87	2099	77.65	21	0.78	235	8.69
1XS0	1011	94	9.30	866	85.66	20	1.98	31	3.07
1XXO	1099	110	10.01	807	73.43	42	3.82	140	12.74
1Y2T	1175	175	14.89	841	71.57	32	2.72	127	10.81
1Y7Y	616	86	13.96	405	65.75	49	7.95	76	12.34
1YAC	1535	218	14.20	1183	77.07	25	1.63	109	7.10
1YHH	1965	184	9.36	1560	79.39	72	3.66	149	7.58
1YN3	807	68	8.43	612	75.84	63	7.81	64	7.93
1YPF	2408	319	13.25	1796	74.58	86	3.57	207	8.60
1YT4	2120	359	16.93	1457	68.73	138	6.51	166	7.83
1YTL	1322	129	9.76	995	75.26	66	4.99	132	9.98
1YU5	607	53	8.73	493	81.22	51	8.40	10	1.65
1YW5	1577	179	11.35	1240	78.63	41	2.60	117	7.42
1YXY	1784	191	10.71	1418	79.48	77	4.32	98	5.49
1YZM	542	10	1.85	523	96.49	0	0.00	9	1.66
1Z0C	1525	176	11.54	1211	79.41	14	0.92	124	8.13
1Z0P	805	75	9.32	627	77.89	4	0.50	99	12.30
1ZKR	1157	142	12.27	958	82.80	16	1.38	41	3.54
1ZO2	1137	101	8.88	847	74.49	74	6.51	115	10.11
1ZRS	2181	320	14.67	1517	69.56	134	6.14	210	9.63
1ZUH	1426	107	7.50	1101	77.21	40	2.81	178	12.48
1ZV1	626	41	6.55	488	77.96	14	2.24	83	13.26
1ZVA	588	28	4.76	540	91.84	11	1.87	9	1.53
1ZVT	1895	229	12.08	1551	81.85	6	0.32	109	5.75
1ZXT	571	39	6.83	483	84.59	0	0.00	49	8.58
2A35	1577	214	13.57	1089	69.06	73	4.63	201	12.75
2A6W	1819	246	13.52	1132	62.23	258	14.18	183	10.06
2A8F	529	61	11.53	438	82.80	9	1.70	21	3.97
2AHF	3247	475	14.63	2272	69.97	168	5.17	332	10.22

2AHN	1379	192	13.92	1122	81.36	13	0.94	52	3.77
2B0A	1473	115	7.81	1257	85.34	38	2.58	63	4.28
2B0J	2553	296	11.59	2127	83.31	29	1.14	101	3.96
2B2F	2096	337	16.08	1588	75.76	38	1.81	133	6.35
2BAY	453	53	11.70	332	73.29	27	5.96	41	9.05
2BK8	862	69	8.00	733	85.03	3	0.35	57	6.61
2BPD	1189	177	14.89	918	77.21	21	1.77	73	6.14
2BVP	2562	269	10.50	1723	67.25	295	11.51	275	10.73
2CG7	719	65	9.04	557	77.47	19	2.64	78	10.85
2CGH	1656	248	14.98	1232	74.40	13	0.79	163	9.84
2CHC	1334	127	9.52	975	73.09	16	1.20	216	16.19
2CI3	2285	269	11.77	1731	75.75	117	5.12	168	7.35
2CIU	1254	115	9.17	877	69.94	139	11.08	123	9.81
2COV	860	78	9.07	624	72.56	36	4.19	122	14.19
2CWC	2258	353	15.63	1483	65.68	201	8.90	221	9.79
2CWK	1373	116	8.45	1133	82.52	21	1.53	103	7.50
2CWL	2446	299	12.22	1779	72.73	142	5.81	226	9.24
2CWR	682	80	11.73	582	85.34	0	0.00	20	2.93
2CYG	2186	293	13.40	1749	80.01	7	0.32	137	6.27
2D4P	1086	89	8.20	789	72.65	149	13.72	59	5.43
2D68	624	40	6.41	510	81.73	4	0.64	70	11.22
2D8E	1035	93	8.99	772	74.59	38	3.67	132	12.75
2DQW	2044	270	13.21	1424	69.67	67	3.28	283	13.85
