Supplementary Table S1. Summary of structural and interfacial parameters of the TmGpx1–CK2β complex across three independent molecular dynamics simulations.

Parameter	Rep 1	Rep 2	Rep 3	Mean ± SD (n = 3)	Source
Complex backbone RMSD (nm)	1.321 ± 0.241	1.638 ± 0.230	1.282 ± 0.246	1.414 ± 0.195	Figure 2A
Complex Rg (nm)	2.933 ± 0.144	2.838 ± 0.102	2.737 ± 0.102	2.836 ± 0.098	Figure 2B
CK2β backbone RMSD (nm)	1.219 ± 0.261	1.075 ± 0.099	0.968 ± 0.089	1.087 ± 0.126	Figure 2C
TmGpx1 backbone RMSD (nm)	1.067 ± 0.280	1.267 ± 0.305	1.356 ± 0.379	1.230 ± 0.148	Figure 2D
CK2β Rg (nm)	2.016 ± 0.128	1.928 ± 0.045	2.024 ± 0.050	1.989 ± 0.053	Suppl. Fig. S1A
TmGpx1 Rg (nm)	1.950 ± 0.186	1.975 ± 0.166	1.831 ± 0.164	1.919 ± 0.077	Suppl. Fig. S1B
Minimum intermolecular distance (nm)	0.265 ± 0.007	0.266 ± 0.007	0.267 ± 0.006	0.266 ± 0.001	Figure 3A
Heavy-atom contacts (count)	228.1 ± 39.3	248.6 ± 36.6	164.6 ± 22.8	213.8 ± 43.8	Figure 3B
Intermolecular H-bonds (per frame)	11.65 ± 2.976	12.05 ± 2.440	11.52 ± 2.351	11.74 ± 0.276	Figure 3C
Buried surface area (nm²)	19.06 ± 1.548	19.87 ± 1.363	16.86 ± 1.764	18.60 ± 1.558	Figure 3D

Supplementary Table S2. Summary of solvent-accessible surface area and salt-bridge interactions between TmGpx1 and CK2β across three independent molecular dynamics simulations.

Parameter	Rep 1	Rep 2	Rep 3	Mean ± SD (n = 3)	Source
SASA, complex (nm²)	235.7 ± 9.111	231.2 ± 6.434	229.1 ± 7.080	232.0 ± 3.372	Suppl. Fig. S2A
SASA, CK2β (nm²)	136.8 ± 5.214	132.3 ± 4.416	133.1 ± 4.287	134.1 ± 2.401	Suppl. Fig. S2B
SASA, TmGpx1 (nm²)	117.9 ± 4.388	118.7 ± 4.470	112.9 ± 5.223	116.5 ± 3.143	Suppl. Fig. S2C
Salt-bridge distance, TmGpx1(+)–CK2β(–) (nm)	0.273 ± 0.022	0.271 ± 0.008	0.272 ± 0.007	0.272 ± 0.001	Suppl. Fig. S3A
Salt-bridge count, TmGpx1(+)–CK2β(–) (per frame)	6.372 ± 2.378	6.075 ± 1.764	8.075 ± 2.048	6.84 ± 1.079	Suppl. Fig. S3B
Salt-bridge distance, TmGpx1(–)–CK2β(+) (nm)	1.601 ± 0.230	1.391 ± 0.318	0.585 ± 0.251	1.192 ± 0.536	Suppl. Fig. S3C
Salt-bridge count, TmGpx1(–)–CK2β(+) (per frame)	0.000 ± 0.000	0.012 ± 0.143	0.940 ± 1.622	0.317 ± 0.539	Suppl. Fig. S3D

Supplementary Table S3. Intermolecular hydrogen-bond occupancy between TmGpx1 and CK2β across three independent molecular dynamics simulations. Hydrogen bonds are listed according to donor and acceptor residues, with “Main” and “Side” indicating main-chain and side-chain atoms, respectively. Occupancy represents the percentage of trajectory frames in which each hydrogen bond was present during the 200-ns simulation. Only hydrogen bonds with an occupancy of at least 20% are shown. Multiple entries involving the same residue pair represent distinct atom-specific hydrogen bonds.

