

# Supplementary Information

*for*

refined: Improved protein structure refinement using machine learning  
based restrained relaxation

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<b>Supplementary Item</b>	<b>Title</b>
Supplementary Table S1	Effects of multi-resolution probabilistic restraints.
Supplementary Table S2	Refinement performance considering GDT-HA of the first selected refined structure.
Supplementary Table S3	Refinement performance considering GDT-HA of the best of top five refined structures.
Supplementary Figure S1	$\Delta$ GDT-HA of refinedD with cumulative and non-cumulative restraints with SCOP family, superfamily, fold class similarity for any of the training proteins.

Supplementary Table S1. Effects of multi-resolution probabilistic restraints.

PDB	Starting GDT-HA	Refined GDT-HA			
		0.5Å restraints	1.0Å restraints	2.0Å restraints	4.0Å restraints
1a07A	74.05	73.10	73.57	72.38	74.52
1a07A	74.05	73.10	73.57	72.38	74.52
1a00A	64.18	63.48	64.72	55.5	53.01
101m_	66.56	69.81	67.53	65.75	59.25
1a5v_	55.82	57.36	57.02	51.03	52.57
1atlA	64	67.37	64.75	63.88	64.38
1afqC	55.73	56.51	52.34	48.7	47.4
1awqA	57.32	57.32	56.4	55.18	56.55
1b0b_	62.94	62.59	59.4	51.77	55.67
1b11A	54.2	52.65	47.79	46.68	45.58
1b66A	57.07	55.62	55.07	53.44	51.45
1b1cA	66.27	65.51	69.28	67.02	60.09
1bs4A	59.23	60.12	57.89	57.44	54.91
1bh5A	53.1	50.16	49.02	44.61	40.36
1be9A	58.56	59.26	53.94	52.08	45.6
1bzsA	41.52	40.30	40.61	39.39	41.52
1bvqA	59.53	61.33	60.43	57.19	59.71
1c9kB	20.56	20.28	20	21.11	21.39
1cfvH	63.66	62.39	58.82	55.04	60.08
1ccwA	60.04	60.04	60.04	57.85	57.48
1cv8_	36.13	36.42	36.13	32.66	32.51
1cpq_	66.47	67.83	67.25	60.66	57.36
1d0iA	38.83	39.17	37.17	38.5	34.67
1d01D	56.85	56.10	52.08	52.68	47.32
1d2uA	32.61	31.79	30.16	30.16	29.35
1d1jC	53.28	56.93	52.37	51.64	50.18
1d8uA	48.48	49.55	47.73	44.39	38.79
1d7bA	10.41	10.14	9.73	10.14	10.14
1df8A	62.29	62.08	58.69	53.39	56.78
1ddrA	63.68	62.89	61.01	58.65	51.73
1dt1A	32.75	31.78	31.78	31.2	28.1
1ds7A	51.41	51.79	52.82	48.97	45.51
1dveA	43.93	43.93	43.22	40.65	39.84
1dud_	59.07	60.08	57.46	51.81	49.6
1d xpA	25.86	25.86	23.86	23.14	22.43
1dw0A	32.81	31.47	32.14	32.37	25
1d zrA	45.22	46.58	48.09	50.96	49.59
1e29A	42.22	41.30	40.19	35.37	35.19
1e20A	51.76	51.49	49.73	49.46	48.24
1ejbA	65.33	67.26	67.56	65.63	63.84

le6iA	72.05	72.95	71.14	69.09	66.59
lelrA	60.74	62.70	64.65	66.99	61.13
lelkA	58.99	60.29	58.17	54.58	57.68
lelwA	68.59	72.65	76.07	80.13	85.47
leumA	75.31	72.52	74.07	72.52	66.93
leqmA	57.28	57.59	57.75	55.38	47.31
lf7lA	51.27	54.03	56.57	53.81	56.36
leyhA	54.34	55.56	53.13	51.91	56.42
lew4A	59.43	61.32	63.44	65.57	65.57
lff3A	52.62	49.29	47.14	46.79	45.36
lfdk_	25.81	24.39	22.97	21.34	23.98
lg5tA	42.04	41.88	41.4	41.4	41.56
lfm0D	70.67	71.33	70.33	61.67	64.33
lgoyA	36.57	34.03	32.41	30.09	27.55
lgcvB	60.85	62.32	59.19	53.68	51.65
lgy7A	63.84	64.67	62.6	61.57	57.64
lgxuA	58.81	60.80	59.09	55.68	52.56
lgpqA	45.28	45.08	44.88	44.09	49.61
lh97A	54.08	53.40	54.42	52.72	56.29
lh4hA	47.82	46.72	46.48	44.17	38.96
lhb_	59.86	61.56	57.65	58.84	55.78
lhlb_	50.16	50.32	50	52.55	43.95
lhdoA	56.71	58.54	60	62.07	61.59
lj3wA	59.51	63.25	60.26	59.51	57.65
li4sA	44.9	44.39	41.84	43.88	44.05
lhn_	28.65	28.46	29.04	26.92	30.96
lkafA	24.77	24.07	22.92	22.69	21.53
lj77A	43.97	45.73	46.11	44.47	39.82
lmn8A	24.74	26.05	25.53	25	27.37
lmk0A	44.59	45.10	44.33	43.56	37.89
l19lA	59.8	59.12	58.11	63.85	49.32
lnlqA	23.1	22.86	25.24	24.05	20.24
loh0A	62.8	66.00	65.6	65.8	62.2
lo82A	30.36	30.36	30	33.21	25
lnwaA	24.11	24.70	24.55	24.7	25.15
lou8A	41.51	42.45	43.87	43.63	46.7
loohA	48.21	50.00	50.79	49.6	49.8
lok0A	18.24	16.55	17.23	16.89	15.54
low4A	54.79	55.21	54.79	51.04	48.33
lq4kA	7.88	8.45	8.56	7.55	8.56
lq1fA	62.5	65.71	63.18	61.82	55.91
lrfyA	61.8	61.80	64.04	59.83	57.58
lsz7A	46.86	48.11	46.23	44.97	44.03