2DYU	2592	362	13.97	1961	75.66	76	2.93	193	7.45
2E01	3867	450	11.64	2785	72.02	223	5.77	409	10.58
2E10	1680	199	11.85	1273	75.77	111	6.61	97	5.77
2E3Z	3844	579	15.06	2471	64.28	408	10.61	386	10.04
2E64	1780	193	10.84	1373	77.13	78	4.38	136	7.64
2E7A	1170	127	10.85	928	79.32	13	1.11	102	8.72
2E8F	1237	69	5.58	992	80.19	34	2.75	142	11.48
2E8G	2117	246	11.62	1676	79.17	8	0.38	187	8.83
2E9Y	2289	303	13.24	1685	73.61	89	3.89	212	9.26
2EBB	970	90	9.28	725	74.74	53	5.46	102	10.52
2EBE	849	73	8.60	718	84.57	29	3.42	29	3.42
2ECR	1089	143	13.13	753	69.15	43	3.95	150	13.77
2EGJ	1237	105	8.49	862	69.68	125	10.11	145	11.72
2EHG	1258	112	8.90	999	79.41	17	1.35	130	10.33
2EPI	880	54	6.14	738	83.86	10	1.14	78	8.86
2ETX	1429	179	12.53	1089	76.21	15	1.05	146	10.22
2EX0	3609	419	11.61	2831	78.44	120	3.33	239	6.62
2F23	1396	115	8.24	1012	72.49	154	11.03	115	8.24
2F5G	1228	73	5.94	906	73.78	58	4.72	191	15.55
2F6L	1398	159	11.37	1044	74.68	70	5.01	125	8.94
2FBN	1537	158	10.28	1292	84.06	0	0.00	87	5.66
2FBQ	1827	153	8.37	1367	74.82	109	5.97	198	10.84
2FD5	1397	188	13.46	1047	74.95	32	2.29	130	9.31
2FHZ	882	91	10.32	720	81.63	13	1.47	58	6.58
2FJZ	523	64	12.24	425	81.26	6	1.15	28	5.35
2FL4	1514	121	7.99	1085	71.66	59	3.90	249	16.45
2FLU	2107	413	19.60	1366	64.83	122	5.79	206	9.78
2FRG	824	48	5.83	607	73.67	41	4.98	128	15.53
2FVH	906	78	8.61	715	78.92	8	0.88	105	11.59
2FW7	934	81	8.67	784	83.94	22	2.36	47	5.03

2G2U	2131	358	16.80	1482	69.54	159	7.46	132	6.19
2G30	2021	160	7.92	1614	79.86	110	5.44	137	6.78
2G40	1173	138	11.76	943	80.39	19	1.62	73	6.22
2G69	749	37	4.94	612	81.71	48	6.41	52	6.94
2G7I	1084	101	9.32	876	80.81	26	2.40	81	7.47
2G7O	664	32	4.82	600	90.36	1	0.15	31	4.67
2GAS	2580	293	11.36	1944	75.35	90	3.49	253	9.81
2GDQ	3113	425	13.65	2067	66.40	253	8.13	368	11.82
2GEC	1233	160	12.98	942	76.40	14	1.14	117	9.49
2GGV	401	20	4.99	320	79.80	0	0.00	61	15.21
2GIY	1314	153	11.64	1032	78.54	24	1.83	105	7.99
2GKG	956	107	11.19	736	76.99	17	1.78	96	10.04
2GKV	885	154	17.40	717	81.02	0	0.00	14	1.58
2GOM	691	51	7.38	602	87.12	0	0.00	38	5.50
2GQV	467	55	11.78	324	69.38	82	17.56	6	1.28
2GXG	1351	78	5.77	1133	83.86	31	2.29	109	8.07
2H14	2241	373	16.64	1715	76.53	33	1.47	120	5.35
2H2R	1190	169	14.20	789	66.30	103	8.66	129	10.84
2H2Z	2274	248	10.91	1749	76.91	151	6.64	126	5.54
2H7W	831	74	8.90	680	81.83	40	4.81	37	4.45
2H7Z	586	67	11.43	473	80.72	1	0.17	45	7.68
