

Support Information

Xiaoyong Cao[†] and Pu Tian^{*,†,‡}

[†]*School of Life Sciences, Jilin University, Changchun, China 130012*

[‡]*School of Artificial Intelligence, Jilin University, Changchun, China 130012*

E-mail: tianpu@jlu.edu.cn

Phone: +86 (0)431 85155287

1.Coordinates transformation with NeRF (Natural Extension Reference Frame) algorithm:

$$\tilde{c}_k = [r_k \cos(\theta_k), r_k \cos(\psi_k) \sin(\theta_k), r_k \sin(\psi_k) \cos(\theta_k)] \quad (1)$$

$$m_k = c_{k-1} - c_{k-2} \quad (2)$$

$$M_k = \widehat{m}_k, \widehat{m}_k \times \widehat{n}_k, \widehat{n}_k \quad (3)$$

$$c_k = M_k \tilde{c}_k + c_{k-1} \quad (4)$$

Here, r_k is the bond length between atoms $k - 1$ and k , θ_k is the bond angle composed of atoms $k - 2, k - 1, k$, and ψ_k is the dihedral angle of $k - 2, k - 1$ as the axis of rotation, \widehat{m}_k the unit vector of m_k , \times is the vector cross product, and c_k is the cartesian coordinate of the updated k atom.

Table S1: GSFE-Refinement best of top 5 results for 150-target refined dataset

ID	start GDT-HA	Δ GDT-HA	start RMSD	Δ RMSD
101m_	0.6656	0.0146	3.9267	-0.027
1a00A	0.6418	-0.0035	16.9914	0.0029
1a07A	0.7405	0.0024	3.29	-0.0044
1a5v_	0.5582	0.0034	1.8435	-0.0214
1afqC	0.5573	0.0078	6.2068	-0.0098
1at1A	0.64	0.0062	6.5628	-0.0287
1awqA	0.5732	0.003	9.9856	-0.0217
1b0b_	0.6294	-0.0017	1.837	-0.0268
1b11A	0.542	-0.0022	12.6573	-0.0301
1b1cA	0.6627	-0.0016	5.5089	-0.0074
1b66A	0.5707	0	0.8874	-0.0338
1be9A	0.5856	0.0024	5.3811	-0.012
1bh5A	0.531	0.0017	4.3604	-0.0173
1bs4A	0.5923	0.0015	5.9913	-0.02
1bvqA	0.5953	0.0072	4.5375	-0.0135
1bzsA	0.4152	-0.0016	7.6959	-0.022
1c9kB	0.2056	0.0027	5.0313	0.0054
1ccwA	0.6004	0.0036	2.454	-0.0131
1cfvH	0.6366	0	5.5613	-0.0291
1cpq_	0.6647	0.0117	5.7355	-0.0141
1cv8_	0.3613	0	3.5176	-0.003
1d01D	0.5685	0	6.0945	-0.0368
1d0iA	0.3883	0.0067	4.754	-0.0419
1d1jC	0.5328	0.0037	5.4926	-0.0096
1d2uA	0.3261	0.0027	4.994	-0.0426

1d7bA	0.1041	0.0013	2.0833	-0.0153
1d8uA	0.4848	0.0016	2.8479	-0.0197
1ddrA	0.6368	0.0173	6.7574	-0.0177
1df8A	0.6229	0.0085	1.9512	-0.0144
1ds7A	0.5141	0.0077	2.1074	-0.012
1dt1A	0.3275	0.0078	1.794	-0.0247
1dud_	0.5907	0.002	15.8571	-0.047
1dveA	0.4393	0.0093	1.1959	-0.0107
1dw0A	0.3281	0.0045	12.2524	-0.0144
1dxpA	0.2586	0.0043	11.966	0.008
1dzcA	0.4522	0.0082	2.3676	0.0009
1e20A	0.5176	0.0081	5.2297	-0.0219
1e29A	0.4222	0.0019	11.7805	-0.0348
1e6iA	0.7227	0	5.8339	-0.0261
1ejbA	0.6548	0.0014	5.8128	-0.0672
1elkA	0.5899	0.0065	3.8924	-0.031
1elrA	0.6074	0.0215	1.7917	-0.0799
1elwA	0.6859	0.0064	1.9984	-0.0253
1eqmA	0.5728	0.0031	11.3548	-0.0094
1eumA	0.7531	0.014	1.9421	0.0023
1ew4A	0.5943	0.0024	1.857	-0.015
1eyhA	0.5434	0.0035	3.5525	-0.0493
1f71A	0.5127	0.0106	1.9146	-0.0194
1fdk_	0.2581	-0.002	10.8596	-0.0139
1ff3A	0.5262	0.0048	2.1792	-0.068
1fm0D	0.7067	0	1.6562	-0.0126
1g5tA	0.4204	0.0032	6.5559	-0.0181

1gcvB	0.6085	0.011	3.5266	-0.081
1goyA	0.3657	0	1.6183	-0.0304
1gpqA	0.4528	0.0019	5.4125	-0.0131
1gxuA	0.5881	0.0057	1.5192	-0.0176
1gy7A	0.6384	0.0124	4.0669	-0.0019
1h4hA	0.4782	0.0012	1.9931	-0.0642
1h97A	0.5408	0	1.4124	0.002
1hbg_	0.5986	0.0119	6.304	-0.0138
1hdoA	0.5671	0.0122	2.708	-0.0462
1hlb_	0.5016	0.0143	1.4586	-0.0285
1hnl_	0.2865	0.002	3.3574	-0.0286
1i4sA	0.449	0.0085	9.4846	-0.0421
1j3wA	0.5951	0.0131	2.7615	0.0016
1j77A	0.4397	0.0063	3.8841	-0.0585
1kafA	0.2477	0.0023	3.6507	-0.0028
1l9lA	0.598	-0.0034	2.6332	0.0024
1mk0A	0.4459	0.0077	3.4147	-0.0091
1mn8A	0.2474	0	2.804	-0.0494
1nlqA	0.231	0.0047	11.5067	-0.0315
1nwaA	0.2411	0.0015	2.4345	-0.0875
1o82A	0.3036	0	3.9845	-0.0081
1oh0A	0.628	0.008	9.0235	-0.0166
1ok0A	0.1824	0	2.2832	0.008
1oohA	0.4821	0.008	2.8792	-0.0174
1ou8A	0.4151	0.0024	5.0654	-0.0272
1ow4A	0.5479	0.0021	5.3922	-0.0106
1q1fA	0.625	0.0169	4.1534	-0.0291

