Supporting Information

Identification for Probable Structure of sAPPα-GABABR1a

Complex and Theoretical Solutions for Such Cases

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ANALYSIS METHOD DETAILS

Trajectory Analysis. We used the rms and rmsf option to get the RMSD and RMSF analysis of Cα atoms in the APP9mer-SD1 complexes, respectively. The hydrogen bond (H-bond) was considered with the hbond option, which was recognized when the cutoff distance was less than 0.35nm and the truncation of angle was less than 30° between APP9mer and SD1. The salt-bridge was considered with the saltar option to be recognized when the distance of the two charged groups from different parts was less than 0.3 nm.[1]

PCA and FEL. The main motions can be described in several main modes in MD simulation.[2] PCA (principal component analysis) can provide a detailed picture of the motion of a biomolecule and calculate its eigenvalues and eigenvectors by reducing the dimension.[3-4] When selecting groups to analyze, we were only interested in the backbone behavior of the first two main components (PC1 and PC2) of the APPmer-SD1 for eliminating the interference of side chain atoms.[4-6] The main components possessed high eigenvectors with eigenvalues. The free energy landscape (FEL) can describe the value of free energy and probability density P(x) of various conformations (X) of macromolecules. The free energy of whole complex was calculated as the equations below.[7]

$$\Delta G(X) = \square K_B T \cdot LnP(x) + A$$

Where $\Delta G(X)$ is the change of free energy, and K_B, $P(x)$ and T indicate Boltzmann constant, probability distribution along a certain coordinate and simulation temperature, respectively. A is the constant term, which is related to the partition function. Undoubtedly, the simplified free energy landscape map is mainly used to analyze the composite conformation of the lowest energy with relatively large $P(X)$.[8] The dominant conformation was projected onto a two-dimensional plane in the form of clusters of points. The grid cell containing the most multipoint clusters was designated as the reference cell, and its free energy value is set to zero. Every frame covariance matrix, eigenvalue and eigenvector were generated using the gmx_covar option by GROMACS and gmx_anaeig option can project trajectories onto selected eigenvectors. In the end,

we will use the *ddtpd* package and the Sigmaplot software to draw the 2D/3D map of FEL.[9]

For the six complexes of APP9mer-SD1 in this study, each group will generate 8,000 structures, including solvated and non-solvated structures, which are used to construct their respective energy landscapes. Moreover, the value of P=0 is meaningless in the calculation formula of free energy when using 3D Cartesian coordinates to plot the graphs by principal component analysis method. So, we had only plotted the free energy landscapes with respect to the lowest energy (set to 0) of each system.

MM/PBSA Binding Free Energy Calculations. Molecular Mechanics/Poisson-Boltzmann Surface Area (MM/PBSA) is a widely used common method for post-processing MD trajectories to estimate the binding free energy.[10-12] Binding free energy is an important indicator to measure the binding strength effectively of the acceptor and ligand.[13] In the calculation, the solvent is regarded as a uniform continuum, and many frames in the equilibrium trajectory are averaged that based on the force field and an implicit continuum model.[14] In this method, the complex binding free energy (ΔG_{bind}) is given blow.[15]

$$\Delta G_{bind}=G_c-G_a-G_l$$

In the above formula, ΔG_{bind}、G_c、G_a、G_l represented the binding energy of the system, complex, acceptor and ligand, respectively. This mean divides the binding free energy into multiple calculations separately, and the specific decomposition is as follows:

$$\Delta G_{bind}=\Delta H-T\Delta S=\Delta E_{MM} + \Delta G_{solv} -T\Delta S$$

$$\Delta E_{MM}=\Delta E_{VDW}+\Delta E_{COU}$$

$$\Delta G_{solv}=\Delta G_{PB}+\Delta G_{SA}$$

Here, we can see clearly that ΔG_{bind} consists of enthalpy changes (ΔH) and entropy changes ($-T\Delta S$) of the system. In this work, difference of kinetic energy (ΔE_{MM}) and solvent effect term (ΔG_{solv}) before and after APP9mer-SD1 binding in vacuum is of importance for ΔH. Meanwhile, ΔE_{MM} and ΔG_{solv} also is divided into two terms. ΔE_{COU} is electrostatic interaction and ΔE_{VDW} is van der Waals interactions between APP9mer

and SD1. [16-17]ΔG_{PB} and ΔG_{SA}, respectively, represents the polar and non-polar solvation energy. ΔE_{MM} is completed by the script itself, ΔG_{PB} is completed by the APBS program, and the ΔG_{SA} term is calculated by the following empirical formula:

$$\Delta G_{SA} = \gamma \text{ SASA} + \beta$$

In which, SASA is the solution accessible surface area.[17] The values of γ and β are respectively 2.2kJ/(mol·nm^2) and β=3.84kJ/mol. Furthermore, ΔG_{bind} is a relative energy, the estimation of -TΔS cannot significantly change the relative free energy, so the contribution of entropy is negligible.[18]

Dynamic Cross-Correlation Map. DCCM is usually used to detect the relative movement of residue pairs in complex structures. The mdmat option and xpm2ps tools of GROMACS was used to make residue contact maps to analyze the mutual mapping relationship of dynamic residue pairs. This method generally uses the covariance of the fluctuation of the C-alpha position of the skeleton atom. We took out a complex conformation every 1 ns from the equilibrium trajectory, then used the following equation to calculate the dynamic cross-correlation matrix C_{ij}:

$$C_{ij} = \frac{\langle \Delta r_i \cdot \Delta r_j \rangle}{\sqrt{\langle \Delta r_i^2 \cdot \Delta r_j^2 \rangle}}$$

Among them, the term C_{ij} represents Cross-correlation coefficient. Δr_i is the average position of C-alpha of ith residue in i^{th} residue, Δr_j is the average position of C-alpha of jth residue of another component in j^{th} residue. Usually, a positive value of C_{ij} means the relative motion of the residue pair in the same direction; when the value is negative, it means the opposite direction.

Table S1. FlexPepDocking Results

	CN		NC	
	score	conformation	score	conformation
1	-24.155		-21.678	
2	-23.819		-17.994	
3	-23.043		-17.806	
4	-22.998		-16.167	
5	-22.955		-16.106	
6	-22.919		-15.734	
7	-21.596		-15.637	
8	-21.623		-14.822	
9	-21.465		-14.612	
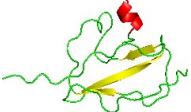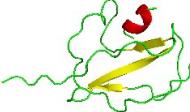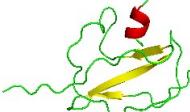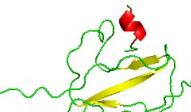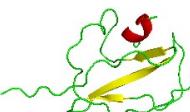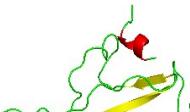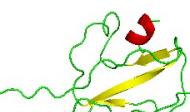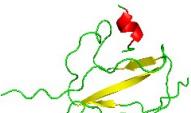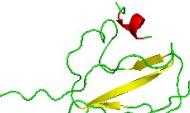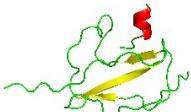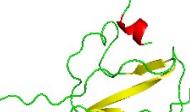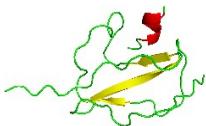
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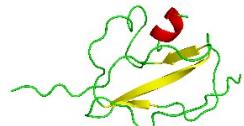
Table S2. Coordination file of sAPPα-SD1 in 2NC

0ACE	CH3	1	5.273	4.116	1.646
0ACE	HH31	2	5.347	4.192	1.679
0ACE	HH32	3	5.301	4.013	1.677
0ACE	HH33	4	5.289	4.127	1.537
0ACE	C	5	5.135	4.154	1.686
0ACE	O	6	5.040	4.083	1.654
1GLY	N	7	5.120	4.280	1.732
1GLY	HN	8	5.202	4.333	1.751
1GLY	CA	9	4.993	4.338	1.763
1GLY	HA1	10	5.003	4.445	1.751
1GLY	HA2	11	4.917	4.305	1.695
1GLY	C	12	4.948	4.314	1.903
1GLY	O	13	5.025	4.254	1.978
2PRO	N	14	4.832	4.359	1.941
2PRO	CD	15	4.764	4.461	1.863
2PRO	HD1	16	4.730	4.425	1.764
2PRO	HD2	17	4.825	4.554	1.856
2PRO	CA	18	4.758	4.326	2.060
2PRO	HA	19	4.802	4.388	2.136
2PRO	CB	20	4.614	4.364	2.025
2PRO	HB1	21	4.566	4.291	1.956
2PRO	HB2	22	4.542	4.385	2.107
2PRO	CG	23	4.639	4.493	1.947
2PRO	HG1	24	4.548	4.508	1.885
2PRO	HG2	25	4.654	4.583	2.010
2PRO	C	26	4.767	4.185	2.105

2PRO	O	27	4.750	4.095	2.023
3THR	N	28	4.794	4.165	2.236
3THR	HN	29	4.790	4.236	2.305
3THR	CA	30	4.828	4.037	2.290
3THR	HA	31	4.922	4.018	2.241
3THR	CB	32	4.859	4.048	2.436
3THR	HB	33	4.779	4.115	2.474
3THR	OG1	34	4.990	4.101	2.448
3THR	HG1	35	5.003	4.184	2.402
3THR	CG2	36	4.854	3.913	2.509
3THR	HG21	37	4.898	3.917	2.611
3THR	HG22	38	4.747	3.891	2.528
3THR	HG23	39	4.914	3.835	2.457
3THR	C	40	4.730	3.926	2.270
3THR	O	41	4.615	3.932	2.312
4SER	N	42	4.777	3.822	2.198
4SER	HN	43	4.870	3.842	2.167
4SER	CA	44	4.719	3.695	2.168
4SER	HA	45	4.637	3.722	2.104
4SER	CB	46	4.814	3.610	2.081
4SER	HB1	47	4.829	3.665	1.986
4SER	HB2	48	4.904	3.594	2.144
4SER	OG	49	4.753	3.487	2.043
4SER	HG1	50	4.825	3.426	2.028
4SER	C	51	4.686	3.612	2.287
4SER	O	52	4.575	3.559	2.297
5GLU	N	53	4.778	3.596	2.384
5GLU	HN	54	4.872	3.625	2.372
5GLU	CA	55	4.761	3.510	2.497
5GLU	HA	56	4.686	3.438	2.465