2H8E	1098	89	8.11	807	73.50	57	5.19	145	13.21
2H8O	2200	289	13.14	1641	74.59	99	4.50	171	7.77
2HC8	803	65	8.09	730	90.91	0	0.00	8	1.00
2HLR	497	71	14.29	389	78.27	1	0.20	36	7.24
2HLY	1589	214	13.47	1185	74.58	51	3.21	139	8.75
2HOQ	2196	237	10.79	1580	71.95	85	3.87	294	13.39
2HPL	878	84	9.57	716	81.55	0	0.00	78	8.88
2HWW	1374	142	10.33	1067	77.66	54	3.93	111	8.08
2HY5	1200	125	10.42	888	74.00	58	4.83	129	10.75
2HZF	950	100	10.53	762	80.21	24	2.53	64	6.74
2I3F	1865	269	14.42	1418	76.03	38	2.04	140	7.51
2I49	3145	466	14.82	2134	67.85	250	7.95	295	9.38
2I5D	1622	168	10.36	1237	76.26	83	5.12	134	8.26
2I6V	822	58	7.06	623	75.79	32	3.89	109	13.26
2IBL	870	58	6.67	764	87.82	25	2.87	23	2.64
2IC6	690	52	7.54	568	82.32	1	0.14	69	10.00
2IC7	1512	146	9.66	1125	74.40	128	8.47	113	7.47
2IIA	665	51	7.67	593	89.17	0	0.00	21	3.16
2IJK	582	55	9.45	497	85.40	2	0.34	28	4.81
2IP2	2536	271	10.69	1850	72.95	173	6.82	242	9.54
2IPR	1095	124	11.32	885	80.82	12	1.10	74	6.76
2IRU	2077	334	16.08	1467	70.63	81	3.90	195	9.39
2IUM	1255	180	14.34	1020	81.27	10	0.80	45	3.59
2IXM	2570	358	13.93	1911	74.36	131	5.10	170	6.61
2IY9	2111	367	17.39	1547	73.28	59	2.79	138	6.54
2IZ6	938	114	12.15	797	84.97	0	0.00	27	2.88
2J2J	1327	219	16.50	1009	76.04	22	1.66	77	5.80
2J5Y	481	43	8.94	409	85.03	0	0.00	29	6.03
2J6B	954	79	8.28	810	84.91	3	0.31	62	6.50
2J71	958	114	11.90	667	69.62	26	2.71	151	15.76
2J8B	722	91	12.60	588	81.44	29	4.02	14	1.94
2J9W	997	86	8.63	715	71.72	74	7.42	122	12.24

2JCP	1211	185	15.28	976	80.59	4	0.33	46	3.80
2NML	1000	62	6.20	833	83.30	33	3.30	72	7.20
2NNU	1831	208	11.36	1466	80.07	75	4.10	82	4.48
2NPT	861	72	8.36	637	73.98	49	5.69	103	11.96
2NRR	1237	97	7.84	785	63.46	142	11.48	213	17.22
2NV0	1597	190	11.90	1237	77.46	57	3.57	113	7.08
2O0Q	910	103	11.32	630	69.23	75	8.24	102	11.21
2O2K	2966	347	11.70	2107	71.04	269	9.07	243	8.19
2O6S	1473	168	11.41	1196	81.19	14	0.95	95	6.45
2O6X	2681	401	14.96	1970	73.48	135	5.04	175	6.53
2OEB	1280	148	11.56	988	77.19	60	4.69	84	6.56
2OHW	1184	105	8.87	984	83.11	14	1.18	81	6.84
2OIX	1510	144	9.54	1050	69.54	127	8.41	189	12.52
2OL7	1774	170	9.58	1491	84.05	38	2.14	75	4.23
2OSA	1701	252	14.81	1216	71.49	36	2.12	197	11.58
2OTU	826	111	13.44	647	78.33	18	2.18	50	6.05
2P1G	1918	192	10.01	1518	79.14	121	6.31	87	4.54
2P38	1429	141	9.87	1047	73.27	77	5.39	164	11.48
2P4H	2324	249	10.71	1849	79.56	71	3.06	155	6.67