1q4kA	0.0788	0.0023	1.7395	-0.0002
1rfyA	0.618	0.0084	2.8979	-0.0364
1sz7A	0.4686	0.0047	8.7317	-0.0081
1t1vA	0.6156	0	8.2837	-0.0289
1t3yA	0.6221	0.0039	6.2022	-0.0147
1t7dA	0.0481	0	2.8585	-0.0349
1tkuA	0.0944	0	16.7339	-0.1489
1tp6A	0.4206	0.004	3.0161	0.0064
1tqgA	0.7214	0.0048	1.1602	-0.0205
1tugB	0.4118	0	10.803	-0.0408
1tzvA	0.5177	0.0071	5.935	-0.0097
1u2hA	0.8021	0.0052	2.613	0.0013
1u55A	0.4846	0.0126	2.4141	-0.0309
1u84A	0.3364	0.0031	2.9302	-0.0031
1ufyA	0.3417	0.0023	21.5158	-0.0354
1ugiA	0.1687	0	1.9191	0.0623
1usqA	0.3291	0.0036	13.1353	-0.004
1uuyA	0.6491	0.0031	6.3911	-0.0047
1uxzA	0.6145	-0.0019	4.1702	-0.0192
1w53A	0.503	0.0059	1.4101	-0.0343
1wlzA	0.3618	0.0029	19.0621	-0.0217
1wmhA	0.7289	0.003	9.198	-0.0028
1wmhB	0.5945	0	3.616	-0.0027
1wpaA	0.2477	-0.0024	1.3425	-0.0051
1wzdA	0.4641	0.0024	1.5859	0.0076
1x6iA	0.5337	0.0028	3.1087	-0.0005
1x91A	0.7232	-0.0017	6.7188	-0.0578

1xa8A	0.2296	0	13.2079	-0.0558
1xmtA	0.5579	0.0026	1.5011	-0.0078
1xppA	0.6237	0.0051	10.4144	-0.0018
1y3dI	0.3906	0.0078	5.3931	-0.0326
1y9tA	0.2023	0	1.5181	-0.0034
1yd0A	0.4494	0	2.3645	-0.0371
1z3eB	0.6607	0.0089	2.4512	-0.0033
2b5aA	0.776	0.013	6.9385	-0.0475
2bwfA	0.6461	0.0097	2.6113	-0.005
2c92A	0.6378	0.0034	3.1986	0.0076
2cb8A	0.7674	0.0117	1.591	-0.0114
2chhA	0.1726	0.0022	2.2773	0.001
2ev1A	0.1797	0	3.5855	-0.0426
2fcwA	0.4646	0.0024	3.4804	-0.0177
2gkgA	0.7049	-0.0061	3.2566	-0.0037
2grrB	0.2102	0.0048	5.4023	-0.0397
2h7zA	0.53	0.0033	8.9504	-0.0064
2hl0A	0.5105	0	7.5891	-0.0084
2ifrA	0.1176	0.0013	5.0274	-0.074
2ip6A	0.7328	0.0057	5.6535	-0.0169
2iu5A	0.2891	0.0056	7.0724	-0.023
2j8wA	0.5547	0.0078	3.3315	-0.0088
2jekA	0.1411	0	1.632	-0.0005
2nmlA	0.205	0	2.7006	-0.0192
2o37A	0.5556	0.0061	8.8581	-0.0286
2ofcA	0.2234	-0.0018	1.8955	0.0106
2oznA	0.3985	0.0038	4.5841	-0.0238

2p6wA	0.2124	0.006	8.5653	-0.0531
2pmrA	0.727	0.0033	2.5528	-0.0423
2pv2A	0.6796	-0.0024	4.5033	-0.0038
2pvbA	0.4042	0	2.0095	0.0095
2rb8A	0.7957	0.0027	1.9139	-0.0008
2rk3A	0.5963	-0.0027	2.3792	-0.0369
2v2pA	0.8	0.0132	1.1419	0.0117
2v33A	0.1978	0.0027	2.3929	-0.011
2vyyA	0.4727	0.0046	7.0412	-0.01
2zs0D	0.6793	0.0035	8.395	-0.0025
3bfoA	0.7118	0.0029	2.3744	0.0006
3bqpA	0.5969	0	16.4106	-0.0442
3bqsA	0.2824	0	1.9198	0.0053
3by4A	0.3939	0.0014	1.9598	-0.0237
3c7mA	0.4526	0.0077	11.8375	-0.0006
3cjsB	0.5729	0.0174	2.2228	-0.0061
3d9nA	0.5543	0.0091	1.5299	-0.0188
mean	-	0.0041	-	-0.0203

Table S2: GSFE-Refinement top 1 results for 150-target refined dataset

ID	start GDT-HA	Δ GDT-HA	start RMSD	Δ RMSD
101m_	0.6656	0.0113	3.9267	-0.0189
1a00A	0.6418	0	16.9914	-0.0037
1a07A	0.7405	0	3.29	0.0074
1a5v_	0.5582	0	1.8435	-0.013
1afqC	0.5573	-0.0026	6.2068	0.0095
1at1A	0.64	0.0012	6.5628	-0.0081

1awqA	0.5732	-0.0031	9.9856	-0.0013
1b0b_	0.6294	-0.0159	1.837	0.0052
1b11A	0.542	0	12.6573	-0.0088
1b1cA	0.6627	0	5.5089	0.0151
1b66A	0.5707	0.0036	0.8874	0.0153
1be9A	0.5856	0.0024	5.3811	-0.0146
1bh5A	0.531	-0.0016	4.3604	-0.0021
1bs4A	0.5923	0	5.9913	0.01
1bvqA	0.5953	0.0018	4.5375	-0.0093
1bzsA	0.4152	0	7.6959	-0.0079
1c9kB	0.2056	-0.0014	5.0313	0.0296
1ccwA	0.6004	-0.0055	2.454	0.0077
1cfvH	0.6366	-0.0021	5.5613	-0.0122
1cpq_	0.6647	0.0058	5.7355	-0.0191
1cv8_	0.3613	-0.0029	3.5176	0.0071
1d01D	0.5685	0	6.0945	0.017
1d0iA	0.3883	0	4.754	0.001
1d1jC	0.5328	0.0055	5.4926	-0.0115
1d2uA	0.3261	-0.0014	4.994	-0.0026
1d7bA	0.1041	0.0013	2.0833	0.0004
1d8uA	0.4848	0.0031	2.8479	-0.0081
1ddrA	0.6368	0.0047	6.7574	-0.0026
1df8A	0.6229	0.0085	1.9512	-0.0011
1ds7A	0.5141	0	2.1074	0.0058
1dt1A	0.3275	0.0058	1.794	0.0076
1dud_	0.5907	0.0061	15.8571	-0.005
1dveA	0.4393	-0.0024	1.1959	0.0109