Replicate	Donor	Acceptor	Occupancy_%
1	GLY40 - Main (TmGpx1)	GLU57 - Side (CK2B)	46.3877
1	GLN76 - Side (TmGpx1)	GLU57 - Side (CK2B)	43.8078
1	GLY40 - Main (TmGpx1)	GLU57 - Side (CK2B)	43.4478
1	GLN76 - Side (TmGpx1)	GLU57 - Side (CK2B)	42.6029
1	LYS117 - Side (TmGpx1)	GLU5 - Side (CK2B)	36.3182
1	GLY106 - Main (TmGpx1)	GLU5 - Side (CK2B)	31.7334
1	ARG128 - Side (TmGpx1)	GLU5 - Main (CK2B)	28.5886
1	LYS153 - Side (TmGpx1)	GLU60 - Side (CK2B)	28.1986
1	LYS117 - Side (TmGpx1)	GLU5 - Side (CK2B)	27.0536
1	SER107 - Main (TmGpx1)	GLU6 - Side (CK2B)	26.9587
1	LYS153 - Side (TmGpx1)	GLU60 - Side (CK2B)	24.8688
1	SER107 - Main (TmGpx1)	GLU6 - Side (CK2B)	24.5138
2	LYS117 - Side (TmGpx1)	GLU5 - Side (CK2B)	65.6317
2	LYS117 - Side (TmGpx1)	GLU5 - Side (CK2B)	54.2423
2	GLY106 - Main (TmGpx1)	GLU5 - Side (CK2B)	44.8828
2	SER107 - Main (TmGpx1)	GLU6 - Side (CK2B)	36.5982
2	ARG17 - Side (CK2B)	LEU123 - Main (TmGpx1)	36.3232
2	SER107 - Main (TmGpx1)	GLU6 - Side (CK2B)	33.2533
2	SER107 - Side (TmGpx1)	GLU6 - Side (CK2B)	32.1384
2	GLN76 - Side (TmGpx1)	GLU57 - Side (CK2B)	30.7885
2	SER107 - Side (TmGpx1)	GLU6 - Side (CK2B)	30.3985
2	GLN76 - Side (TmGpx1)	GLU57 - Side (CK2B)	22.9889
2	GLY106 - Main (TmGpx1)	GLU5 - Side (CK2B)	22.9039
3	TRP12 - Side (CK2B)	LEU130 - Main (TmGpx1)	96.5002
3	ARG17 - Main (CK2B)	GLN72 - Main (TmGpx1)	89.3455
3	GLY74 - Main (TmGpx1)	GLY15 - Main (CK2B)	86.7157
3	SER69 - Side (CK2B)	LEU124 - Main (TmGpx1)	72.9314
3	ARG128 - Side (TmGpx1)	GLU73 - Side (CK2B)	63.8318
3	ARG128 - Side (TmGpx1)	GLU73 - Side (CK2B)	47.2276

Supplementary Table S4. RMSD clustering of the TmGpx1–CK2β complex during 150–200 ns using the GROMOS method with a 0.5-nm cutoff. The dominant-cluster population and cumulative contribution of the three largest clusters are shown for each replicate.

Replicate	Time window	Total frames	Cutoff (nm)	Total clusters	Cluster 1 frames (%)	Top 3 clusters (%)
Rep 1	150–200 ns	5001	0.5	11	3296 / 5001 (65.91%)	89.46%
Rep 2	150–200 ns	5001	0.5	12	3295 / 5001 (65.89%)	92.58%
Rep 3	150–200 ns	5001	0.5	7	2786 / 5001 (55.71%)	87.80%

Supplementary Table S5. Distribution of frames among RMSD clusters for the TmGpx1–CK2β complex during 150–200 ns. Values indicate the number and percentage of frames assigned to each cluster in the three replicates.