5GLU	CB	57	4.883	3.424	2.532
5GLU	HB1	58	4.967	3.494	2.552
5GLU	HB2	59	4.868	3.363	2.624
5GLU	CG	60	4.912	3.329	2.416
5GLU	HG1	61	4.822	3.264	2.416
5GLU	HG2	62	4.928	3.384	2.321
5GLU	CD	63	5.030	3.235	2.439
5GLU	OE1	64	5.110	3.207	2.345
5GLU	OE2	65	5.045	3.182	2.552
5GLU	C	66	4.697	3.576	2.614
5GLU	O	67	4.723	3.549	2.731
6GLY	N	68	4.601	3.665	2.584
6GLY	HN	69	4.594	3.685	2.487
6GLY	CA	70	4.516	3.740	2.672
6GLY	HA1	71	4.480	3.828	2.620
6GLY	HA2	72	4.437	3.670	2.698
6GLY	C	73	4.579	3.799	2.793
6GLY	O	74	4.697	3.831	2.803
7CYS	N	75	4.491	3.813	2.894
7CYS	HN	76	4.394	3.803	2.873
7CYS	CA	77	4.524	3.837	3.031
7CYS	HA	78	4.629	3.849	3.053
7CYS	CB	79	4.471	3.965	3.097
7CYS	HB1	80	4.362	3.972	3.113
7CYS	HB2	81	4.520	3.976	3.197
7CYS	SG	82	4.517	4.104	2.989
7CYS	C	83	4.488	3.715	3.107
7CYS	O	84	4.373	3.670	3.108
8GLN	N	85	4.590	3.657	3.173
8GLN	HN	86	4.684	3.688	3.166

8GLN	CA	87	4.574	3.543	3.258
8GLN	HA	88	4.527	3.469	3.195
8GLN	CB	89	4.714	3.484	3.283
8GLN	HB1	90	4.776	3.563	3.331
8GLN	HB2	91	4.708	3.395	3.349
8GLN	CG	92	4.782	3.442	3.153
8GLN	HG1	93	4.712	3.388	3.086
8GLN	HG2	94	4.830	3.530	3.105
8GLN	CD	95	4.883	3.331	3.178
8GLN	OE1	96	4.863	3.210	3.164
8GLN	NE2	97	5.008	3.372	3.210
8GLN	HE21	98	5.022	3.470	3.229
8GLN	HE22	99	5.091	3.316	3.212
8GLN	C	100	4.489	3.559	3.379
8GLN	O	101	4.497	3.659	3.451
9ILE	N	102	4.407	3.458	3.412
9ILE	HN	103	4.409	3.377	3.353
9ILE	CA	104	4.321	3.459	3.527
9ILE	HA	105	4.336	3.549	3.584
9ILE	CB	106	4.178	3.457	3.481
9ILE	HB	107	4.161	3.527	3.397
9ILE	CG2	108	4.138	3.316	3.433
9ILE	HG21	109	4.119	3.241	3.513
9ILE	HG22	110	4.040	3.324	3.381
9ILE	HG23	111	4.208	3.284	3.353
9ILE	CG1	112	4.071	3.502	3.582
9ILE	HG11	113	3.970	3.484	3.542
9ILE	HG12	114	4.092	3.427	3.662
9ILE	CD	115	4.073	3.648	3.627
9ILE	HD1	116	4.154	3.653	3.703

9ILE	HD2	117	4.084	3.721	3.545
9ILE	HD3	118	3.979	3.670	3.683
9ILE	C	119	4.350	3.350	3.624
9ILE	O	120	4.426	3.257	3.595
10ILE	N	121	4.310	3.366	3.751
10ILE	HN	122	4.266	3.452	3.775
10ILE	CA	123	4.314	3.273	3.859
10ILE	HA	124	4.421	3.266	3.876
10ILE	CB	125	4.258	3.335	3.984
10ILE	HB	126	4.261	3.253	4.059
10ILE	CG2	127	4.351	3.448	4.032
10ILE	HG21	128	4.326	3.483	4.134
10ILE	HG22	129	4.455	3.412	4.041
10ILE	HG23	130	4.349	3.531	3.958
10ILE	CG1	131	4.114	3.387	3.972
10ILE	HG11	132	4.100	3.452	4.062
10ILE	HG12	133	4.110	3.456	3.885
10ILE	CD	134	4.004	3.282	3.979
10ILE	HD1	135	4.033	3.201	4.050
10ILE	HD2	136	3.905	3.326	4.004
10ILE	HD3	137	4.003	3.233	3.879
10ILE	C	138	4.263	3.136	3.829
10ILE	O	139	4.190	3.108	3.734
11HIS	N	140	4.297	3.043	3.920
11HIS	HN	141	4.343	3.062	4.006
11HIS	CA	142	4.253	2.908	3.907
11HIS	HA	143	4.188	2.900	3.821
11HIS	CB	144	4.374	2.814	3.896
11HIS	HB1	145	4.458	2.847	3.962
11HIS	HB2	146	4.359	2.704	3.903

11HIS	ND1	147	4.359	2.728	3.659
11HIS	CG	148	4.421	2.806	3.754
11HIS	CE1	149	4.433	2.737	3.550
11HIS	HE1	150	4.413	2.699	3.450
11HIS	NE2	151	4.545	2.813	3.568
11HIS	HE2	152	4.618	2.800	3.502
11HIS	CD2	153	4.538	2.850	3.701
11HIS	HD2	154	4.627	2.896	3.743
11HIS	C	155	4.183	2.876	4.035
11HIS	O	156	4.210	2.942	4.135
12PRO	N	157	4.099	2.777	4.035
12PRO	CD	158	4.049	2.711	3.915
12PRO	HD1	159	4.138	2.679	3.856
12PRO	HD2	160	3.976	2.771	3.856
12PRO	CA	161	4.035	2.721	4.151
12PRO	HA	162	4.000	2.804	4.211
12PRO	CB	163	3.924	2.635	4.093
12PRO	HB1	164	3.889	2.553	4.159
12PRO	HB2	165	3.831	2.688	4.062
12PRO	CG	166	3.976	2.583	3.958
12PRO	HG1	167	4.054	2.505	3.974
12PRO	HG2	168	3.892	2.562	3.888
12PRO	C	169	4.122	2.636	4.237
12PRO	O	170	4.220	2.585	4.182
13PRO	N	171	4.105	2.612	4.363
13PRO	CD	172	4.175	2.501	4.426
13PRO	HD1	173	4.285	2.502	4.407
13PRO	HD2	174	4.134	2.402	4.397
13PRO	CA	175	4.012	2.675	4.453
13PRO	HA	176	3.911	2.673	4.416

13PRO	CB	177	4.010	2.597	4.584
13PRO	HB1	178	4.001	2.662	4.674
13PRO	HB2	179	3.930	2.519	4.586
13PRO	CG	180	4.150	2.534	4.574
13PRO	HG1	181	4.230	2.599	4.614
13PRO	HG2	182	4.154	2.447	4.642
13PRO	C	183	4.040	2.820	4.471
13PRO	O	184	4.157	2.854	4.487
14TRP	N	185	3.939	2.909	4.464
14TRP	HN	186	3.850	2.869	4.444
14TRP	CA	187	3.961	3.049	4.480
14TRP	HA	188	4.051	3.065	4.539
14TRP	CB	189	3.965	3.117	4.342
14TRP	HB1	190	4.018	3.045	4.275
14TRP	HB2	191	3.861	3.132	4.306
14TRP	CG	192	4.041	3.245	4.337
14TRP	CD1	193	3.991	3.371	4.328
14TRP	HD1	194	3.887	3.393	4.308
14TRP	NE1	195	4.085	3.466	4.357
14TRP	HE1	196	4.076	3.562	4.341
14TRP	CE2	197	4.199	3.398	4.392
14TRP	CD2	198	4.177	3.262	4.378
14TRP	CE3	199	4.278	3.174	4.403
14TRP	HE3	200	4.269	3.069	4.381
14TRP	CZ3	201	4.401	3.225	4.440
14TRP	HZ3	202	4.478	3.154	4.465
14TRP	CZ2	203	4.319	3.449	4.433
14TRP	HZ2	204	4.336	3.555	4.426
14TRP	CH2	205	4.420	3.360	4.460
14TRP	HH2	206	4.518	3.396	4.488

14TRP	C	207	3.850	3.111	4.557
14TRP	O	208	3.737	3.062	4.565
15GLU	N	209	3.873	3.232	4.611
15GLU	HN	210	3.963	3.276	4.609
15GLU	CA	211	3.777	3.317	4.675
15GLU	HA	212	3.704	3.254	4.724
15GLU	CB	213	3.823	3.408	4.790
15GLU	HB1	214	3.917	3.454	4.753
15GLU	HB2	215	3.756	3.495	4.807
15GLU	CG	216	3.837	3.330	4.921
15GLU	HG1	217	3.752	3.258	4.929
15GLU	HG2	218	3.926	3.264	4.918
15GLU	CD	219	3.848	3.416	5.047
15GLU	OE1	220	3.759	3.405	5.136
15GLU	OE2	221	3.949	3.491	5.054
15GLU	C	222	3.700	3.406	4.584
15GLU	O	223	3.758	3.493	4.519
16GLY	N	224	3.568	3.387	4.568
16GLY	HN	225	3.518	3.319	4.621
16GLY	CA	226	3.490	3.457	4.471
16GLY	HA1	227	3.389	3.441	4.503
16GLY	HA2	228	3.518	3.562	4.468
16GLY	C	229	3.485	3.406	4.332
16GLY	O	230	3.554	3.311	4.293
17GLY	N	231	3.410	3.469	4.240
17GLY	HN	232	3.342	3.537	4.268
17GLY	CA	233	3.392	3.425	4.105
17GLY	HA1	234	3.473	3.363	4.070
17GLY	HA2	235	3.294	3.380	4.105
17GLY	C	236	3.386	3.540	4.010

17GLY	O	237	3.389	3.655	4.052
18ILE	N	238	3.361	3.518	3.880
18ILE	HN	239	3.357	3.426	3.842
18ILE	CA	240	3.361	3.620	3.780
18ILE	HA	241	3.327	3.714	3.823
18ILE	CB	242	3.496	3.632	3.716
18ILE	HB	243	3.488	3.693	3.623
18ILE	CG2	244	3.584	3.715	3.811
18ILE	HG21	245	3.538	3.810	3.846
18ILE	HG22	246	3.615	3.660	3.902
18ILE	HG23	247	3.681	3.740	3.763
18ILE	CG1	248	3.557	3.495	3.684
18ILE	HG11	249	3.570	3.435	3.777
18ILE	HG12	250	3.478	3.438	3.631
18ILE	CD	251	3.690	3.492	3.609
18ILE	HD1	252	3.711	3.390	3.571
18ILE	HD2	253	3.684	3.564	3.525
18ILE	HD3	254	3.779	3.521	3.669
18ILE	C	255	3.253	3.599	3.680
18ILE	O	256	3.211	3.490	3.640
19ARG	N	257	3.192	3.710	3.633
19ARG	HN	258	3.219	3.799	3.670
19ARG	CA	259	3.088	3.709	3.536
19ARG	HA	260	3.080	3.613	3.487
19ARG	CB	261	2.948	3.734	3.594
19ARG	HB1	262	2.870	3.693	3.526
19ARG	HB2	263	2.952	3.677	3.689
19ARG	CG	264	2.906	3.879	3.624
19ARG	HG1	265	2.989	3.915	3.690
19ARG	HG2	266	2.909	3.945	3.535