1dw0A	0.3281	-0.0044	12.2524	0.0008
1dxpA	0.2586	0.0014	11.966	0.0242
1dzrA	0.4522	-0.0014	2.3676	-0.0008
1e20A	0.5176	0	5.2297	-0.0076
1e29A	0.4222	0	11.7805	-0.0003
1e6iA	0.7227	-0.0113	5.8339	0.0343
1ejbA	0.6548	-0.006	5.8128	-0.0151
1elkA	0.5899	0.0016	3.8924	-0.0276
1elrA	0.6074	0.0156	1.7917	-0.0894
1elwA	0.6859	-0.0085	1.9984	0.0374
1eqmA	0.5728	0.0016	11.3548	0.0197
1eumA	0.7531	0	1.9421	-0.0049
1ew4A	0.5943	0.0048	1.857	-0.0065
1eyhA	0.5434	-0.0035	3.5525	-0.0851
1f71A	0.5127	0	1.9146	-0.0004
1fdk_	0.2581	-0.004	10.8596	0.0076
1ff3A	0.5262	-0.0024	2.1792	0.0105
1fm0D	0.7067	-0.0034	1.6562	-0.0157
1g5tA	0.4204	0	6.5559	0.0004
1gcvB	0.6085	0.0018	3.5266	-0.009
1goyA	0.3657	0.0024	1.6183	0.0001
1gpqA	0.4528	0.0039	5.4125	-0.0012
1gxuA	0.5881	0.0057	1.5192	-0.0129
1gy7A	0.6384	0.0062	4.0669	0.012
1h4hA	0.4782	-0.0025	1.9931	0.0015
1h97A	0.5408	0	1.4124	-0.0064
1hbg_	0.5986	0.0102	6.304	-0.0236

1hdoA	0.5671	0.0024	2.708	-0.0048
1hlb_	0.5016	0	1.4586	-0.0121
1hnl_	0.2865	-0.0019	3.3574	0.0107
1i4sA	0.449	0.0068	9.4846	-0.0085
1j3wA	0.5951	0.0094	2.7615	0.0037
1j77A	0.4397	0.005	3.8841	0.0023
1kafA	0.2477	0.0046	3.6507	0.0114
1l9lA	0.598	-0.0034	2.6332	0.0025
1mk0A	0.4459	-0.0052	3.4147	0.0002
1mn8A	0.2474	-0.0027	2.804	-0.0414
1nlqA	0.231	0.0023	11.5067	-0.0044
1nwaA	0.2411	0.0015	2.4345	-0.0059
1o82A	0.3036	0	3.9845	-0.0014
1oh0A	0.628	0.008	9.0235	0.0107
1ok0A	0.1824	-0.0067	2.2832	0.0202
1oohA	0.4821	0.004	2.8792	-0.0013
1ou8A	0.4151	0	5.0654	-0.0295
1ow4A	0.5479	0.0021	5.3922	-0.0196
1q1fA	0.625	0.0118	4.1534	-0.0203
1q4kA	0.0788	0.0012	1.7395	0.018
1rfyA	0.618	-0.0028	2.8979	-0.001
1sz7A	0.4686	-0.0016	8.7317	0.014
1t1vA	0.6156	0.0027	8.2837	-0.0257
1t3yA	0.6221	0.0039	6.2022	-0.0084
1t7dA	0.0481	0	2.8585	-0.0319
1tkuA	0.0944	0	16.7339	-0.0069
1tp6A	0.4206	0.002	3.0161	0.0289

1tqgA	0.7214	0.0048	1.1602	-0.0117
1tugB	0.4118	0	10.803	0.0133
1tzvA	0.5177	0	5.935	-0.0118
1u2hA	0.8021	0	2.613	0.0007
1u55A	0.4846	0.0042	2.4141	0.0006
1u84A	0.3364	0	2.9302	-0.0032
1ufyA	0.3417	0.0023	21.5158	0.0061
1ugiA	0.1687	-0.003	1.9191	0.0474
1usqA	0.3291	0.0036	13.1353	0.0028
1uuyA	0.6491	-0.0031	6.3911	0.0039
1uxzA	0.6145	0	4.1702	-0.0058
1w53A	0.503	0.003	1.4101	-0.0128
1wlzA	0.3618	-0.003	19.0621	-0.0336
1wmhA	0.7289	0	9.198	0.0112
1wmhB	0.5945	-0.0061	3.616	0.0024
1wpaA	0.2477	-0.0047	1.3425	0.1414
1wzdA	0.4641	0	1.5859	0.0075
1x6iA	0.5337	0	3.1087	0.0018
1x91A	0.7232	0.0016	6.7188	-0.0358
1xa8A	0.2296	0.0025	13.2079	-0.0074
1xmtA	0.5579	0.0053	1.5011	-0.0077
1xppA	0.6237	-0.0126	10.4144	0.1296
1y3dI	0.3906	0.0039	5.3931	-0.0249
1y9tA	0.2023	0.0022	1.5181	0.0296
1yd0A	0.4494	-0.0056	2.3645	-0.0069
1z3eB	0.6607	0.0089	2.4512	-0.0244
2b5aA	0.776	0.0065	6.9385	-0.004

2bwfA	0.6461	0.0033	2.6113	0.014
2c92A	0.6378	-0.0017	3.1986	0.0072
2cb8A	0.7674	0	1.591	-0.0038
2chhA	0.1726	-0.0022	2.2773	0.0297
2ev1A	0.1797	0.0014	3.5855	-0.008
2fcwA	0.4646	0	3.4804	-0.0136
2gkgA	0.7049	-0.0061	3.2566	-0.0029
2grrB	0.2102	0.0048	5.4023	-0.0127
2h7zA	0.53	-0.0067	8.9504	0.0084
2hl0A	0.5105	0	7.5891	0.012
2ifrA	0.1176	0.0013	5.0274	0.0034
2ip6A	0.7328	0.0028	5.6535	0.0104
2iu5A	0.2891	0.0014	7.0724	-0.0131
2j8wA	0.5547	0.0019	3.3315	-0.0211
2jekA	0.1411	-0.0018	1.632	-0.0091
2nmlA	0.205	0.0025	2.7006	0.0044
2o37A	0.5556	0.0123	8.8581	-0.0356
2ofcA	0.2234	-0.0018	1.8955	0.0123
2oznA	0.3985	-0.0019	4.5841	-0.002
2p6wA	0.2124	-0.0012	8.5653	0.0246
2pmrA	0.727	0	2.5528	0.0046
2pv2A	0.6796	0.0073	4.5033	-0.0095
2pvbA	0.4042	-0.0023	2.0095	0.0169
2rb8A	0.7957	0	1.9139	-0.0047
2rk3A	0.5963	-0.0027	2.3792	0.0209
2v2pA	0.8	0.0029	1.1419	0.0013
2v33A	0.1978	0.0082	2.3929	-0.0045