Cluster	Rep 1 frames (%)	Rep 2 frames (%)	Rep 3 frames (%)
1	3296 (65.91)	3295 (65.89)	2786 (55.71)
2	821 (16.42)	822 (16.44)	930 (18.60)
3	357 (7.14)	513 (10.26)	675 (13.50)
4	186 (3.72)	197 (3.94)	311 (6.22)
5	124 (2.48)	76 (1.52)	242 (4.84)
6	120 (2.40)	45 (0.90)	56 (1.12)
7	55 (1.10)	25 (0.50)	1 (0.02)
8	22 (0.44)	12 (0.24)	—
9	15 (0.30)	12 (0.24)	—
10	4 (0.08)	2 (0.04)	—
11	1 (0.02)	1 (0.02)	—
12	—	1 (0.02)	—

Supplementary Table S6A–C. Residue–residue contact analysis of the TmGpx1–CK2β complex across three independent molecular dynamics simulations.

(A) Replicate 1, (B) Replicate 2, and (C) Replicate 3. Interfacial residue pairs were identified over each 200-ns trajectory (20,001 analyzed frames per replicate). A residue pair was considered in contact in a frame when any heavy atoms of the two residues were within 0.60 nm. Only pairs in contact in ≥30% of frames are listed, ranked by contact frequency. contact_freq_%, percentage of analyzed frames in which the residue pair was in contact; mean_min_dist_nm, average shortest heavy-atom distance between the two residues during contact frames; CK2B_dG_kcal_mol and TmGpx1_dG_kcal_mol, total per-residue MM/GBSA binding free-energy contribution (kcal/mol) of each residue in that replicate (the overall contribution of the residue to binding, not a pair-specific value); "–", residue not included in the per-residue decomposition output of that replicate; n_frames_in_contact, number of frames in which the residue pair was in contact. The ΔG values reported in Table 2 are the means of these replicate-level values.

Table S6A — Replicate 1

No.	CK2B_ residue	TmGpx1_residue	contact_freq_%	mean_min_dist_nm	CK2B_dG_kcal_mol	TmGpx1_dG_kcal_mol	n_frames_in_contact
1	PRO:58	PHE:41	99.97	0.3533	−2.18	−2.00	19995
2	GLU:57	TRP:131	99.915	0.3466	−0.14	−5.11	19984
3	LEU:62	ILE:151	99.83	0.4063	−0.65	−4.52	19967
4	TRP:12	ARG:128	99.79	0.3461	−3.03	−4.82	19959
5	GLU:57	GLN:76	99.7	0.306	−0.14	−2.41	19941
6	GLU:63	ILE:151	99.69	0.3776	−0.18	−4.52	19939
7	LEU:56	TRP:131	99.53	0.3769	−0.34	−5.11	19907
8	ASP:55	TRP:131	99.175	0.3879	0.71	−5.11	19836
9	PRO:58	TRP:131	99.015	0.3661	−2.18	−5.11	19804
10	TRP:12	VAL:126	98.8151	0.3927	−3.03	−1.14	19764
11	GLU:5	GLY:106	97.9951	0.3346	−2.02	−2.17	19600