19ARG	CD	267	2.783	3.897	3.711
19ARG	HD1	268	2.810	3.832	3.797
19ARG	HD2	269	2.768	4.002	3.742
19ARG	NE	270	2.663	3.853	3.633
19ARG	HE	271	2.663	3.849	3.533
19ARG	CZ	272	2.534	3.846	3.676
19ARG	NH1	273	2.509	3.841	3.810
19ARG	HH11	274	2.591	3.828	3.866
19ARG	HH12	275	2.423	3.801	3.842
19ARG	NH2	276	2.435	3.838	3.583
19ARG	HH21	277	2.452	3.841	3.485
19ARG	HH22	278	2.340	3.834	3.614
19ARG	C	279	3.132	3.817	3.443
19ARG	O	280	3.159	3.932	3.479
20TYR	N	281	3.132	3.789	3.312
20TYR	HN	282	3.106	3.696	3.284
20TYR	CA	283	3.163	3.877	3.204
20TYR	HA	284	3.265	3.909	3.222
20TYR	CB	285	3.171	3.784	3.082
20TYR	HB1	286	3.242	3.700	3.096
20TYR	HB2	287	3.072	3.733	3.072
20TYR	CG	288	3.196	3.849	2.950
20TYR	CD1	289	3.321	3.859	2.893
20TYR	HD1	290	3.396	3.797	2.939
20TYR	CE1	291	3.339	3.936	2.781
20TYR	HE1	292	3.435	3.933	2.731
20TYR	CZ	293	3.234	3.986	2.708
20TYR	OH	294	3.256	4.047	2.583
20TYR	HH	295	3.171	4.072	2.546
20TYR	CD2	296	3.092	3.906	2.881

20TYR	HD2	297	2.996	3.909	2.932
20TYR	CE2	298	3.110	3.981	2.767
20TYR	HE2	299	3.022	4.012	2.712
20TYR	C	300	3.072	3.994	3.194
20TYR	O	301	2.956	3.989	3.235
21ARG	N	302	3.133	4.106	3.149
21ARG	HN	303	3.228	4.118	3.122
21ARG	CA	304	3.060	4.229	3.138
21ARG	HA	305	2.954	4.211	3.135
21ARG	CB	306	3.077	4.339	3.243
21ARG	HB1	307	3.187	4.357	3.256
21ARG	HB2	308	3.029	4.435	3.216
21ARG	CG	309	3.021	4.300	3.380
21ARG	HG1	310	3.073	4.208	3.415
21ARG	HG2	311	3.038	4.376	3.458
21ARG	CD	312	2.869	4.279	3.376
21ARG	HD1	313	2.814	4.367	3.336
21ARG	HD2	314	2.837	4.194	3.312
21ARG	NE	315	2.829	4.250	3.516
21ARG	HE	316	2.896	4.273	3.587
21ARG	CZ	317	2.706	4.210	3.560
21ARG	NH1	318	2.591	4.203	3.488
21ARG	HH11	319	2.597	4.211	3.388
21ARG	HH12	320	2.509	4.167	3.533
21ARG	NH2	321	2.686	4.223	3.694
21ARG	HH21	322	2.762	4.253	3.752
21ARG	HH22	323	2.595	4.197	3.726
21ARG	C	324	3.091	4.294	3.007
21ARG	O	325	3.209	4.300	2.972
22GLY	N	326	2.991	4.347	2.935

22GLY	HN	327	2.900	4.347	2.976
22GLY	CA	328	2.995	4.405	2.804
22GLY	HA1	329	2.950	4.502	2.814
22GLY	HA2	330	3.098	4.411	2.775
22GLY	C	331	2.935	4.313	2.704
22GLY	O	332	2.868	4.213	2.732
23LEU	N	333	2.968	4.338	2.576
23LEU	HN	334	3.033	4.407	2.545
23LEU	CA	335	2.893	4.282	2.467
23LEU	HA	336	2.794	4.316	2.488
23LEU	CB	337	2.921	4.349	2.331
23LEU	HB1	338	2.845	4.324	2.254
23LEU	HB2	339	2.922	4.460	2.333
23LEU	CG	340	3.061	4.321	2.274
23LEU	HG	341	3.056	4.213	2.251
23LEU	CD1	342	3.067	4.396	2.140
23LEU	HD11	343	3.158	4.374	2.080
23LEU	HD12	344	2.980	4.361	2.080
23LEU	HD13	345	3.066	4.506	2.152
23LEU	CD2	346	3.184	4.367	2.354
23LEU	HD21	347	3.189	4.323	2.456
23LEU	HD22	348	3.281	4.346	2.302
23LEU	HD23	349	3.181	4.478	2.359
23LEU	C	350	2.897	4.133	2.454
23LEU	O	351	3.000	4.067	2.465
24THR	N	352	2.778	4.075	2.427
24THR	HN	353	2.709	4.141	2.399
24THR	CA	354	2.758	3.933	2.434
24THR	HA	355	2.785	3.897	2.532
24THR	CB	356	2.613	3.900	2.414

24THR	HB	357	2.569	3.954	2.327
24THR	OG1	358	2.541	3.938	2.531
24THR	HG1	359	2.520	4.032	2.534
24THR	CG2	360	2.594	3.749	2.397
24THR	HG21	361	2.485	3.728	2.388
24THR	HG22	362	2.639	3.716	2.301
24THR	HG23	363	2.628	3.700	2.491
24THR	C	364	2.850	3.856	2.346
24THR	O	365	2.838	3.840	2.225
25ARG	N	366	2.948	3.792	2.412
25ARG	HN	367	2.968	3.806	2.509
25ARG	CA	368	3.040	3.701	2.351
25ARG	HA	369	2.998	3.655	2.263
25ARG	CB	370	3.176	3.765	2.320
25ARG	HB1	371	3.225	3.812	2.408
25ARG	HB2	372	3.246	3.685	2.287
25ARG	CG	373	3.167	3.879	2.219
25ARG	HG1	374	3.093	3.954	2.254
25ARG	HG2	375	3.261	3.934	2.198
25ARG	CD	376	3.126	3.831	2.079
25ARG	HD1	377	3.216	3.777	2.043
25ARG	HD2	378	3.030	3.775	2.082
25ARG	NE	379	3.128	3.949	1.989
25ARG	HE	380	3.214	3.969	1.941
25ARG	CZ	381	3.018	4.019	1.947
25ARG	NH1	382	2.895	4.000	2.002
25ARG	HH11	383	2.887	3.944	2.085
25ARG	HH12	384	2.826	4.067	1.977
25ARG	NH2	385	3.042	4.112	1.850
25ARG	HH21	386	3.127	4.102	1.798

25ARG	HH22	387	2.971	4.177	1.823
25ARG	C	388	3.062	3.593	2.452
25ARG	O	389	3.098	3.619	2.567
26ASP	N	390	3.051	3.467	2.407
26ASP	HN	391	3.031	3.437	2.314
26ASP	CA	392	3.079	3.362	2.500
26ASP	HA	393	3.060	3.393	2.602
26ASP	CB	394	2.991	3.240	2.472
26ASP	HB1	395	2.891	3.279	2.444
26ASP	HB2	396	3.021	3.177	2.385
26ASP	CG	397	2.968	3.149	2.592
26ASP	OD1	398	2.916	3.037	2.566
26ASP	OD2	399	2.974	3.201	2.707
26ASP	C	400	3.218	3.308	2.505
26ASP	O	401	3.273	3.262	2.406
27GLN	N	402	3.284	3.316	2.622
27GLN	HN	403	3.230	3.325	2.705
27GLN	CA	404	3.421	3.296	2.659
27GLN	HA	405	3.477	3.334	2.574
27GLN	CB	406	3.450	3.366	2.792
27GLN	HB1	407	3.397	3.314	2.874
27GLN	HB2	408	3.557	3.357	2.821
27GLN	CG	409	3.423	3.517	2.790
27GLN	HG1	410	3.312	3.524	2.794
27GLN	HG2	411	3.465	3.565	2.881
27GLN	CD	412	3.479	3.584	2.665
27GLN	OE1	413	3.600	3.579	2.646
27GLN	NE2	414	3.398	3.659	2.585
27GLN	HE21	415	3.301	3.663	2.609
27GLN	HE22	416	3.441	3.736	2.538

27GLN	C	417	3.462	3.153	2.661
27GLN	O	418	3.398	3.064	2.716
28VAL	N	419	3.584	3.128	2.608
28VAL	HN	420	3.634	3.203	2.566
28VAL	CA	421	3.640	2.997	2.607
28VAL	HA	422	3.559	2.935	2.573
28VAL	CB	423	3.747	2.998	2.502
28VAL	HB	424	3.830	3.062	2.539
28VAL	CG1	425	3.812	2.860	2.483
28VAL	HG11	426	3.882	2.867	2.397
28VAL	HG12	427	3.880	2.823	2.563
28VAL	HG13	428	3.736	2.783	2.461
28VAL	CG2	429	3.697	3.044	2.364
28VAL	HG21	430	3.659	3.148	2.352
28VAL	HG22	431	3.789	3.033	2.303
28VAL	HG23	432	3.616	2.982	2.320
28VAL	C	433	3.686	2.954	2.742
28VAL	O	434	3.775	3.012	2.805
29LYS	N	435	3.639	2.837	2.788
29LYS	HN	436	3.576	2.788	2.728
29LYS	CA	437	3.656	2.784	2.919
29LYS	HA	438	3.674	2.860	2.994
29LYS	CB	439	3.530	2.700	2.946
29LYS	HB1	440	3.537	2.624	2.865
29LYS	HB2	441	3.534	2.643	3.041
29LYS	CG	442	3.398	2.778	2.949
29LYS	HG1	443	3.384	2.829	2.851
29LYS	HG2	444	3.317	2.704	2.963
29LYS	CD	445	3.395	2.864	3.076
29LYS	HD1	446	3.423	2.804	3.165

29LYS	HD2	447	3.472	2.942	3.058
29LYS	CE	448	3.263	2.938	3.089
29LYS	HE1	449	3.263	3.013	3.172
29LYS	HE2	450	3.233	2.980	2.990
29LYS	NZ	451	3.162	2.834	3.120
29LYS	HZ1	452	3.206	2.742	3.102
29LYS	HZ2	453	3.138	2.833	3.221
29LYS	HZ3	454	3.085	2.844	3.050
29LYS	C	455	3.783	2.705	2.925
29LYS	O	456	3.816	2.656	3.033
30ALA	N	457	3.853	2.690	2.812
30ALA	HN	458	3.814	2.735	2.731
30ALA	CA	459	3.959	2.597	2.790
30ALA	HA	460	3.955	2.524	2.870
30ALA	CB	461	3.930	2.530	2.654
30ALA	HB1	462	4.002	2.448	2.632
30ALA	HB2	463	3.825	2.494	2.657
30ALA	HB3	464	3.941	2.600	2.569
30ALA	C	465	4.090	2.667	2.793
30ALA	O	466	4.193	2.600	2.793
31ILE	N	467	4.094	2.800	2.813
31ILE	HN	468	4.007	2.847	2.830
31ILE	CA	469	4.207	2.887	2.816
31ILE	HA	470	4.295	2.824	2.818
31ILE	CB	471	4.202	2.994	2.711
31ILE	HB	472	4.280	3.068	2.740
31ILE	CG2	473	4.232	2.928	2.576
31ILE	HG21	474	4.141	2.881	2.532
31ILE	HG22	475	4.269	3.004	2.504
31ILE	HG23	476	4.315	2.856	2.591