2vyyA	0.4727	0.0023	7.0412	0.0048
2zs0D	0.6793	-0.0034	8.395	-0.0017
3bfoA	0.7118	0	2.3744	0.0006
3bqpA	0.5969	0.0031	16.4106	0.0045
3bqsA	0.2824	0	1.9198	-0.0101
3by4A	0.3939	-0.0015	1.9598	0.0131
3c7mA	0.4526	0	11.8375	-0.005
3cjsB	0.5729	0.007	2.2228	-0.0123
3d9nA	0.5543	0.0055	1.5299	-0.0182
mean	-	0.0008	-	-0.0003

Table S3: GSFE-Refinement best of top 5 results for CASP12 dataset

ID	start GDT-HA	Δ GDT-HA	start RMSD	Δ RMSD
TR520	0.581	-0.0031	3.9267	-0.0012
TR594	0.3427	0	16.9914	-0.0057
TR862	0.4032	0.0027	3.29	-0.0449
TR866	0.55	0	1.8435	-0.0181
TR868	0.5733	0.0043	6.2068	-0.006
TR869	0.2885	0	6.5628	-0.004
TR870	0.2276	0.0021	9.9856	-0.0051
TR872	0.5682	0	1.837	-0.021
TR877	0.4894	0.0053	12.6573	-0.0319
TR879	0.6352	-0.0079	5.5089	-0.0899
TR882	0.6899	0.0031	0.8874	-0.034
TR884	0.4401	0.0036	5.3811	-0.0155
TR885	0.7412	0	4.3604	-0.0135
TR891	0.7567	0.0022	5.9913	-0.0003
TR893	0.6908	0.0015	4.5375	-0.0094
TR894	0.5463	0	7.6959	-0.0095
TR895	0.5146	0.0042	5.0313	-0.0721
TR896	0.468	0.0029	2.454	-0.0065
TR898	0.2524	0.0023	5.5613	-0.0148
TR905	0.3244	0.0051	5.7355	-0.0421
TR909	0.4264	-0.003	3.5176	-0.0336
TR913	0.4534	-0.003	6.0945	-0.0429
TR917	0.6535	0.0211	4.754	-0.0668
TR920	0.6039	0.0023	5.4926	-0.0238
TR921	0.4801	0.0036	4.994	-0.0093
TR922	0.6791	0.0067	2.0833	-0.0078
TR928	0.4274	0.0059	2.8479	-0.0215
TR944	0.5603	0.002	6.7574	-0.0275
TR945	0.4113	-0.002	1.9512	-0.0604
TR947	0.5157	0.0143	2.1074	-0.0456
TR948	0.5956	0.0084	1.794	-0.0105
mean	-	0.0027	-	-0.0146

Table S4: GSFE-Refinement top 1 results for CASP12 dataset

ID	start GDT-HA	Δ GDT-HA	start RMSD	Δ RMSD
TR520	0.581	-0.0062	3.9267	-0.0012
TR594	0.3427	0	16.9914	0.0046
TR862	0.4032	0	3.29	0.0209
TR866	0.55	-0.0065	1.8435	0.0012
TR868	0.5733	0.0043	6.2068	0.0029
TR869	0.2885	0	6.5628	-0.0035
TR870	0.2276	-0.002	9.9856	0.0198
TR872	0.5682	0	1.837	0.0052
TR877	0.4894	-0.0052	12.6573	0.007
TR879	0.6352	-0.0079	5.5089	0.0764
TR882	0.6899	0	0.8874	0.0154
TR884	0.4401	0.0036	5.3811	-0.0143
TR885	0.7412	-0.0044	4.3604	-0.0135
TR891	0.7567	0.0022	5.9913	-0.0003
TR893	0.6908	0	4.5375	0.0084
TR894	0.5463	-0.0046	7.6959	0.0031
TR895	0.5146	-0.0063	5.0313	0.0438
TR896	0.468	0.0029	2.454	0.0012
TR898	0.2524	0	5.5613	-0.0001
TR905	0.3244	0.0051	5.7355	-0.0421
TR909	0.4264	-0.003	3.5176	0.015
TR913	0.4534	-0.0089	6.0945	-0.0429
TR917	0.6535	-0.0269	4.754	0.0792
TR920	0.6039	0.0023	5.4926	-0.0213
TR921	0.4801	-0.0091	4.994	0.0197
TR922	0.6791	0.0033	2.0833	0.0039
TR928	0.4274	-0.0146	2.8479	0.0557
TR944	0.5603	-0.001	6.7574	-0.0243
TR945	0.4113	-0.0206	1.9512	0.0684
TR947	0.5157	-0.0086	2.1074	-0.0456
TR948	0.5956	-0.0033	1.794	0.0136
mean	-	-0.0037	-	0.0083

Table S5: GSFE-Refinement best of top 5 results for CASP11 dataset

ID	start GDT-HA	Δ GDT-HA	start RMSD	Δ RMSD
TR217	0.644	0.0072	3.9267	-0.0128
TR228	0.5476	0	16.9914	-0.0325
TR274	0.2896	0.0041	3.29	-0.0186
TR280	0.5938	0	1.8435	-0.0266
TR283	0.4119	0.0128	6.2068	-0.0038
TR759	0.4395	0	6.5628	-0.0176
TR762	0.7043	0.001	9.9856	-0.0168
TR765	0.5789	0.0033	1.837	-0.0136
TR768	0.6381	0.0035	12.6573	-0.0175
TR769	0.5851	0	5.5089	0.0079
TR772	0.524	0	0.8874	-0.0062
TR774	0.3767	0.005	5.3811	-0.0105
TR776	0.6279	0.0148	4.3604	-0.0103
TR780	0.5395	0	5.9913	-0.0083
TR782	0.6477	0.0046	4.5375	-0.0207
TR783	0.573	0	7.6959	-0.0184
TR786	0.4781	0	5.0313	-0.0155
TR792	0.5813	0.0062	2.454	-0.0145
TR795	0.5864	0	5.5613	0.0078
TR803	0.3321	0.0037	5.7355	0.005
TR810	0.54	-0.0044	3.5176	-0.0269
TR811	0.7331	-0.002	6.0945	0.0023
TR816	0.5221	-0.0037	4.754	-0.0143
TR821	0.4833	0.0128	5.4926	-0.0059
TR822	0.3026	0.0044	4.994	-0.0047
TR827	0.3394	0.009	2.0833	-0.048
TR828	0.4881	0.0059	2.8479	-0.0255
TR829	0.5037	0	6.7574	-0.0065
TR833	0.6134	-0.0023	1.9512	-0.0206
TR837	0.4339	0	2.1074	-0.0485
TR848	0.5815	-0.0018	1.794	-0.0267
TR854	0.5857	0.0036	15.8571	-0.0189
TR856	0.6148	0	1.1959	-0.0012
TR857	0.3307	0.0052	12.2524	-0.0066
mean	-	0.0027	-	-0.0145