12	PRO:58	ILE:151	97.9001	0.4398	−2.18	−4.52	19581
13	GLU:73	ARG:149	97.8501	0.3295	−0.95	−8.39	19571
14	GLU:6	GLN:72	97.3151	0.3749	−1.67	−0.91	19464
15	ASP:59	ILE:151	96.8202	0.3771	−0.16	−4.52	19365
16	GLU:57	GLY:40	96.5302	0.3188	−0.14	−2.01	19307
17	TRP:9	ARG:128	95.9002	0.4001	−0.86	−4.82	19181
18	GLU:5	ASN:105	95.4002	0.3893	−2.02	−1.75	19081
19	ASP:70	ARG:149	94.6603	0.3263	−0.96	−8.39	18933
20	VAL:7	ARG:128	94.4653	0.3381	−1.60	−4.82	18894
21	SER:69	ILE:151	94.3603	0.4364	0.23	−4.52	18873
22	MET:52	LEU:130	94.2603	0.4027	−0.64	−1.68	18853
23	GLU:57	CYS:39	93.7803	0.3606	−0.14	−3.13	18757
24	GLU:57	PHE:41	93.4353	0.4294	−0.14	−2.00	18688
25	SER:69	ARG:149	93.4003	0.4212	0.23	−8.39	18681
26	ASP:59	PHE:41	92.9554	0.4744	−0.16	−2.00	18592
27	PRO:58	SER:150	92.0404	0.4692	−2.18	−0.10	18409
28	ASP:55	ARG:128	91.9454	0.4547	0.71	−4.82	18390
29	SER:8	ARG:128	91.5054	0.4145	–	−4.82	18302
30	LEU:16	VAL:126	90.4305	0.4479	−0.50	−1.14	18087
31	GLU:6	ASN:105	89.4755	0.4108	−1.67	−1.75	17896
32	GLU:60	ILE:151	88.2906	0.3913	−0.57	−4.52	17659
33	GLU:63	THR:152	87.9156	0.446	−0.18	−0.96	17584
34	GLU:6	GLY:106	87.6956	0.3824	−1.67	−2.17	17540
35	GLU:57	LYS:38	86.6257	0.4962	−0.14	−1.05	17326
36	ILE:72	ARG:149	85.0507	0.4059	−0.36	−8.39	17011
37	GLU:73	LEU:130	85.0107	0.4316	−0.95	−1.68	17003
38	GLU:60	LYS:153	84.7758	0.3338	−0.57	−3.92	16956
39	GLN:74	LEU:123	84.7108	0.3988	−0.06	−1.51	16943
40	GLU:6	LYS:108	84.5508	0.4411	−1.67	−1.44	16911
41	GLU:60	PHE:41	83.7208	0.4475	−0.57	−2.00	16745
42	TRP:12	LYS:127	83.0458	0.5092	−3.03	−1.24	16610
43	GLU:5	SER:107	82.3109	0.4882	−2.02	–	16463

44	TRP:9	LEU:130	80.391	0.4516	−0.86	−1.68	16079
45	GLU:5	ARG:128	80.206	0.336	−2.02	−4.82	16042
46	GLU:6	SER:107	80.161	0.3533	−1.67	–	16033
47	GLU:63	LYS:153	78.1311	0.3968	−0.18	−3.92	15627
48	GLU:6	ARG:128	76.9362	0.5178	−1.67	−4.82	15388
49	GLU:73	LEU:123	72.5264	0.4553	−0.95	−1.51	14506
50	LEU:71	ARG:149	71.4864	0.5286	−0.21	−8.39	14298
51	GLU:73	VAL:126	69.4115	0.485	−0.95	−1.14	13883
52	PRO:58	LEU:130	68.8916	0.5176	−2.18	−1.68	13779
53	GLU:5	LYS:127	66.1517	0.4236	−2.02	−1.24	13231
54	GLU:5	GLN:72	63.3318	0.5158	−2.02	−0.91	12667
55	GLU:5	LYS:117	62.4919	0.3223	−2.02	–	12499
56	ASP:55	LEU:130	61.9369	0.5119	0.71	−1.68	12388
57	ASP:55	GLY:74	58.4121	0.5474	0.71	−0.11	11683
58	GLU:60	GLN:44	57.3221	0.4938	−0.57	−0.57	11465
59	GLU:5	GLU:114	56.6872	0.4278	−2.02	–	11338
60	HIS:153	LEU:124	55.4622	0.4195	–	−1.03	11093
61	ASP:55	PHE:73	54.9223	0.5513	0.71	−0.64	10985
62	GLU:61	ILE:151	53.4573	0.5726	−0.24	−4.52	10692
63	GLU:5	VAL:104	53.4373	0.4531	−2.02	–	10688
64	ILE:72	LEU:130	50.8825	0.5214	−0.36	−1.68	10177
65	GLU:5	VAL:129	50.8225	0.5293	−2.02	–	10165
66	GLU:73	GLY:122	47.5276	0.5304	−0.95	–	9506
67	VAL:7	ASN:105	46.4127	0.5625	−1.60	−1.75	9283
68	GLU:5	ALA:109	45.2727	0.5488	−2.02	–	9055
69	GLU:6	ASP:103	43.8828	0.5047	−1.67	1.30	8777
70	VAL:7	GLN:72	42.2079	0.5507	−1.60	−0.91	8442
71	LEU:62	ARG:149	39.933	0.4883	−0.65	−8.39	7987
72	GLU:77	LEU:124	39.758	0.5295	0.30	−1.03	7952
73	SER:4	ARG:128	37.0581	0.5662	0.24	−4.82	7412
74	ASP:70	LEU:123	36.8932	0.5085	−0.96	−1.51	7379