31ILE	CG1	477	4.077	3.084	2.717
31ILE	HG11	478	3.994	3.021	2.678
31ILE	HG12	479	4.062	3.133	2.816
31ILE	CD	480	4.084	3.199	2.617
31ILE	HD1	481	4.172	3.258	2.650
31ILE	HD2	482	4.078	3.173	2.509
31ILE	HD3	483	4.001	3.271	2.634
31ILE	C	484	4.214	2.951	2.950
31ILE	O	485	4.113	2.973	3.018
32ASN	N	486	4.337	2.984	2.992
32ASN	HN	487	4.416	2.976	2.931
32ASN	CA	488	4.363	3.043	3.120
32ASN	HA	489	4.300	3.001	3.197
32ASN	CB	490	4.497	2.992	3.176
32ASN	HB1	491	4.586	3.031	3.122
32ASN	HB2	492	4.516	3.030	3.279
32ASN	CG	493	4.521	2.842	3.169
32ASN	OD1	494	4.624	2.801	3.117
32ASN	ND2	495	4.417	2.763	3.206
32ASN	HD21	496	4.329	2.807	3.226
32ASN	HD22	497	4.421	2.664	3.196
32ASN	C	498	4.357	3.191	3.118
32ASN	O	499	4.424	3.255	3.198
33PHE	N	500	4.291	3.244	3.013
33PHE	HN	501	4.252	3.183	2.944
33PHE	CA	502	4.299	3.385	2.992
33PHE	HA	503	4.299	3.441	3.084
33PHE	CB	504	4.425	3.421	2.911
33PHE	HB1	505	4.438	3.530	2.901
33PHE	HB2	506	4.507	3.379	2.973

33PHE	CG	507	4.436	3.360	2.775
33PHE	CD1	508	4.517	3.251	2.754
33PHE	HD1	509	4.577	3.221	2.839
33PHE	CE1	510	4.556	3.210	2.629
33PHE	HE1	511	4.629	3.132	2.612
33PHE	CZ	512	4.490	3.267	2.523
33PHE	HZ	513	4.514	3.234	2.423
33PHE	CD2	514	4.370	3.408	2.664
33PHE	HD2	515	4.313	3.497	2.685
33PHE	CE2	516	4.394	3.365	2.535
33PHE	HE2	517	4.335	3.413	2.459
33PHE	C	518	4.170	3.434	2.935
33PHE	O	519	4.074	3.362	2.907
34LEU	N	520	4.163	3.568	2.929
34LEU	HN	521	4.236	3.623	2.969
34LEU	CA	522	4.051	3.648	2.890
34LEU	HA	523	3.973	3.580	2.860
34LEU	CB	524	3.995	3.729	3.008
34LEU	HB1	525	3.978	3.669	3.101
34LEU	HB2	526	4.083	3.789	3.039
34LEU	CG	527	3.864	3.800	2.971
34LEU	HG	528	3.875	3.846	2.870
34LEU	CD1	529	3.745	3.702	2.974
34LEU	HD11	530	3.746	3.637	2.884
34LEU	HD12	531	3.738	3.637	3.064
34LEU	HD13	532	3.653	3.764	2.965
34LEU	CD2	533	3.845	3.921	3.063
34LEU	HD21	534	3.852	3.904	3.173
34LEU	HD22	535	3.906	4.004	3.021
34LEU	HD23	536	3.744	3.962	3.041

34LEU	C	537	4.107	3.728	2.778
34LEU	O	538	4.210	3.789	2.808
35PRO	N	539	4.047	3.732	2.663
35PRO	CD	540	3.973	3.621	2.604
35PRO	HD1	541	3.869	3.638	2.639
35PRO	HD2	542	4.016	3.530	2.651
35PRO	CA	543	4.086	3.820	2.557
35PRO	HA	544	4.185	3.789	2.527
35PRO	CB	545	4.000	3.783	2.435
35PRO	HB1	546	3.900	3.831	2.443
35PRO	HB2	547	4.037	3.828	2.341
35PRO	CG	548	3.992	3.631	2.451
35PRO	HG1	549	3.914	3.585	2.387
35PRO	HG2	550	4.088	3.585	2.419
35PRO	C	551	4.103	3.966	2.582
35PRO	O	552	4.028	4.010	2.670
36VAL	N	553	4.189	4.041	2.512
36VAL	HN	554	4.255	3.994	2.454
36VAL	CA	555	4.199	4.184	2.504
36VAL	HA	556	4.234	4.203	2.604
36VAL	CB	557	4.296	4.229	2.400
36VAL	HB	558	4.268	4.183	2.303
36VAL	CG1	559	4.304	4.380	2.371
36VAL	HG11	560	4.211	4.413	2.321
36VAL	HG12	561	4.312	4.444	2.461
36VAL	HG13	562	4.388	4.395	2.298
36VAL	CG2	563	4.431	4.192	2.463
36VAL	HG21	564	4.464	4.086	2.470
36VAL	HG22	565	4.507	4.239	2.397
36VAL	HG23	566	4.444	4.240	2.563

36VAL	C	567	4.073	4.262	2.492
36VAL	O	568	3.974	4.226	2.429
37ASP	N	569	4.066	4.377	2.562
37ASP	HN	570	4.146	4.408	2.612
37ASP	CA	571	3.954	4.465	2.577
37ASP	HA	572	3.986	4.551	2.635
37ASP	CB	573	3.910	4.537	2.449
37ASP	HB1	574	3.901	4.461	2.369
37ASP	HB2	575	3.814	4.591	2.464
37ASP	CG	576	4.009	4.642	2.400
37ASP	OD1	577	4.110	4.675	2.469
37ASP	OD2	578	3.990	4.709	2.296
37ASP	C	579	3.834	4.410	2.646
37ASP	O	580	3.745	4.484	2.687
38TYR	N	581	3.818	4.278	2.663
38TYR	HN	582	3.872	4.222	2.599
38TYR	CA	583	3.713	4.225	2.743
38TYR	HA	584	3.622	4.279	2.722
38TYR	CB	585	3.689	4.073	2.731
38TYR	HB1	586	3.785	4.030	2.766
38TYR	HB2	587	3.608	4.033	2.797
38TYR	CG	588	3.655	4.036	2.591
38TYR	CD1	589	3.571	4.108	2.510
38TYR	HD1	590	3.551	4.211	2.537
38TYR	CE1	591	3.521	4.058	2.392
38TYR	HE1	592	3.466	4.114	2.318
38TYR	CZ	593	3.568	3.935	2.352
38TYR	OH	594	3.528	3.888	2.225
38TYR	HH	595	3.467	3.958	2.200
38TYR	CD2	596	3.677	3.904	2.558

38TYR	HD2	597	3.735	3.838	2.621
38TYR	CE2	598	3.638	3.853	2.437
38TYR	HE2	599	3.652	3.748	2.413
38TYR	C	600	3.728	4.256	2.888
38TYR	O	601	3.839	4.270	2.940
39GLU	N	602	3.614	4.269	2.959
39GLU	HN	603	3.525	4.250	2.918
39GLU	CA	604	3.595	4.294	3.098
39GLU	HA	605	3.691	4.299	3.148
39GLU	CB	606	3.505	4.417	3.120
39GLU	HB1	607	3.413	4.395	3.062
39GLU	HB2	608	3.474	4.426	3.226
39GLU	CG	609	3.578	4.541	3.070
39GLU	HG1	610	3.670	4.565	3.128
39GLU	HG2	611	3.608	4.527	2.963
39GLU	CD	612	3.492	4.666	3.065
39GLU	OE1	613	3.462	4.722	2.956
39GLU	OE2	614	3.460	4.720	3.174
39GLU	C	615	3.519	4.186	3.167
39GLU	O	616	3.440	4.107	3.114
40ILE	N	617	3.553	4.167	3.296
40ILE	HN	618	3.629	4.216	3.338
40ILE	CA	619	3.498	4.073	3.389
40ILE	HA	620	3.396	4.051	3.362
40ILE	CB	621	3.570	3.943	3.408
40ILE	HB	622	3.534	3.901	3.504
40ILE	CG2	623	3.541	3.845	3.293
40ILE	HG21	624	3.574	3.901	3.203
40ILE	HG22	625	3.608	3.758	3.311
40ILE	HG23	626	3.434	3.815	3.290

40ILE	CG1	627	3.723	3.960	3.422
40ILE	HG11	628	3.771	3.999	3.330
40ILE	HG12	629	3.746	4.039	3.496
40ILE	CD	630	3.793	3.839	3.482
40ILE	HD1	631	3.754	3.808	3.582
40ILE	HD2	632	3.785	3.751	3.414
40ILE	HD3	633	3.901	3.865	3.496
40ILE	C	634	3.482	4.136	3.523
40ILE	O	635	3.571	4.193	3.585
41GLU	N	636	3.364	4.124	3.587
41GLU	HN	637	3.291	4.078	3.538
41GLU	CA	638	3.338	4.177	3.717
41GLU	HA	639	3.401	4.265	3.730
41GLU	CB	640	3.191	4.223	3.715
41GLU	HB1	641	3.181	4.301	3.637
41GLU	HB2	642	3.137	4.131	3.684
41GLU	CG	643	3.153	4.290	3.847
41GLU	HG1	644	3.202	4.239	3.932
41GLU	HG2	645	3.189	4.392	3.821
41GLU	CD	646	3.002	4.300	3.863
41GLU	OE1	647	2.934	4.326	3.760
41GLU	OE2	648	2.949	4.286	3.977
41GLU	C	649	3.365	4.072	3.819
41GLU	O	650	3.323	3.958	3.806
42TYR	N	651	3.435	4.102	3.931
42TYR	HN	652	3.473	4.192	3.946
42TYR	CA	653	3.459	4.010	4.038
42TYR	HA	654	3.469	3.909	4.003
42TYR	CB	655	3.592	4.051	4.104
42TYR	HB1	656	3.673	4.050	4.029

42TYR	HB2	657	3.578	4.159	4.131
42TYR	CG	658	3.628	3.984	4.232
42TYR	CD1	659	3.642	3.847	4.231
42TYR	HD1	660	3.633	3.796	4.136
42TYR	CE1	661	3.668	3.771	4.342
42TYR	HE1	662	3.686	3.665	4.331
42TYR	CZ	663	3.701	3.840	4.457
42TYR	OH	664	3.743	3.769	4.571
42TYR	HH	665	3.767	3.680	4.546
42TYR	CD2	666	3.663	4.045	4.350
42TYR	HD2	667	3.661	4.153	4.362
42TYR	CE2	668	3.699	3.977	4.464
42TYR	HE2	669	3.743	4.033	4.545
42TYR	C	670	3.347	4.014	4.137
42TYR	O	671	3.298	4.120	4.175
43VAL	N	672	3.304	3.893	4.176
43VAL	HN	673	3.345	3.811	4.137
43VAL	CA	674	3.185	3.870	4.251
43VAL	HA	675	3.151	3.966	4.287
43VAL	CB	676	3.066	3.814	4.177
43VAL	HB	677	3.085	3.709	4.148
43VAL	CG1	678	2.943	3.807	4.269
43VAL	HG11	679	2.906	3.905	4.307
43VAL	HG12	680	2.855	3.757	4.222
43VAL	HG13	681	2.960	3.749	4.363
43VAL	CG2	682	3.044	3.896	4.049
43VAL	HG21	683	2.954	3.862	3.996
43VAL	HG22	684	3.034	4.006	4.062
43VAL	HG23	685	3.129	3.884	3.978
43VAL	C	686	3.220	3.787	4.370