2P52	1660	242	14.58	1147	69.10	112	6.75	159	9.58
2P5D	1451	153	10.54	1081	74.50	104	7.17	113	7.79
2P5K	654	46	7.03	504	77.06	65	9.94	39	5.96
2P65	1539	189	12.28	1224	79.53	39	2.53	87	5.65
2P84	1313	113	8.61	903	68.77	139	10.59	158	12.03
2PBP	2198	232	10.56	1622	73.79	63	2.87	281	12.78
2PBQ	1234	125	10.13	997	80.79	6	0.49	106	8.59
2PEF	3073	305	9.93	2420	78.75	82	2.67	266	8.66
2PET	1887	148	7.84	1360	72.07	201	10.65	178	9.43
2PGE	2958	335	11.33	2105	71.16	286	9.67	232	7.84
2PKF	2294	244	10.64	1554	67.74	226	9.85	270	11.77
2PMR	756	71	9.39	566	74.87	42	5.56	77	10.19
2PND	1134	92	8.11	870	76.72	52	4.59	120	10.58
2PST	642	74	11.53	517	80.53	11	1.71	40	6.23
2PTV	938	61	6.50	665	70.90	79	8.42	133	14.18
2PV2	848	45	5.31	646	76.18	49	5.78	108	12.74
2Q8O	1031	73	7.08	908	88.07	10	0.97	40	3.88
2QIY	1131	107	9.46	878	77.63	26	2.30	120	10.61
2QOL	2308	344	14.90	1742	75.48	60	2.60	162	7.02
2QPW	1278	139	10.88	978	76.53	50	3.91	111	8.69
2QR3	949	70	7.38	829	87.36	0	0.00	50	5.27
2QT4	698	132	18.91	531	76.07	0	0.00	35	5.01
2R6U	910	115	12.64	768	84.40	17	1.87	10	1.10
2R77	1623	216	13.31	1233	75.97	72	4.44	102	6.28
2R99	1373	155	11.29	1118	81.43	33	2.40	67	4.88
2RCZ	721	42	5.83	628	87.10	2	0.28	49	6.80
2RFA	1776	183	10.30	1381	77.76	94	5.29	118	6.64
2RIK	2277	169	7.42	1866	81.95	111	4.87	131	5.75
2RJD	2732	358	13.10	2077	76.02	129	4.72	168	6.15
2RK5	763	65	8.52	627	82.18	22	2.88	49	6.42
2VC8	492	29	5.89	456	92.68	7	1.42	0	0.00
2YXF	978	71	7.26	798	81.60	5	0.51	104	10.63
2YYV	1754	216	12.31	1353	77.14	28	1.60	157	8.95
2YZ1	869	77	8.86	720	82.85	31	3.57	41	4.72

2Z14	1079	82	7.60	842	78.04	67	6.21	88	8.16
2Z1E	2253	236	10.47	1800	79.89	35	1.55	182	8.08
2Z37	1838	329	17.90	1241	67.52	111	6.04	157	8.54
2ZFY	2141	219	10.23	1654	77.25	54	2.52	214	10.00
3ADO	2595	230	8.86	2143	82.58	52	2.00	170	6.55
3BB7	2285	316	13.83	1806	79.04	59	2.58	104	4.55
3BN6	1342	259	19.30	885	65.95	45	3.35	153	11.40
3C4S	445	21	4.72	378	84.94	2	0.45	44	9.89
3PHS	2006	182	9.07	1601	79.81	39	1.94	184	9.17
3SSW	983	50	5.09	718	73.04	132	13.43	83	8.44
4RWU	741	88	11.88	610	82.32	0	0.00	43	5.80
5WOF	769	79	10.27	605	78.67	8	1.04	77	10.01
6XIA	3234	444	13.73	2385	73.75	84	2.60	321	9.93
Total	572783	66178	11.55	433156	75.62	24346	4.25	49103	8.57
Avg.	-	-	10.76	-	76.97	-	3.86	-	8.41
Std.	-	-	3.19	-	5.92	-	3.23	-	3.25

Note: Avg. stands for average; Std. stands for standard deviation.