75	MET:52	ARG:149	33.1283	0.5202	−0.64	−8.39	6626
76	SER:4	GLY:106	32.9734	0.5754	0.24	−2.17	6595
77	GLU:63	SER:156	31.2584	0.53	−0.18	0.08	6252
78	GLU:60	GLY:40	31.0434	0.5219	−0.57	−2.01	6209
79	GLU:77	LEU:123	30.2185	0.5063	0.30	−1.51	6044

Table S6B— Replicate 2

No.	CK2B_residue	TmGpx1_residue	contact_freq_%	mean_min_dist_nm	CK2B_dG_kcal_mol	TmGpx1_dG_kcal_mol	n_frames_in_contact
1	TRP:9	ARG:128	99.995	0.3422	−4.06	−5.62	20000
2	TRP:12	ARG:128	99.94	0.3305	−3.67	−5.62	19989
3	LEU:62	ILE:151	99.91	0.3854	−0.68	−4.18	19983
4	MET:52	LEU:130	99.905	0.3906	−0.64	−2.67	19982
5	VAL:7	ARG:128	99.835	0.2846	–	−5.62	19968
6	SER:69	ILE:151	99.83	0.365	−0.35	−4.18	19967
7	TRP:12	VAL:126	99.825	0.4176	−3.67	−1.98	19966
8	SER:69	ARG:149	99.73	0.3188	−0.35	−8.44	19947
9	SER:8	ARG:128	99.35	0.4409	–	−5.62	19871
10	GLU:6	GLY:106	99.095	0.3666	−1.24	–	19820
11	GLU:5	GLY:106	98.8201	0.3223	–	–	19765
12	GLU:5	ARG:128	98.5851	0.3216	–	−5.62	19718
13	ASP:70	ARG:149	98.0301	0.3566	−0.54	−8.44	19607
14	GLU:5	ASN:105	97.9451	0.3419	–	–	19590
15	GLU:63	ILE:151	97.9451	0.4027	0.65	−4.18	19590
16	GLU:57	TRP:131	97.9051	0.3743	−0.14	−3.55	19582
17	GLU:6	SER:107	97.7151	0.322	−1.24	–	19544
18	GLU:6	ASN:105	97.6951	0.4476	−1.24	–	19540
19	GLU:6	ARG:128	97.6301	0.4595	−1.24	−5.62	19527
20	GLU:73	ARG:149	97.4651	0.2988	−2.62	−8.44	19494
21	GLU:5	LYS:117	97.2551	0.2888	–	–	19452
22	TRP:9	LEU:130	96.6052	0.3938	−4.06	−2.67	19322