43VAL	O	687	3.235	3.666	4.352
44CYS	N	688	3.222	3.846	4.491
44CYS	HN	689	3.202	3.943	4.500
44CYS	CA	690	3.226	3.768	4.610
44CYS	HA	691	3.298	3.688	4.600
44CYS	CB	692	3.281	3.860	4.721
44CYS	HB1	693	3.377	3.901	4.684
44CYS	HB2	694	3.205	3.935	4.752
44CYS	SG	695	3.330	3.775	4.874
44CYS	C	696	3.100	3.694	4.640
44CYS	O	697	2.990	3.729	4.599
45ARG	N	698	3.109	3.577	4.706
45ARG	HN	699	3.198	3.553	4.743
45ARG	CA	700	3.012	3.477	4.738
45ARG	HA	701	2.958	3.455	4.647
45ARG	CB	702	3.072	3.346	4.790
45ARG	HB1	703	3.118	3.373	4.887
45ARG	HB2	704	2.994	3.274	4.824
45ARG	CG	705	3.163	3.280	4.687
45ARG	HG1	706	3.257	3.338	4.676
45ARG	HG2	707	3.192	3.181	4.728
45ARG	CD	708	3.088	3.260	4.555
45ARG	HD1	709	3.007	3.185	4.562
45ARG	HD2	710	3.058	3.359	4.513
45ARG	NE	711	3.196	3.210	4.466
45ARG	HE	712	3.273	3.168	4.514
45ARG	CZ	713	3.187	3.190	4.331
45ARG	NH1	714	3.079	3.228	4.257
45ARG	HH11	715	3.004	3.281	4.296
45ARG	HH12	716	3.072	3.193	4.163

45ARG	NH2	717	3.284	3.116	4.270
45ARG	HH21	718	3.344	3.073	4.338
45ARG	HH22	719	3.258	3.065	4.189
45ARG	C	720	2.913	3.523	4.840
45ARG	O	721	2.939	3.607	4.926
46GLY	N	722	2.792	3.466	4.844
46GLY	HN	723	2.765	3.381	4.798
46GLY	CA	724	2.683	3.521	4.918
46GLY	HA1	725	2.595	3.466	4.888
46GLY	HA2	726	2.707	3.512	5.023
46GLY	C	727	2.641	3.663	4.904
46GLY	O	728	2.623	3.720	4.796
47GLU	N	729	2.613	3.723	5.020
47GLU	HN	730	2.605	3.678	5.109
47GLU	CA	731	2.564	3.858	5.027
47GLU	HA	732	2.515	3.891	4.937
47GLU	CB	733	2.461	3.855	5.141
47GLU	HB1	734	2.518	3.840	5.234
47GLU	HB2	735	2.422	3.959	5.141
47GLU	CG	736	2.337	3.766	5.123
47GLU	HG1	737	2.307	3.770	5.016
47GLU	HG2	738	2.363	3.663	5.155
47GLU	CD	739	2.216	3.818	5.198
47GLU	OE1	740	2.104	3.772	5.161
47GLU	OE2	741	2.209	3.904	5.291
47GLU	C	742	2.672	3.958	5.054
47GLU	O	743	2.658	4.080	5.050
48ARG	N	744	2.794	3.914	5.087
48ARG	HN	745	2.814	3.816	5.083
48ARG	CA	746	2.912	3.995	5.104

48ARG	HA	747	2.878	4.078	5.164
48ARG	CB	748	3.038	3.920	5.151
48ARG	HB1	749	3.052	3.825	5.097
48ARG	HB2	750	3.126	3.987	5.144
48ARG	CG	751	3.029	3.882	5.299
48ARG	HG1	752	3.009	3.972	5.360
48ARG	HG2	753	2.939	3.816	5.304
48ARG	CD	754	3.152	3.820	5.365
48ARG	HD1	755	3.234	3.894	5.355
48ARG	HD2	756	3.136	3.796	5.473
48ARG	NE	757	3.173	3.695	5.286
48ARG	HE	758	3.093	3.652	5.245
48ARG	CZ	759	3.287	3.649	5.226
48ARG	NH1	760	3.404	3.719	5.243
48ARG	HH11	761	3.424	3.811	5.275
48ARG	HH12	762	3.487	3.678	5.205
48ARG	NH2	763	3.293	3.539	5.146
48ARG	HH21	764	3.220	3.473	5.162
48ARG	HH22	765	3.382	3.498	5.128
48ARG	C	766	2.952	4.064	4.978
48ARG	O	767	2.944	4.001	4.873
49GLU	N	768	3.000	4.189	4.975
49GLU	HN	769	2.984	4.241	5.059
49GLU	CA	770	3.039	4.258	4.855
49GLU	HA	771	2.998	4.206	4.770
49GLU	CB	772	2.972	4.396	4.853
49GLU	HB1	773	2.984	4.442	4.954
49GLU	HB2	774	3.025	4.462	4.780
49GLU	CG	775	2.821	4.388	4.832
49GLU	HG1	776	2.788	4.383	4.725

49GLU	HG2	777	2.764	4.302	4.873
49GLU	CD	778	2.755	4.505	4.904
49GLU	OE1	779	2.699	4.594	4.835
49GLU	OE2	780	2.760	4.510	5.030
49GLU	C	781	3.187	4.271	4.849
49GLU	O	782	3.262	4.260	4.946
50VAL	N	783	3.235	4.304	4.728
50VAL	HN	784	3.175	4.315	4.651
50VAL	CA	785	3.373	4.324	4.695
50VAL	HA	786	3.436	4.251	4.747
50VAL	CB	787	3.392	4.309	4.547
50VAL	HB	788	3.316	4.369	4.493
50VAL	CG1	789	3.531	4.351	4.496
50VAL	HG11	790	3.558	4.452	4.534
50VAL	HG12	791	3.612	4.288	4.537
50VAL	HG13	792	3.523	4.359	4.385
50VAL	CG2	793	3.378	4.163	4.504
50VAL	HG21	794	3.276	4.118	4.512
50VAL	HG22	795	3.404	4.147	4.397
50VAL	HG23	796	3.442	4.098	4.568
50VAL	C	797	3.431	4.451	4.747
50VAL	O	798	3.367	4.555	4.760
51VAL	N	799	3.560	4.446	4.785
51VAL	HN	800	3.612	4.362	4.773
51VAL	CA	801	3.635	4.559	4.832
51VAL	HA	802	3.577	4.644	4.864
51VAL	CB	803	3.713	4.530	4.957
51VAL	HB	804	3.766	4.437	4.928
51VAL	CG1	805	3.808	4.647	4.986
51VAL	HG11	806	3.886	4.665	4.908

51VAL	HG12	807	3.753	4.741	5.006
51VAL	HG13	808	3.871	4.631	5.076
51VAL	CG2	809	3.619	4.516	5.078
51VAL	HG21	810	3.556	4.604	5.102
51VAL	HG22	811	3.552	4.431	5.052
51VAL	HG23	812	3.681	4.503	5.169
51VAL	C	813	3.719	4.609	4.720
51VAL	O	814	3.791	4.540	4.649
52GLY	N	815	3.712	4.742	4.704
52GLY	HN	816	3.648	4.795	4.759
52GLY	CA	817	3.762	4.822	4.596
52GLY	HA1	818	3.744	4.928	4.611
52GLY	HA2	819	3.864	4.788	4.597
52GLY	C	820	3.703	4.795	4.462
52GLY	O	821	3.584	4.768	4.448
53PRO	N	822	3.774	4.828	4.357
53PRO	CD	823	3.892	4.912	4.360
53PRO	HD1	824	3.985	4.853	4.378
53PRO	HD2	825	3.884	4.995	4.434
53PRO	CA	826	3.729	4.803	4.223
53PRO	HA	827	3.638	4.860	4.216
53PRO	CB	828	3.830	4.870	4.129
53PRO	HB1	829	3.910	4.803	4.092
53PRO	HB2	830	3.780	4.920	4.043
53PRO	CG	831	3.883	4.980	4.223
53PRO	HG1	832	3.988	5.008	4.200
53PRO	HG2	833	3.833	5.079	4.217
53PRO	C	834	3.693	4.663	4.190
53PRO	O	835	3.770	4.570	4.215
54LYS	N	836	3.576	4.645	4.127

54LYS	HN	837	3.519	4.723	4.102
54LYS	CA	838	3.527	4.512	4.108
54LYS	HA	839	3.578	4.442	4.173
54LYS	CB	840	3.376	4.510	4.136
54LYS	HB1	841	3.325	4.581	4.067
54LYS	HB2	842	3.335	4.409	4.119
54LYS	CG	843	3.319	4.567	4.267
54LYS	HG1	844	3.384	4.526	4.347
54LYS	HG2	845	3.329	4.677	4.272
54LYS	CD	846	3.172	4.526	4.281
54LYS	HD1	847	3.163	4.420	4.311
54LYS	HD2	848	3.138	4.581	4.371
54LYS	CE	849	3.089	4.561	4.157
54LYS	HE1	850	3.090	4.667	4.125
54LYS	HE2	851	3.117	4.502	4.067
54LYS	NZ	852	2.944	4.536	4.177
54LYS	HZ1	853	2.885	4.528	4.092
54LYS	HZ2	854	2.923	4.455	4.239
54LYS	HZ3	855	2.910	4.619	4.230
54LYS	C	856	3.551	4.465	3.968
54LYS	O	857	3.550	4.346	3.938
55VAL	N	858	3.554	4.559	3.872
55VAL	HN	859	3.546	4.656	3.894
55VAL	CA	860	3.565	4.527	3.733
55VAL	HA	861	3.533	4.427	3.709
55VAL	CB	862	3.480	4.617	3.649
55VAL	HB	863	3.486	4.722	3.685
55VAL	CG1	864	3.512	4.599	3.500
55VAL	HG11	865	3.561	4.500	3.491
55VAL	HG12	866	3.423	4.598	3.433