Table S6: GSFE-Refinement top 1 results for CASP11 dataset

ID	start GDT-HA	Δ GDT-HA	start RMSD	Δ RMSD
TR217	0.644	0.006	3.9267	-0.0096
TR228	0.5476	-0.0059	16.9914	-0.0356
TR274	0.2896	0	3.29	0.0016
TR280	0.5938	0.0026	1.8435	-0.0213
TR283	0.4119	0.0032	6.2068	-0.0031
TR759	0.4395	0.004	6.5628	0.0009
TR762	0.7043	0.0039	9.9856	-0.0057
TR765	0.5789	0.0033	1.837	-0.0067
TR768	0.6381	0.0018	12.6573	-0.0059
TR769	0.5851	0.0025	5.5089	-0.0004
TR772	0.524	-0.0013	0.8874	0.002
TR774	0.3767	0.0033	5.3811	-0.0065
TR776	0.6279	0.0045	4.3604	-0.0026
TR780	0.5395	0.0052	5.9913	0.0069
TR782	0.6477	-0.0022	4.5375	-0.0067
TR783	0.573	0	7.6959	0.0106
TR786	0.4781	-0.0034	5.0313	0.0006
TR792	0.5813	0.0031	2.454	-0.0143
TR795	0.5864	-0.0055	5.5613	0.009
TR803	0.3321	0.0019	5.7355	0.02
TR810	0.54	0.0011	3.5176	-0.0113
TR811	0.7331	0.001	6.0945	0.0005
TR816	0.5221	-0.0074	4.754	-0.0018
TR821	0.4833	-0.0019	5.4926	0.0031
TR822	0.3026	0.0022	4.994	-0.0089
TR827	0.3394	0.0065	2.0833	-0.0456
TR828	0.4881	0.0059	2.8479	-0.009
TR829	0.5037	0	6.7574	0.0016
TR833	0.6134	-0.0046	1.9512	0.0015
TR837	0.4339	0.0041	2.1074	-0.0289
TR848	0.5815	0	1.794	-0.0016
TR854	0.5857	0.0107	15.8571	-0.0151
TR856	0.6148	0	1.1959	-0.008
TR857	0.3307	0.0026	12.2524	-0.0018
mean	-	0.0014	-	-0.0056

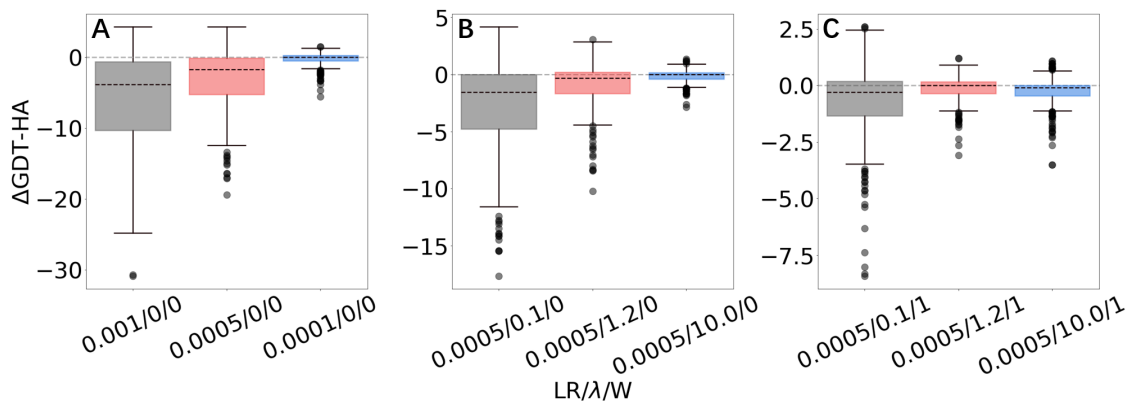


Figure S1: Δ GDT-HA of top 1 models by GFSE-Refinement for various $/LR/\lambda/W$ combinations on 3DRobot dataset

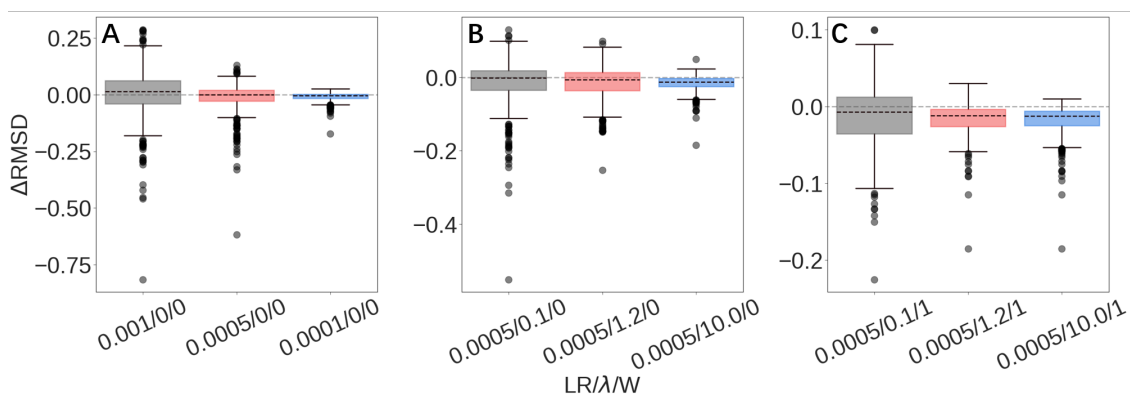


Figure S2: Δ RMSD of best of top 5 models by GFSE-Refinement for various $/LR/\lambda/W$ combinations on 3DRobot dataset