23	PRO:58	TRP:131	96.4502	0.3707	−2.07	−3.55	19291
24	GLU:5	LYS:127	95.9952	0.3859	–	–	19200
25	GLN:74	LEU:123	95.9502	0.3774	−0.38	−4.02	19191
26	ARG:17	LEU:124	95.3952	0.383	–	−2.13	19080
27	GLU:5	GLU:114	94.9603	0.4038	–	–	18993
28	GLU:5	VAL:104	94.0503	0.4562	–	–	18811
29	LEU:56	TRP:131	93.7903	0.399	–	−3.55	18759
30	GLU:5	VAL:129	93.5453	0.5092	–	–	18710
31	GLU:57	GLN:76	93.2203	0.3555	−0.14	−1.79	18645
32	GLU:73	LEU:130	91.9554	0.4442	−2.62	−2.67	18392
33	ILE:72	LEU:130	90.7655	0.4213	−0.46	−2.67	18154
34	GLU:6	LYS:108	90.6255	0.484	−1.24	−0.41	18126
35	TRP:9	VAL:129	90.0755	0.4745	−4.06	–	18016
36	GLU:73	VAL:126	89.6555	0.4659	−2.62	−1.98	17932
37	SER:4	ARG:128	88.9856	0.4523	0.20	−5.62	17798
38	PRO:66	ILE:151	86.0707	0.3925	−0.95	−4.18	17215
39	ASP:55	TRP:131	85.8657	0.4594	1.40	−3.55	17174
40	GLU:73	LEU:123	83.8508	0.4692	−2.62	−4.02	16771
41	GLU:6	GLN:72	82.4609	0.437	−1.24	−0.26	16493
42	GLU:63	LYS:153	80.201	0.3954	0.65	−1.12	16041
43	LEU:71	ARG:149	79.966	0.5192	–	−8.44	15994
44	GLU:63	PHE:41	78.2611	0.4254	0.65	−1.23	15653
45	SER:69	LEU:130	74.3663	0.4649	−0.35	−2.67	14874
46	GLU:5	SER:107	73.7663	0.5629	–	–	14754
47	TRP:9	VAL:126	73.5713	0.5001	−4.06	−1.98	14715
48	LEU:16	VAL:126	72.9514	0.4286	–	−1.98	14591
49	PRO:58	PHE:41	72.4014	0.443	−2.07	−1.23	14481
50	ASN:65	ILE:151	71.6664	0.5135	0.17	−4.18	14334
51	ARG:17	VAL:126	71.4964	0.3902	–	−1.98	14300
52	GLU:5	ALA:109	68.0066	0.5393	–	–	13602
53	ILE:72	ARG:149	64.4368	0.4577	−0.46	−8.44	12888

54	ARG:17	LEU:123	63.3468	0.3442	–	−4.02	12670
55	GLU:57	GLY:74	61.9419	0.4477	−0.14	−0.17	12389
56	GLU:63	GLN:44	61.7269	0.4629	0.65	−0.45	12346
57	GLU:73	GLY:122	60.677	0.506	−2.62	–	12136
58	ASP:55	ARG:128	58.5021	0.5036	1.40	−5.62	11701
59	SER:4	GLY:106	56.8572	0.4912	0.20	–	11372
60	ASN:67	ILE:151	55.7722	0.5499	–	−4.18	11155
61	ASP:70	LEU:123	54.0323	0.4949	−0.54	−4.02	10807
62	PRO:66	THR:152	53.4173	0.4745	−0.95	−0.12	10684
63	ARG:17	GLY:125	52.2774	0.5325	–	–	10456
64	GLU:5	GLN:72	51.1724	0.5503	–	−0.26	10235
65	ASP:55	PHE:73	48.6426	0.5274	1.40	–	9729
66	GLU:73	ARG:128	48.2576	0.5138	−2.62	−5.62	9652
67	GLU:63	GLY:40	47.5776	0.4798	0.65	−0.28	9516
68	SER:69	SER:150	47.2926	0.5353	−0.35	–	9459
69	ASP:55	GLY:74	46.7627	0.5439	1.40	−0.17	9353
70	GLU:57	GLY:40	45.9127	0.4858	−0.14	−0.28	9183
71	GLU:57	LYS:38	45.8477	0.4789	−0.14	−0.09	9170
72	TRP:12	LYS:127	44.5178	0.5699	−3.67	–	8904
73	PRO:58	GLN:76	44.0478	0.5135	−2.07	−1.79	8810
74	GLU:57	CYS:39	43.1978	0.5144	−0.14	−0.48	8640
75	ASP:59	ILE:151	43.0678	0.4968	–	−4.18	8614
76	LEU:62	PHE:41	42.3779	0.497	−0.68	−1.23	8476
77	SER:4	SER:107	39.133	0.448	0.20	–	7827
78	LEU:71	LEU:123	39.088	0.4121	–	−4.02	7818
79	ARG:17	GLY:122	38.9231	0.4838	–	–	7785
80	GLN:74	LEU:124	37.7631	0.4234	−0.38	−2.13	7553
81	GLU:77	LEU:124	36.2432	0.4749	0.17	−2.13	7249
82	ASP:55	GLN:72	34.1033	0.524	1.40	−0.26	6821
83	ASP:59	PHE:41	33.5283	0.5516	–	−1.23	6706
84	ASP:55	LEU:130	33.2083	0.4958	1.40	−2.67	6642