55VAL	HG13	867	3.576	4.684	3.469
55VAL	CG2	868	3.336	4.571	3.678
55VAL	HG21	869	3.330	4.464	3.650
55VAL	HG22	870	3.308	4.591	3.784
55VAL	HG23	871	3.271	4.625	3.606
55VAL	C	872	3.710	4.539	3.700
55VAL	O	873	3.775	4.637	3.738
56ARG	N	874	3.768	4.438	3.633
56ARG	HN	875	3.719	4.360	3.594
56ARG	CA	876	3.896	4.451	3.572
56ARG	HA	877	3.931	4.552	3.592
56ARG	CB	878	3.999	4.353	3.631
56ARG	HB1	879	4.100	4.374	3.591
56ARG	HB2	880	3.999	4.379	3.739
56ARG	CG	881	3.958	4.206	3.628
56ARG	HG1	882	3.855	4.184	3.662
56ARG	HG2	883	3.951	4.182	3.519
56ARG	CD	884	4.065	4.126	3.703
56ARG	HD1	885	4.044	4.017	3.706
56ARG	HD2	886	4.167	4.135	3.661
56ARG	NE	887	4.073	4.167	3.846
56ARG	HE	888	3.979	4.186	3.877
56ARG	CZ	889	4.178	4.210	3.922
56ARG	NH1	890	4.307	4.175	3.894
56ARG	HH11	891	4.323	4.117	3.814
56ARG	HH12	892	4.369	4.183	3.972
56ARG	NH2	893	4.154	4.270	4.042
56ARG	HH21	894	4.076	4.332	4.046
56ARG	HH22	895	4.236	4.309	4.085
56ARG	C	896	3.886	4.430	3.425

56ARG	O	897	3.798	4.360	3.375
57LYS	N	898	3.984	4.483	3.348
57LYS	HN	899	4.046	4.542	3.398
57LYS	CA	900	3.991	4.486	3.205
57LYS	HA	901	3.918	4.418	3.164
57LYS	CB	902	3.970	4.629	3.155
57LYS	HB1	903	3.868	4.658	3.188
57LYS	HB2	904	4.031	4.713	3.195
57LYS	CG	905	3.954	4.631	3.002
57LYS	HG1	906	4.049	4.611	2.948
57LYS	HG2	907	3.883	4.548	2.981
57LYS	CD	908	3.883	4.756	2.951
57LYS	HD1	909	3.862	4.746	2.843
57LYS	HD2	910	3.794	4.770	3.016
57LYS	CE	911	3.964	4.884	2.972
57LYS	HE1	912	3.970	4.897	3.082
57LYS	HE2	913	4.060	4.890	2.916
57LYS	NZ	914	3.884	4.991	2.909
57LYS	HZ1	915	3.945	5.071	2.934
57LYS	HZ2	916	3.886	4.985	2.805
57LYS	HZ3	917	3.792	5.004	2.956
57LYS	C	918	4.121	4.434	3.155
57LYS	O	919	4.222	4.485	3.205
58CYS	N	920	4.122	4.346	3.054
58CYS	HN	921	4.041	4.306	3.012
58CYS	CA	922	4.249	4.316	2.996
58CYS	HA	923	4.327	4.309	3.070
58CYS	CB	924	4.237	4.177	2.930
58CYS	HB1	925	4.203	4.096	2.997
58CYS	HB2	926	4.159	4.195	2.853

58CYS	SG	927	4.379	4.107	2.840
58CYS	C	928	4.297	4.422	2.902
58CYS	O	929	4.222	4.461	2.813
59LEU	N	930	4.420	4.472	2.918
59LEU	HN	931	4.484	4.445	2.990
59LEU	CA	932	4.468	4.575	2.830
59LEU	HA	933	4.382	4.631	2.796
59LEU	CB	934	4.555	4.679	2.903
59LEU	HB1	935	4.649	4.631	2.937
59LEU	HB2	936	4.587	4.758	2.831
59LEU	CG	937	4.483	4.741	3.024
59LEU	HG	938	4.486	4.662	3.102
59LEU	CD1	939	4.570	4.856	3.078
59LEU	HD11	940	4.672	4.818	3.097
59LEU	HD12	941	4.578	4.941	3.006
59LEU	HD13	942	4.541	4.894	3.178
59LEU	CD2	943	4.338	4.787	3.001
59LEU	HD21	944	4.332	4.851	2.910
59LEU	HD22	945	4.269	4.700	3.004
59LEU	HD23	946	4.302	4.854	3.082
59LEU	C	947	4.549	4.513	2.722
59LEU	O	948	4.589	4.397	2.723
60ALA	N	949	4.584	4.587	2.615
60ALA	HN	950	4.547	4.679	2.625
60ALA	CA	951	4.629	4.534	2.490
60ALA	HA	952	4.572	4.451	2.451
60ALA	CB	953	4.622	4.631	2.370
60ALA	HB1	954	4.533	4.693	2.390
60ALA	HB2	955	4.709	4.699	2.378
60ALA	HB3	956	4.624	4.586	2.268

60ALA	C	957	4.764	4.473	2.492
60ALA	O	958	4.791	4.384	2.411
61ASN	N	959	4.847	4.502	2.594
61ASN	HN	960	4.811	4.575	2.653
61ASN	CA	961	4.967	4.433	2.627
61ASN	HA	962	5.001	4.377	2.540
61ASN	CB	963	5.072	4.537	2.669
61ASN	HB1	964	5.175	4.496	2.673
61ASN	HB2	965	5.069	4.608	2.584
61ASN	CG	966	5.038	4.627	2.787
61ASN	OD1	967	4.931	4.609	2.844
61ASN	ND2	968	5.124	4.728	2.815
61ASN	HD21	969	5.108	4.790	2.892
61ASN	HD22	970	5.193	4.745	2.744
61ASN	C	971	4.961	4.319	2.723
61ASN	O	972	5.064	4.273	2.771
62GLY	N	973	4.844	4.258	2.750
62GLY	HN	974	4.755	4.286	2.715
62GLY	CA	975	4.847	4.142	2.834
62GLY	HA1	976	4.756	4.085	2.818
62GLY	HA2	977	4.921	4.076	2.791
62GLY	C	978	4.877	4.168	2.977
62GLY	O	979	4.946	4.096	3.050
63SER	N	980	4.819	4.281	3.023
63SER	HN	981	4.747	4.320	2.966
63SER	CA	982	4.822	4.336	3.155
63SER	HA	983	4.861	4.267	3.228
63SER	CB	984	4.911	4.460	3.169
63SER	HB1	985	4.927	4.481	3.277
63SER	HB2	986	5.011	4.435	3.129

63SER	OG	987	4.856	4.578	3.112
63SER	HG1	988	4.876	4.589	3.019
63SER	C	989	4.679	4.355	3.193
63SER	O	990	4.590	4.372	3.110
64TRP	N	991	4.652	4.357	3.325
64TRP	HN	992	4.720	4.333	3.394
64TRP	CA	993	4.534	4.407	3.390
64TRP	HA	994	4.457	4.398	3.315
64TRP	CB	995	4.500	4.309	3.503
64TRP	HB1	996	4.579	4.310	3.582
64TRP	HB2	997	4.409	4.341	3.557
64TRP	CG	998	4.469	4.170	3.458
64TRP	CD1	999	4.550	4.061	3.475
64TRP	HD1	1000	4.654	4.051	3.501
64TRP	NE1	1001	4.482	3.949	3.434
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64TRP	HE3	1006	4.197	4.279	3.395
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64TRP	CH2	1011	4.138	3.967	3.310
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64TRP	O	1014	4.641	4.603	3.478
65THR	N	1015	4.419	4.609	3.442
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65THR	CA 1017	4.405	4.732	3.515
65THR	HA 1018	4.478	4.802	3.477
65THR	CB 1019	4.264	4.782	3.500
65THR	HB 1020	4.232	4.862	3.570
65THR	OG1 1021	4.169	4.678	3.522
65THR	HG1 1022	4.132	4.701	3.607
65THR	CG2 1023	4.247	4.841	3.360
65THR	HG21 1024	4.145	4.883	3.343
65THR	HG22 1025	4.316	4.927	3.353
65THR	HG23 1026	4.261	4.765	3.280
65THR	C 1027	4.443	4.733	3.659
65THR	O 1028	4.491	4.832	3.713
66ASP	N 1029	4.410	4.625	3.731
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66ASP	CG 1036	4.233	4.649	3.979
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66ASP	OD2 1038	4.111	4.617	3.982
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66ASP	O 1040	4.593	4.418	3.799
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67MET	CA 1043	4.797	4.503	3.980
67MET	HA 1044	4.837	4.495	3.880
67MET	CB 1045	4.896	4.587	4.063
67MET	HB1 1046	4.993	4.539	4.086

67MET	HB2 1047	4.925	4.680	4.008
67MET	CG 1048	4.836	4.641	4.192
67MET	HG1 1049	4.740	4.689	4.166
67MET	HG2 1050	4.798	4.549	4.240
67MET	SD 1051	4.925	4.748	4.311
67MET	CE 1052	4.971	4.888	4.204
67MET	HE1 1053	4.882	4.933	4.154
67MET	HE2 1054	5.005	4.966	4.275
67MET	HE3 1055	5.054	4.850	4.141
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69THR	HG1 1077	4.621	3.832	4.337
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70PRO	HA 1089	4.089	4.063	4.249
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71SER	CB 1102	4.229	3.854	4.591
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71SER	OG 1105	4.300	3.977	4.578
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72ARG	HB1 1114	3.961	4.337	4.689
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72ARG	CG 1116	4.144	4.285	4.783
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72ARG	HG2 1118	4.171	4.223	4.695
72ARG	CD 1119	4.208	4.424	4.771
72ARG	HD1 1120	4.316	4.411	4.747
72ARG	HD2 1121	4.156	4.491	4.699
72ARG	NE 1122	4.209	4.482	4.908
72ARG	HE 1123	4.198	4.423	4.988
72ARG	CZ 1124	4.238	4.614	4.921
72ARG	NH1 1125	4.278	4.698	4.821
72ARG	HH11 1126	4.285	4.671	4.725
72ARG	HH12 1127	4.347	4.767	4.841
72ARG	NH2 1128	4.253	4.664	5.047
72ARG	HH21 1129	4.217	4.613	5.125
72ARG	HH22 1130	4.245	4.763	5.059
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72ARG	O 1132	3.706	4.204	4.745
73CYS	N 1133	3.741	4.111	4.947
73CYS	HN 1134	3.803	4.069	5.013
73CYS	CA 1135	3.603	4.112	4.984
73CYS	HA 1136	3.557	4.198	4.936

73CYS	CB 1137	3.551	3.976	4.935
73CYS	HB1 1138	3.568	3.981	4.825
73CYS	HB2 1139	3.629	3.907	4.973
73CYS	SG 1140	3.376	3.946	4.973
73CYS	C 1141	3.588	4.128	5.131
73CYS	O 1142	3.674	4.084	5.207
74VAL	N 1143	3.483	4.205	5.168
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74VAL	HA 1146	3.535	4.312	5.335
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74VAL	HB 1148	3.320	4.340	5.443
74VAL	CG1 1149	3.335	4.449	5.258
74VAL	HG11 1150	3.241	4.503	5.284
74VAL	HG12 1151	3.425	4.512	5.275
74VAL	HG13 1152	3.340	4.428	5.149
74VAL	CG2 1153	3.212	4.226	5.296
74VAL	HG21 1154	3.199	4.139	5.364
74VAL	HG22 1155	3.121	4.287	5.310
74VAL	HG23 1156	3.219	4.196	5.189
74VAL	C 1157	3.455	4.131	5.403
74VAL	O 1158	3.426	4.014	5.378
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75ARG	CB 1163	3.599	4.058	5.732
75ARG	HB1 1164	3.615	4.152	5.788
75ARG	HB2 1165	3.577	3.978	5.806
75ARG	CG 1166	3.726	4.030	5.652