1t3yA	62.21	64.89	64.5	61.26	54.58
1t1vA	61.56	60.48	57.53	48.92	53.76
1tkuA	9.44	9.95	9.31	9.31	9.95
1t7dA	4.81	4.93	5.17	5.05	4.93
1tqgA	72.14	72.14	72.62	67.86	63.33
1tp6A	42.06	42.46	45.63	41.67	40.67
1tugB	41.18	40.52	39.87	39.54	37.58
1u2hA	80.21	85.42	79.43	76.3	69.27
1tzvA	51.77	51.06	53.19	53.9	48.4
1ufyA	34.17	35.09	34.86	33.72	33.49
1u84A	33.64	34.57	31.79	30.25	31.79
1u55A	48.46	48.18	45.25	49.44	43.44
1ugiA	16.87	16.57	16.27	14.76	15.96
1usqA	32.91	33.45	33.63	32.73	29.68
1w53A	50.3	48.51	45.54	44.05	45.83
1uxzA	61.45	60.11	58.21	55.53	52.86
1uuyA	64.91	68.01	69.57	69.72	66.15
1wlzA	36.18	36.47	36.47	36.18	35
1wmhB	59.45	60.67	60.98	57.62	66.77
1wmhA	72.89	74.40	73.49	64.46	66.87
1wzdA	46.41	47.13	47.61	44.26	44.86
1wpaA	24.77	23.36	23.36	24.07	22.66
1x91A	72.32	72.82	71.14	66.61	68.96
1x6iA	53.37	55.62	62.36	64.89	69.1
1xa8A	22.96	23.60	24.74	25	23.09
1xmtA	55.79	55.53	56.84	55	51.32
1y3dl	39.06	38.67	41.02	37.89	38.67
1xppA	62.37	64.39	63.13	54.8	52.02
1yd0A	44.94	44.66	44.94	47.19	42.98
1y9tA	20.23	19.32	19.32	19.32	18.18
1z3eB	66.07	68.30	70.54	66.96	64.73
2bwfA	64.61	65.58	64.29	58.12	54.22
2b5aA	77.6	79.22	70.78	68.83	71.1
2chhA	17.26	16.81	15.71	16.37	14.82
2cb8A	76.74	77.03	77.03	78.78	72.38
2e92A	63.78	66.84	68.2	67.52	69.05
2ev1A	17.97	20.14	18.38	18.65	17.7
2gkgA	70.49	71.52	66.19	64.55	66.39
2fcwA	46.46	47.64	45.05	45.05	45.05
2h7zA	53	57.33	53	52.33	53
2grrB	21.02	21.82	21.34	21.02	23.57
2hi0A	51.05	50.52	51.22	45.63	48.78
2ifrA	11.76	12.13	12.62	11.52	11.03