85	GLU:57	PHE:73	31.4084	0.5578	−0.14	–	6282
86	PRO:66	ARG:149	31.2334	0.5321	−0.95	−8.44	6247

Table S6C— Replicate 3

No.	CK2B_residue	TmGpx1_residue	contact_freq_%	mean_min_dist_nm	CK2B_dG_kcal_mol	TmGpx1_dG_kcal_mol	n_frames_in_contact
1	TRP:12	TRP:131	100	0.3659	−3.41	−2.18	20001
2	GLU:73	ARG:128	100	0.278	−1.93	−7.64	20001
3	SER:69	VAL:126	99.925	0.3909	−1.39	−2.53	19986
4	TRP:12	LEU:130	99.855	0.2928	−3.41	−2.22	19972
5	LEU:16	TRP:131	99.59	0.4315	−2.48	−2.18	19919
6	SER:69	GLY:125	99.57	0.373	−1.39	−0.33	19915
7	SER:69	LEU:124	99.45	0.3019	−1.39	−4.58	19891
8	GLU:73	VAL:126	99.085	0.4382	−1.93	−2.53	19818
9	LEU:16	GLY:74	98.7101	0.4957	−2.48	−0.87	19743
10	GLY:15	TRP:131	98.2351	0.3967	−1.09	−2.18	19648
11	GLY:15	GLY:74	97.9551	0.294	−1.09	−0.87	19592
12	LEU:16	PHE:73	97.8001	0.3787	−2.48	−2.24	19561
13	LEU:62	LEU:124	97.5101	0.4152	−0.56	−4.58	19503
14	GLY:15	PHE:73	97.3751	0.3822	−1.09	−2.24	19476
15	ARG:17	GLN:72	97.1151	0.3044	−1.77	−0.98	19424
16	ARG:17	PHE:73	97.0251	0.4733	−1.77	−2.24	19406
17	PRO:66	GLY:125	96.9602	0.373	−1.18	−0.33	19393
18	LEU:16	GLN:72	96.8902	0.3705	−2.48	−0.98	19379
19	ARG:17	ASN:71	96.4002	0.3416	−1.77	–	19281
20	GLY:15	ASN:75	96.2752	0.4956	−1.09	−0.49	19256
21	GLY:15	GLN:72	96.2202	0.4257	−1.09	−0.98	19245
22	ASP:70	LYS:127	96.0002	0.35	−0.38	−2.43	19201
23	PRO:58	LEU:124	95.9352	0.4068	−0.54	−4.58	19188
24	TRP:12	ARG:128	95.6702	0.4019	−3.41	−7.64	19135
25	LEU:16	LEU:130	95.3952	0.488	−2.48	−2.22	19080