75ARG	HG1 1167	3.744	4.122	5.593
75ARG	HG2 1168	3.814	4.024	5.719
75ARG	CD 1169	3.739	3.913	5.554
75ARG	HD1 1170	3.665	3.927	5.472
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75ARG	NE 1172	3.707	3.793	5.637
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75ARG	CZ 1174	3.665	3.672	5.590
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75ARG	HH11 1176	3.744	3.688	5.409
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75ARG	NH2 1178	3.616	3.575	5.672
75ARG	HH21 1179	3.630	3.600	5.768
75ARG	HH22 1180	3.600	3.483	5.637
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24ASP	CA 1197	2.804	2.720	4.172
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24ASP	HB1 1200	2.610	2.771	4.260
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24ASP	OD1 1203	2.451	2.658	4.092
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24ASP	C 1205	2.884	2.824	4.243
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25ASP	CA 1209	3.009	2.904	4.439
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25ASP	CB 1211	2.972	2.901	4.588
25ASP	HB1 1212	3.004	2.808	4.640
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25ASP	CG 1214	2.826	2.935	4.612
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25ASP	C 1217	3.151	2.861	4.431
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26SER	CA 1221	3.316	2.694	4.360
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27ASP	CB 1234	3.194	2.719	3.891
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27ASP	HB2 1236	3.228	2.745	3.788
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28VAL	HA 1245	3.494	3.098	4.005
28VAL	CB 1246	3.652	3.044	3.868
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28VAL	HG12 1250	3.638	3.198	3.706
28VAL	HG13 1251	3.687	3.251	3.884
28VAL	CG2 1252	3.748	3.017	3.984
28VAL	HG21 1253	3.847	3.013	3.936
28VAL	HG22 1254	3.761	3.099	4.058
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29TRP	HA 1261	3.306	3.226	3.624
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29TRP	HD1 1267	3.504	2.918	3.407
29TRP	NE1 1268	3.590	3.099	3.324
29TRP	HE1 1269	3.679	3.069	3.296
29TRP	CE2 1270	3.530	3.220	3.300
29TRP	CD2 1271	3.409	3.225	3.366
29TRP	CE3 1272	3.336	3.340	3.370
29TRP	HE3 1273	3.238	3.345	3.415
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30TRP	CA 1284	2.938	3.265	3.756
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30TRP	HB1 1287	2.981	3.468	3.783
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30TRP	CG 1289	2.772	3.459	3.803
30TRP	CD1 1290	2.649	3.477	3.746
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30TRP	NE1 1292	2.560	3.519	3.842
30TRP	HE1 1293	2.466	3.543	3.841
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30TRP	CD2 1295	2.750	3.481	3.943
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30TRP	HE3 1297	2.938	3.454	4.032
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30TRP	HZ3 1299	2.859	3.502	4.261
30TRP	CZ2 1300	2.576	3.570	4.085
30TRP	HZ2 1301	2.476	3.605	4.104
30TRP	CH2 1302	2.663	3.548	4.190
30TRP	HH2 1303	2.625	3.579	4.286
30TRP	C 1304	2.837	3.166	3.708
30TRP	O 1305	2.836	3.133	3.590
31GLY	N 1306	2.754	3.112	3.799
31GLY	HN 1307	2.748	3.120	3.898
31GLY	CA 1308	2.646	3.034	3.745
31GLY	HA1 1309	2.684	2.962	3.674
31GLY	HA2 1310	2.604	2.994	3.836
31GLY	C 1311	2.530	3.102	3.681
31GLY	O 1312	2.541	3.213	3.629
32GLY	N 1313	2.411	3.039	3.680
32GLY	HN 1314	2.395	2.959	3.737
32GLY	CA 1315	2.290	3.090	3.625
32GLY	HA1 1316	2.211	3.024	3.659

32GLY	HA2 1317	2.285	3.190	3.666
32GLY	C 1318	2.281	3.111	3.478
32GLY	O 1319	2.375	3.075	3.407
33NME	N 1320	2.175	3.172	3.420
33NME	HN 1321	2.097	3.204	3.472
33NME	CH3 1322	2.160	3.200	3.281
33NME	HH31 1323	2.056	3.189	3.243
33NME	HH32 1324	2.209	3.298	3.262
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7.40210	7.40210	7.40210		

(a)

(b)