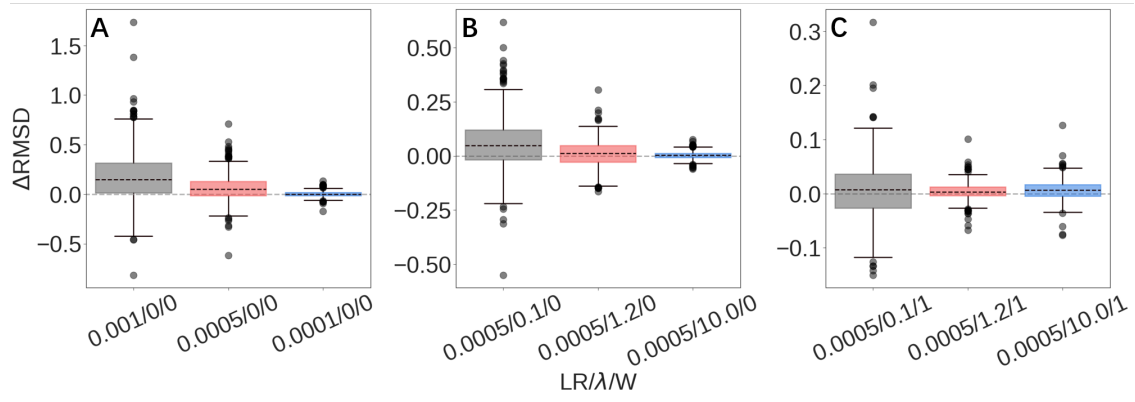


Figure S3: ΔRMSD of top 1 models by GFSE-Refinement for various $\text{LR}/\lambda/\text{W}$ combinations on 3DRobot dataset

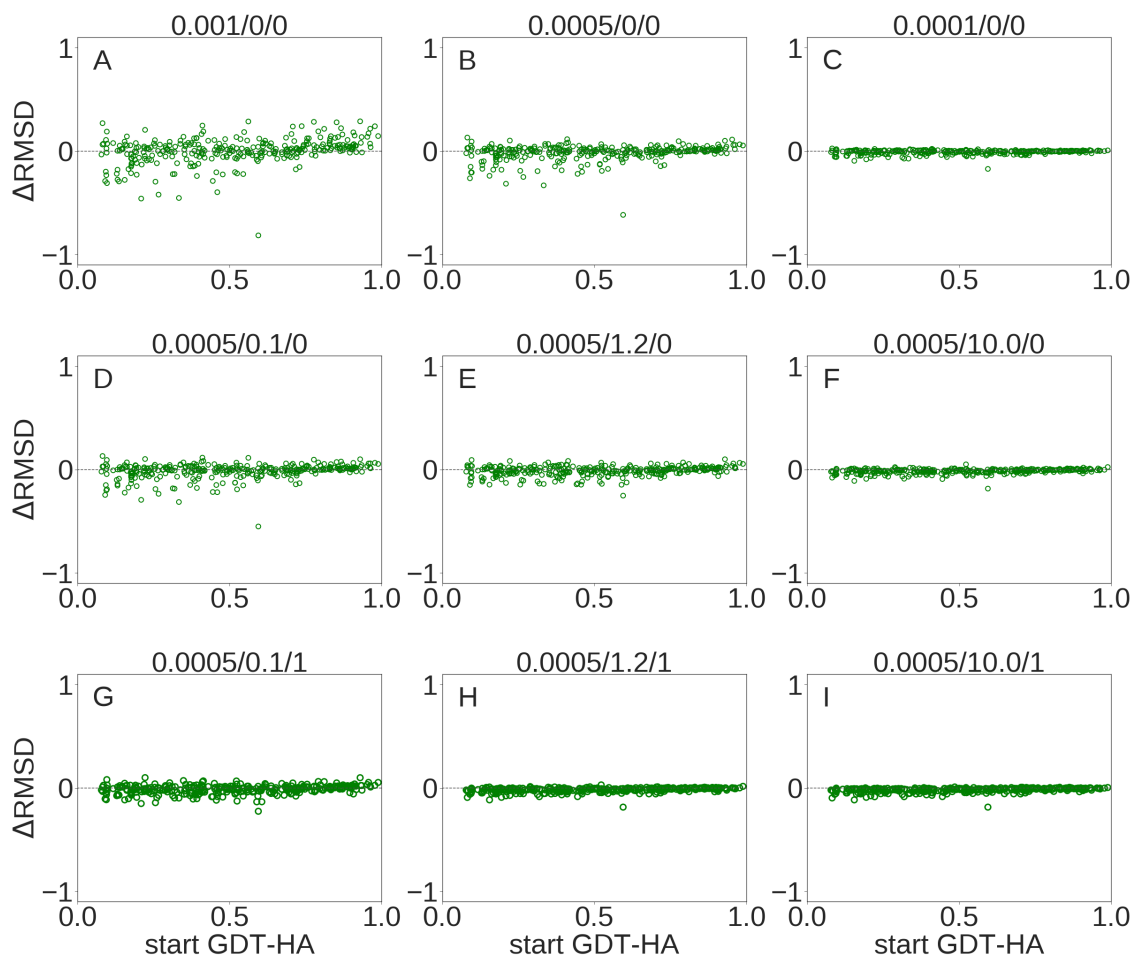


Figure S4: Scatter plots of ΔRMSD as a function of start GDT-HA for best of top 5 models by GSFE-Refinement for various /LR/ λ /W combinations on 3DRobot dataset