26	ARG:17	GLY:74	95.1202	0.506	−1.77	−0.87	19025
27	TRP:12	PHE:73	93.8653	0.5252	−3.41	−2.24	18774
28	ASP:70	GLY:125	93.4953	0.4828	−0.38	−0.33	18700
29	GLU:73	LYS:127	93.4753	0.5253	−1.93	−2.43	18696
30	ARG:17	ASN:75	91.3554	0.3601	−1.77	−0.49	18272
31	LEU:16	ARG:128	89.2105	0.4356	−2.48	−7.64	17843
32	TRP:12	VAL:129	85.7107	0.5459	−3.41	0.01	17143
33	SER:11	TRP:131	84.8808	0.5324	–	−2.18	16977
34	ASP:70	VAL:126	84.5208	0.4782	−0.38	−2.53	16905
35	GLU:77	ARG:128	83.0658	0.4253	−0.68	−7.64	16614
36	PRO:66	VAL:126	82.2359	0.5272	−1.18	−2.53	16448
37	MET:1	LEU:124	82.0709	0.4156	–	−4.58	16415
38	MET:1	LEU:123	80.276	0.4054	–	−0.54	16056
39	GLU:63	LEU:124	80.216	0.4401	−0.13	−4.58	16044
40	ASN:67	GLY:125	78.1861	0.5145	0.01	−0.33	15638
41	PRO:66	LEU:124	76.1362	0.4886	−1.18	−4.58	15228
42	MET:52	LEU:124	76.1212	0.4499	−0.41	−4.58	15225
43	ASP:70	ARG:128	75.4412	0.4917	−0.38	−7.64	15089
44	GLU:5	ILE:151	74.0463	0.462	−1.51	−1.11	14810
45	GLU:6	ILE:151	73.2713	0.4308	−0.80	−1.11	14655
46	MET:1	LEU:130	73.2713	0.4018	–	−2.22	14655
47	MET:52	VAL:126	72.7264	0.5025	−0.41	−2.53	14546
48	SER:2	LEU:124	69.5915	0.3945	–	−4.58	13919
49	PRO:66	PRO:121	69.4615	0.4632	−1.18	−0.33	13893
50	SER:3	ARG:149	69.0365	0.458	–	−5.49	13808
51	SER:149	LYS:108	66.9817	0.4232	–	–	13397
52	MET:1	VAL:126	65.9717	0.4211	–	−2.53	13195
53	GLN:74	ARG:128	65.0867	0.4041	–	−7.64	13018
54	GLU:5	ARG:149	65.0217	0.3057	−1.51	−5.49	13005
55	GLY:18	GLN:72	63.8368	0.5422	–	−0.98	12768
56	MET:1	ARG:149	60.852	0.4894	–	−5.49	12171

57	ASN:65	LEU:124	56.7672	0.542	0.08	−4.58	11354
58	SER:69	LYS:127	55.9472	0.5355	−1.39	−2.43	11190
59	GLU:6	ARG:149	55.8422	0.3273	−0.80	−5.49	11169
60	PRO:66	LYS:127	55.7722	0.5077	−1.18	−2.43	11155
61	HIS:153	SER:107	55.6222	0.455	–	–	11125
62	ASN:65	GLY:125	54.6873	0.5367	0.08	−0.33	10938
63	SER:149	SER:107	50.3025	0.4526	–	–	10061
64	SER:69	LEU:123	46.1127	0.5528	−1.39	−0.54	9223
65	ARG:150	ASP:103	43.4628	0.4023	–	–	8693
66	GLU:5	LEU:123	38.8781	0.5218	−1.51	−0.54	7776
67	ASN:67	LYS:127	36.2932	0.4662	0.01	−2.43	7259
68	ARG:17	ASP:103	34.8933	0.5006	−1.77	–	6979
69	LEU:62	GLY:125	34.6083	0.5195	−0.56	−0.33	6922
70	LEU:16	ASN:105	33.6483	0.5694	−2.48	–	6730
71	SER:3	LEU:123	31.4184	0.4654	–	−0.54	6284
72	PHE:13	TRP:131	31.4034	0.5796	−0.21	−2.18	6281