S50
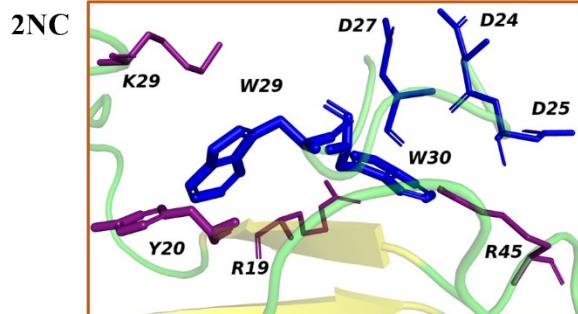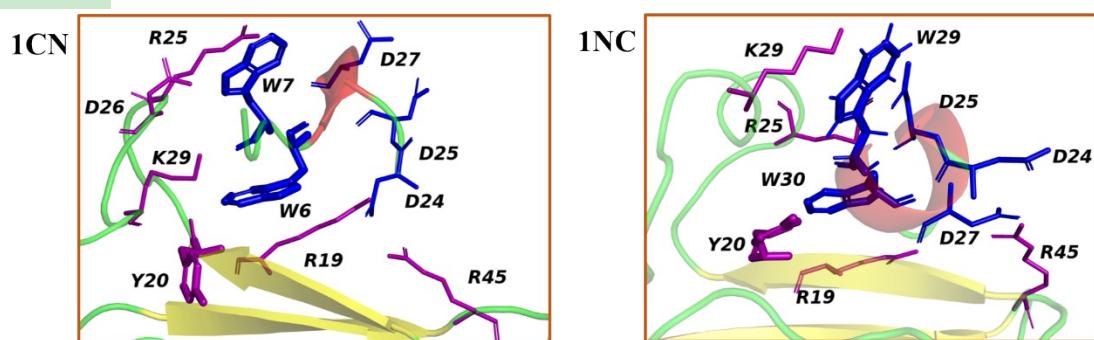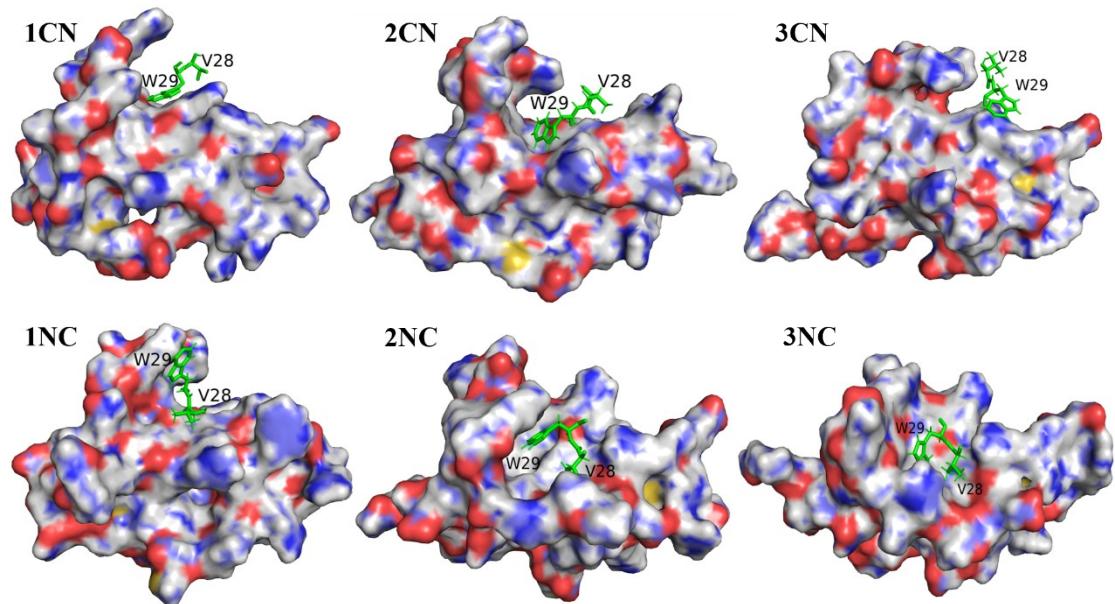
Figure S1. (a) Diagrams of major residue interactions of three complexes (1CN, 1NC, 2NC) of APP9mer-SD1. SD1 and APP9mer are presented in the form of Cartoon, and the key residues are shown in stick (blue residues belong to APP9mer, purple residues belong to SD1). (b) Binding mode of V28 and W29 of APP9mer (stick representation) interacting with the hydrophobic pocket of SD1(molecular surface representation and different colors represent different elements).
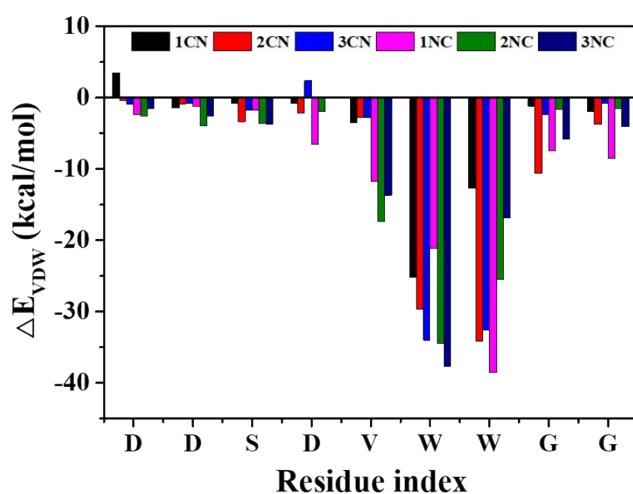
Figure S2. The contribution of each residue in the APP9mer of the six systems to the ΔE_{VDW}.
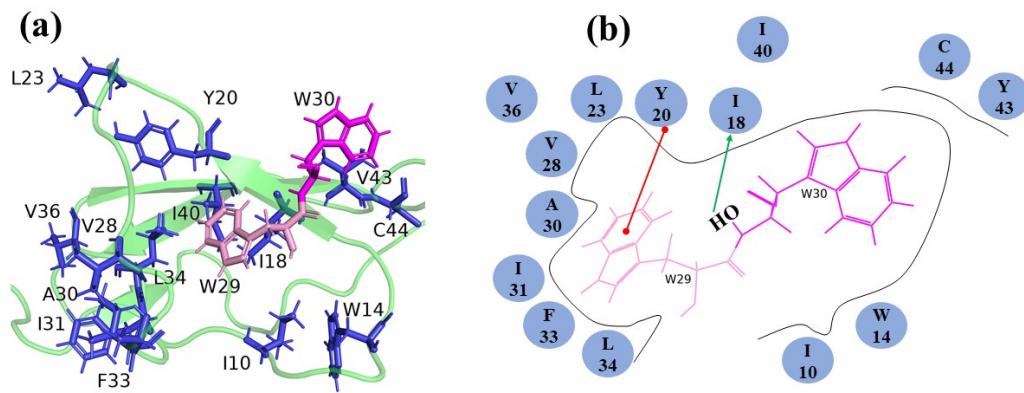
Figure S3. The positional relationship between residues W29, W30 of APP9mer (a) and the hydrophobic pocket in SD1 (indicated by blue balls) (b). The red and green lines stand for the π-π stacking and H-bond interaction, respectively.
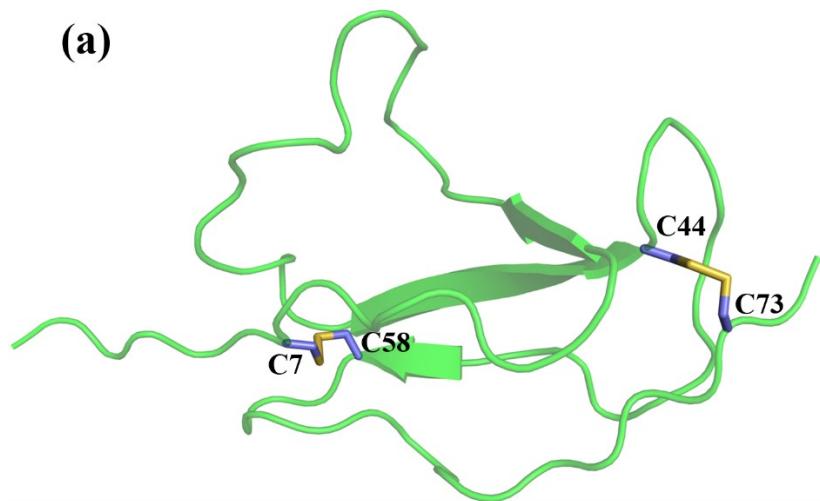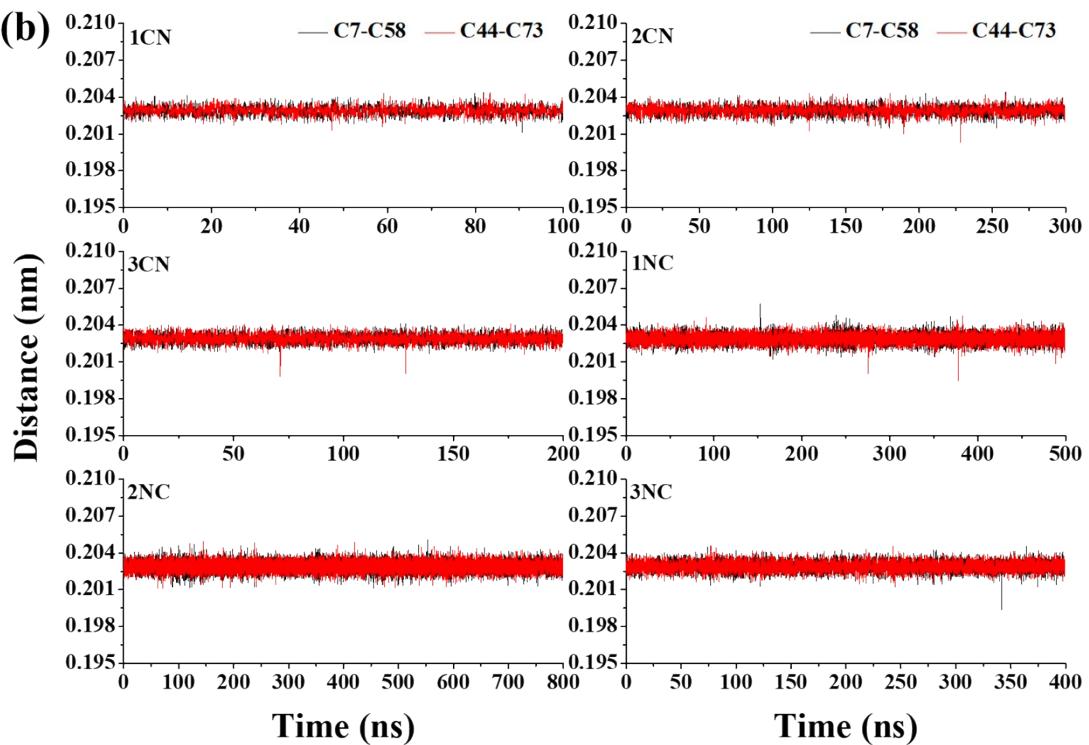
Figure S4. (a) Two disulfide bonds C7-C58, C44-C73 formed by Cys in SD1 (shown in yellow bars). (b) The distances between C7 and C58, and between C44 and C73, changed along with the simulation time during the whole process of MD simulation. Disulfide bonds C7-C58 and C44-C73 are represented by black and red curves respectively.
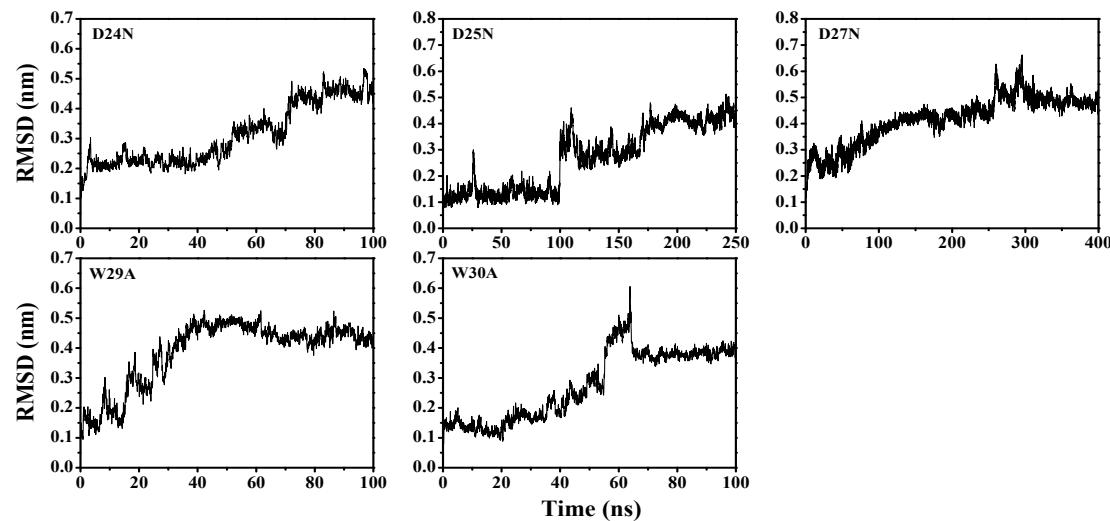
Figure S5. The RMSD curves of the mutant system 1CN-mut.
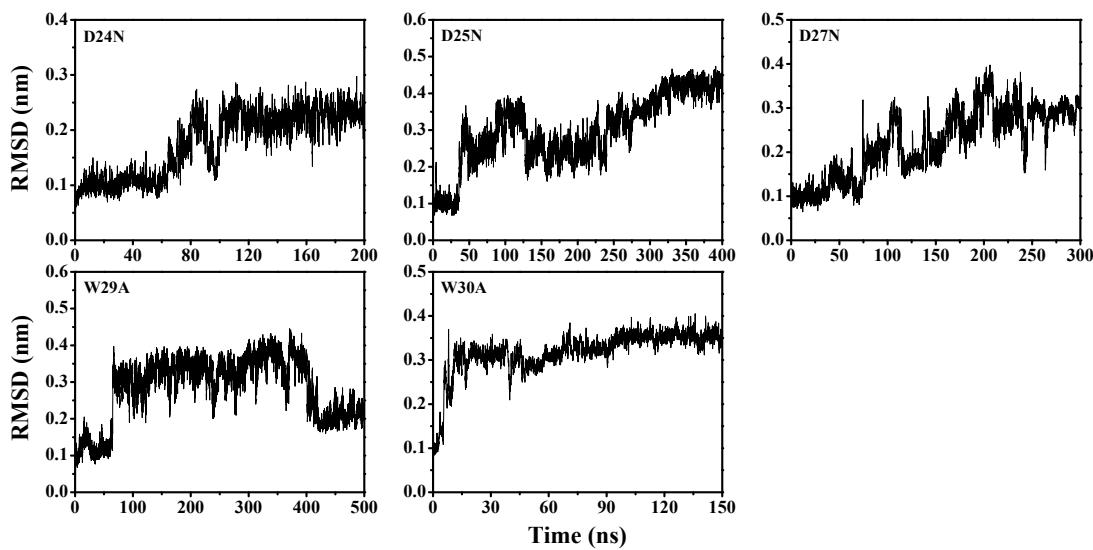
Figure S6. The RMSD curves of the mutant system 1NC-mut.
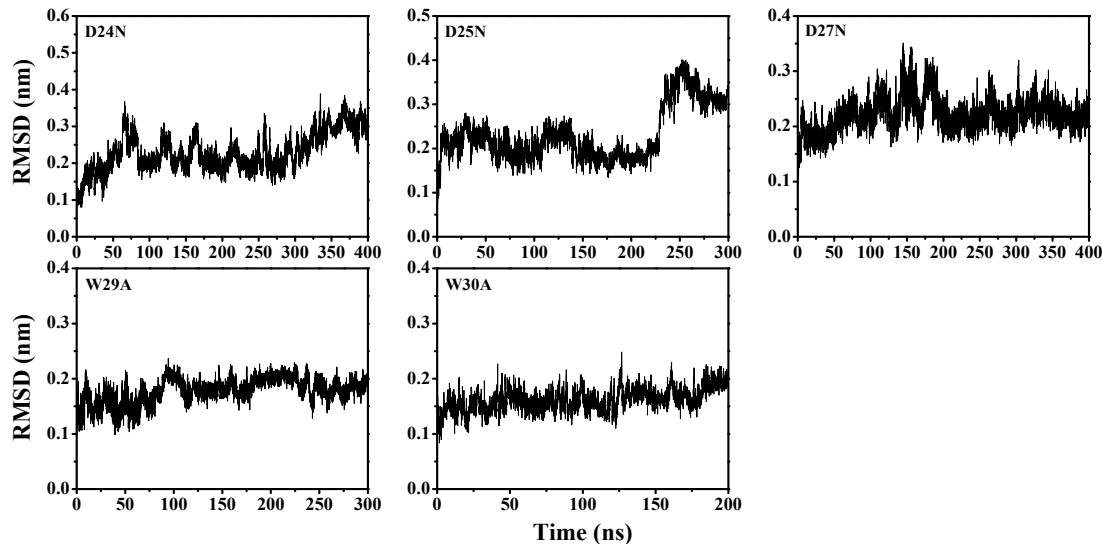
Figure S7. The RMSD curves of the mutant system 2NC-mut.

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