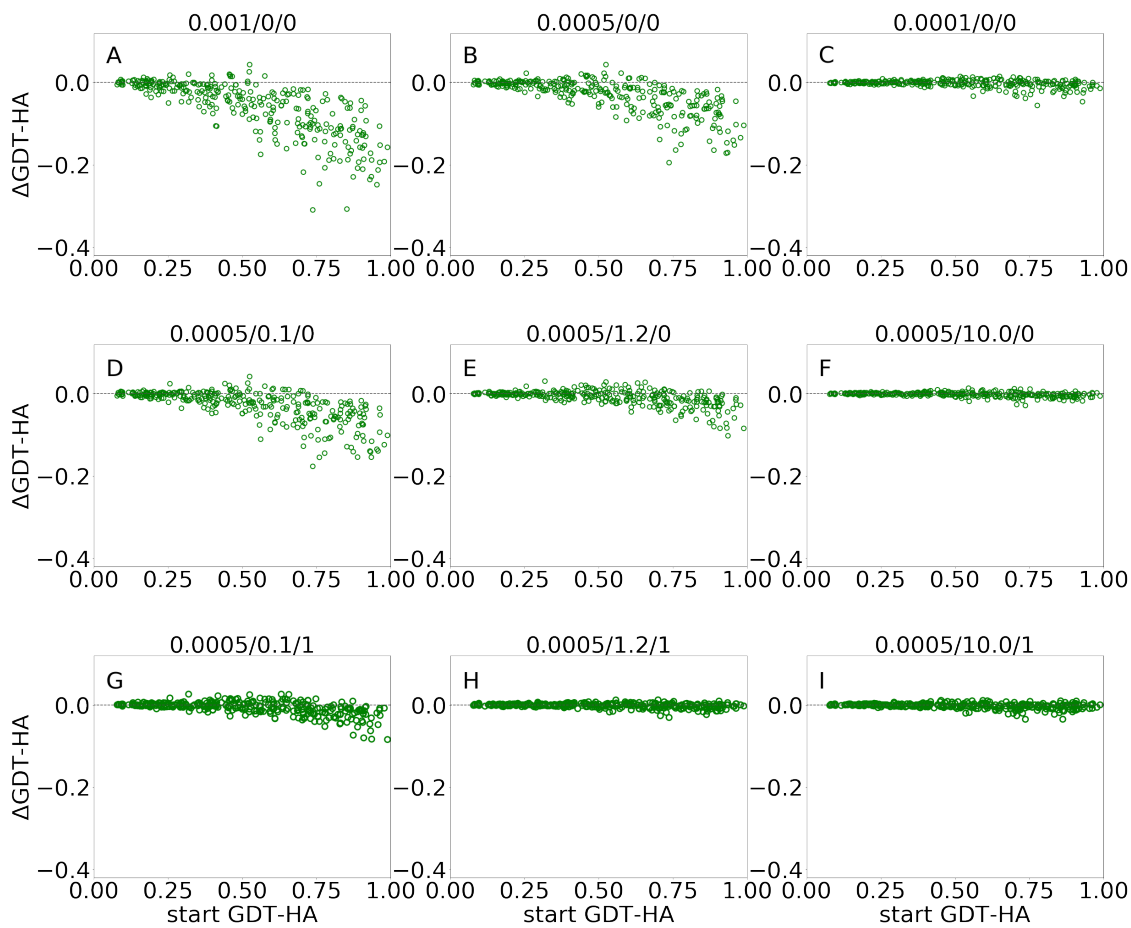


Figure S5: Scatter plots of $\Delta\text{GDT-HA}$ as a function of start GDT-HA for top 1 models by GSFE-Refinement for various $LR/\lambda/W$ combinations on 3DRobot dataset

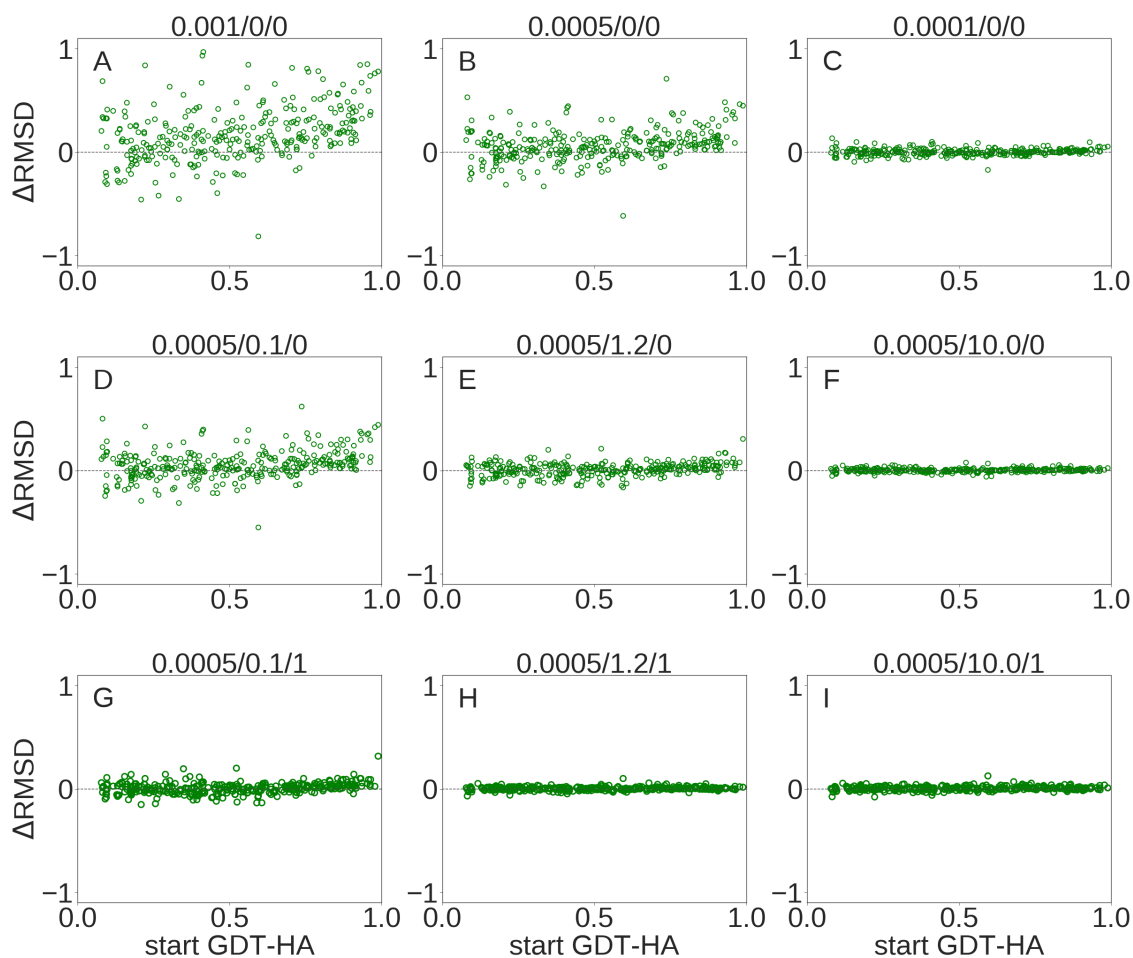


Figure S6: Scatter plots of ΔRMSD as a function of start GDT-HA for top 1 models by GSFE-Refinement for various /LR/ λ /W combinations on 3DRobot dataset