Supporting Figures

Figure S1. FASPR computational time (in seconds) for side-chain packing as a function of number of rotamers (A) or number of residues (B).
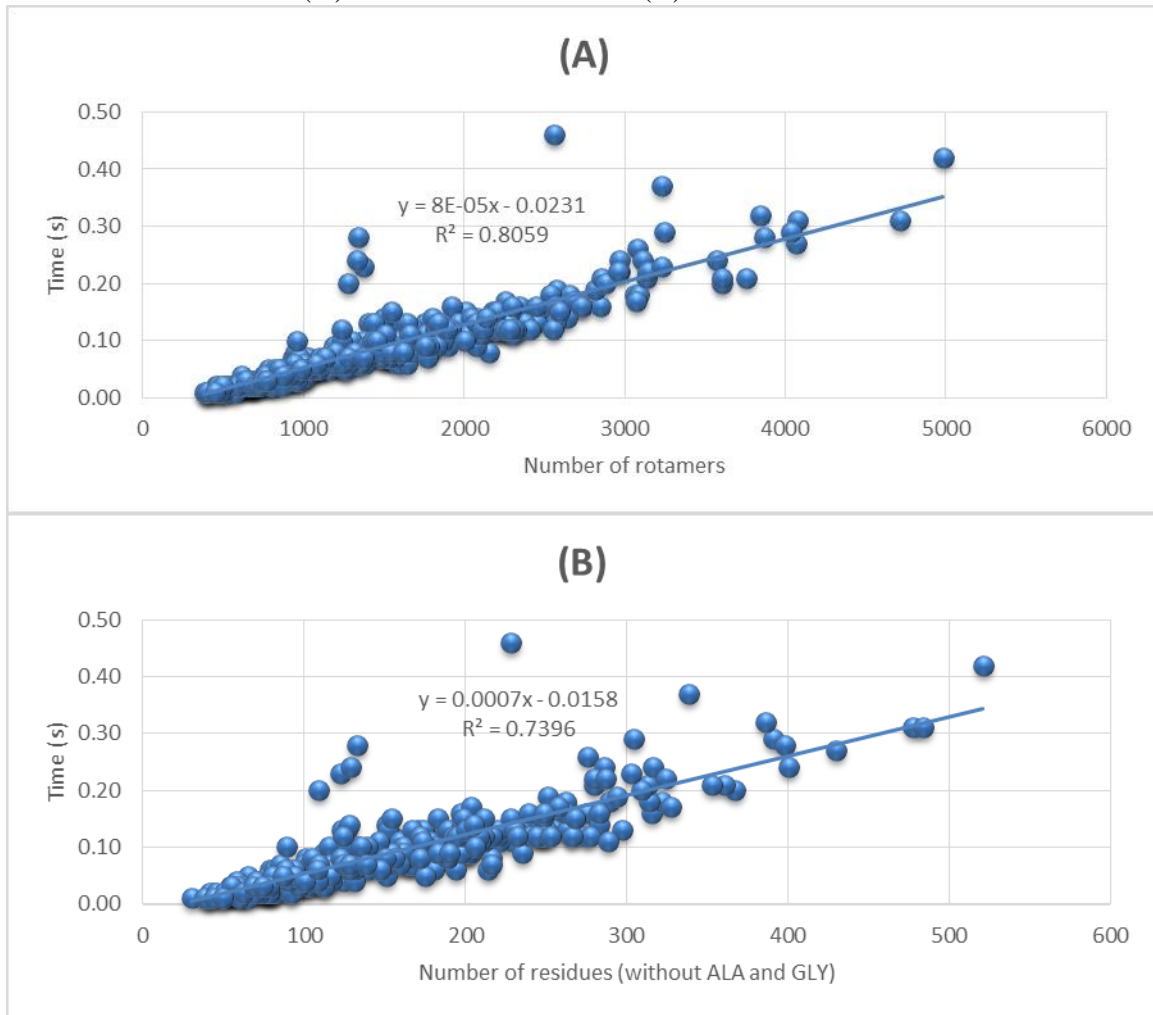
Figure S2. The accuracy of FASPR in terms of χ_{1-4} recovery rate (A) or RMSD (B) as a function of number of residues.