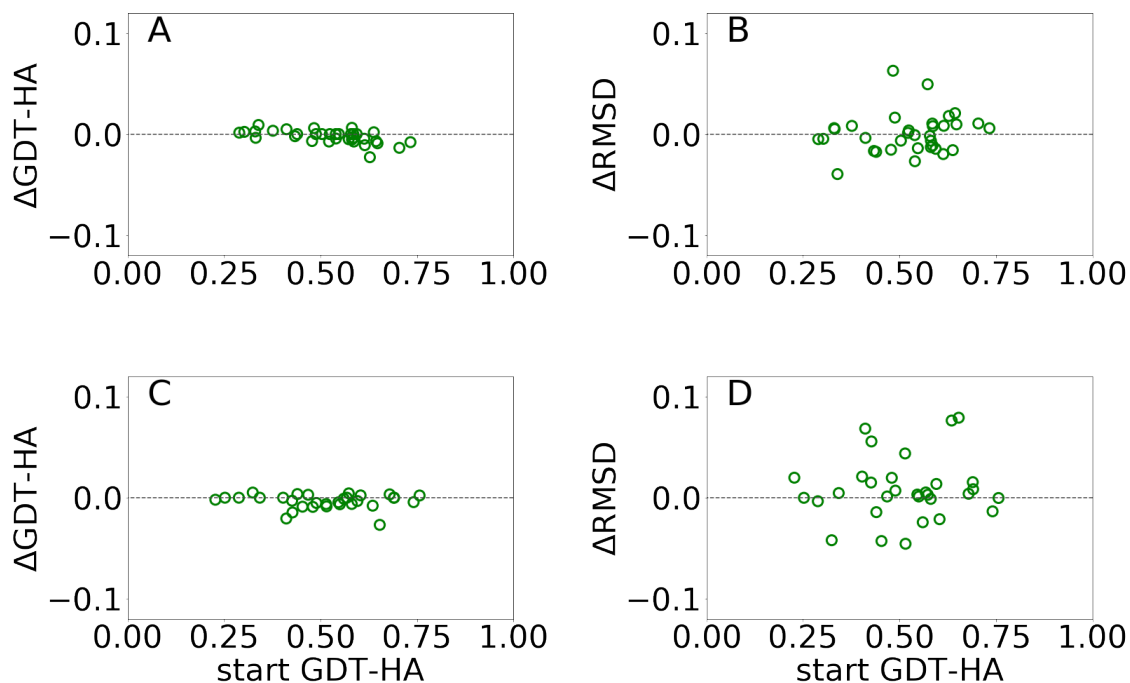


Figure S7: Scatter plots of $\Delta\text{GDT-HA}$ (A,C), ΔRMSD (B,D) as a function of start GDT-HA for top 1 models by GSFE-Refinement for various /LR/ λ /W combinations on CASP11 and CASP12 dataset

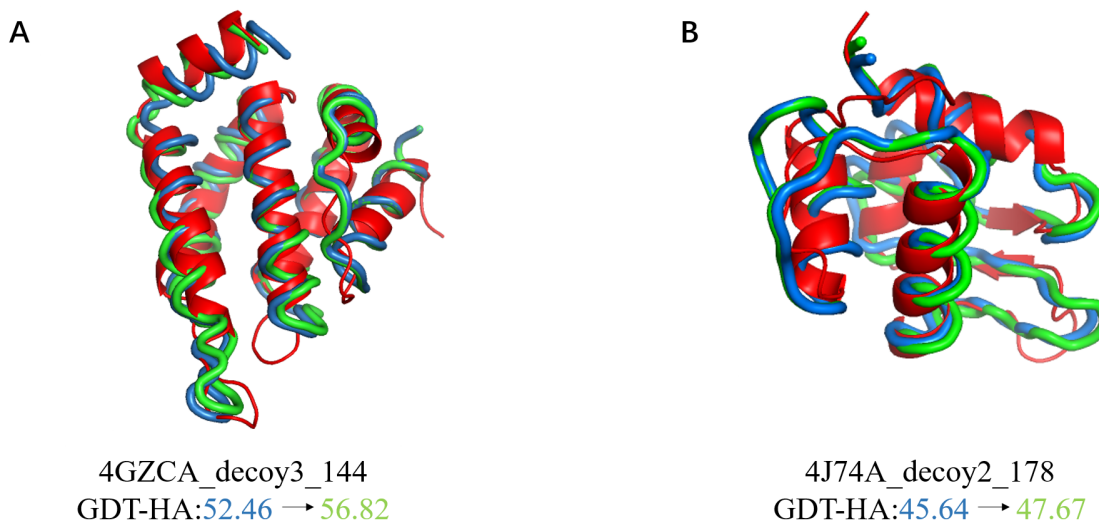


Figure S8: Two examples of GSFE-refinement with larger improvement for learning rate 0.0005 than 0.0001. The starting (red) and refined (green) decoys are overlaid on the experimental (blue) structures with change of GDT-HA at learning rate of 0.0005 indicated. Corresponding change of GDT-HA is 0.57 for 4GZCA_decoy3_144 and 0.58 for 4J74A_decoy2_178 respectively.

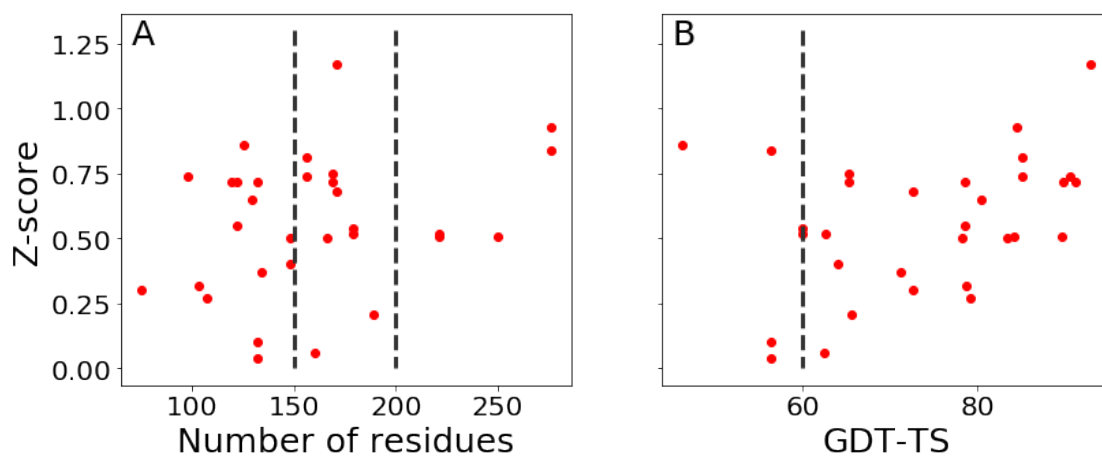


Figure S9: GDT-TS based Z-scores for top 1 model by GSFE-Refinement in CASP14. (A) As a function of the number of residues. (B) As a function of starting GDT-TS score.