2iu5A	28.91	29.19	27.65	30.45	29.75
2ip6A	73.28	76.15	79.02	75.29	78.16
2j8wA	55.47	56.05	58.2	56.05	59.77
2nmlA	20.5	19.75	20	19.25	22
2jekA	14.11	14.11	14.11	14.29	13.21
2o37A	55.56	58.64	58.64	67.59	60.19
2ofcA	22.34	22.16	21.63	18.09	19.15
2pmrA	72.7	69.41	65.13	66.12	69.74
2p6wA	21.24	21.24	21.6	22.57	21
2oznA	39.85	40.41	40.6	38.35	35.9
2pvbA	40.42	40.42	39.95	43.22	37.62
2pv2A	68.2	68.93	72.57	72.09	71.12
2rb8A	79.57	80.91	80.91	77.96	73.66
2v2pA	80	78.53	74.12	69.41	68.09
2rk3A	59.63	62.30	64.44	63.24	64.44
2zs0D	67.93	68.97	65.86	65.52	58.62
2vyyA	47.27	46.14	47.05	43.41	45.45
2v33A	19.78	21.70	23.9	24.18	21.98
3bqpA	59.69	61.87	63.75	55.94	57.5
3bfoA	71.18	70.88	73.24	74.41	70.88
3by4A	39.39	40.99	44.19	40.84	38.95
3bqsA	28.24	28.53	27.35	26.18	26.18
3c7mA	45.26	45.13	45.64	47.31	43.08
3d9nA	55.43	59.60	58.88	67.21	57.25
3cjsB	57.29	59.38	59.38	67.01	61.46
<b>Mean</b>	<b>48.9988</b>	<b>49.54133333</b>	<b>48.9566</b>	<b>47.6046</b>	<b>46.25806667</b>

Supplementary Table S2. Refinement performance considering GDT-HA of the first selected refined structure.

PDB	Starting GDT-HA	Refined GDT-HA									
		refined-C	refined-NC	FG-MD	FastRelax	FastRelax-0.5	FastRelax-1.0	FastRelax-2.0	FastRelax-4.0	ModRefiner-0	ModRefiner-100
1a07A	74.05	76.19	73.81	77.38	69.29	74.05	73.1	68.1	73.33	71.19	73.57
1a00A	64.18	65.07	52.13	64.18	50.89	63.48	60.82	59.93	54.43	62.77	64.36
101m_	66.56	69.64	61.53	69.32	51.14	68.99	65.58	66.4	60.39	68.67	67.86
1a5v_	55.82	57.19	49.83	54.62	45.55	56.51	55.65	50.17	50.86	55.48	56.51
1atlA	64	67.5	64.13	64.38	60.87	66.75	63.88	66.5	63.5	63.88	64.13
1afqC	55.73	56.25	46.88	55.73	38.28	55.99	54.17	50	47.4	44.79	56.25
1awqA	57.32	57.32	58.23	56.86	57.32	57.47	58.23	57.77	53.96	57.77	57.47
1b0b_	62.94	62.41	61.35	63.12	57.09	62.06	59.57	52.48	47.16	59.93	63.48
1b11A	54.2	52.43	51.11	52.88	42.92	51.55	50.44	48.45	47.12	50.22	52.88
1b66A	57.07	58.51	50.36	57.97	56.7	56.7	55.07	53.08	53.62	56.16	57.07
1b1cA	66.27	67.77	66.72	64.31	54.07	66.57	66.42	60.54	59.79	66.57	66.87
1bs4A	59.23	60.57	56.85	59.08	55.36	59.67	59.23	59.08	55.21	56.4	58.93
1bh5A	53.1	50.98	41.67	50.33	40.2	49.84	48.37	41.34	47.39	47.71	50.65
1be9A	58.56	58.33	46.76	59.26	47.45	57.64	54.4	57.64	46.53	53.01	57.41
1bszA	41.52	40	39.09	42.88	40.15	39.85	40.3	40	39.39	39.24	41.36

1bvqA	59.53	61.15	56.29	60.07	58.27	60.97	61.69	57.19	50.54	56.83	57.55
1c9kB	20.56	20.83	21.39	20.56	20	20.14	19.72	20.42	20.69	19.31	21.81
1cfvH	63.66	61.76	62.18	63.45	61.55	61.97	61.76	57.56	56.72	65.13	64.08
1ccwA	60.04	59.85	58.76	61.86	61.5	58.58	56.93	54.56	60.04	60.77	60.22
1cv8_	36.13	35.84	34.83	35.69	28.61	35.26	35.98	32.8	32.95	34.83	35.26
1cpq_	66.47	65.89	63.76	65.89	51.16	66.28	65.89	62.21	52.91	67.64	64.53
1d0iA	38.83	39.67	42.5	40.17	34.83	38.5	38	40	33.33	37.17	38.33
1d01D	56.85	55.51	52.98	56.85	43.01	55.8	51.79	51.79	51.49	56.7	55.8
1d2uA	32.61	32.07	30.98	32.2	28.53	32.2	30.84	29.35	30.84	33.02	32.07
1dljC	53.28	53.83	53.83	54.56	52.01	54.01	54.38	55.11	54.2	51.09	52.55
1d8uA	48.48	48.79	47.27	48.64	36.21	48.48	44.7	43.03	35.61	44.39	47.42
1d7bA	10.41	9.86	9.86	10.14	9.32	9.86	9.19	10	9.86	9.86	10
1d8A	62.29	62.29	50.42	62.08	48.94	61.02	59.53	52.54	51.27	60.81	62.29
1ddrA	63.68	63.52	51.26	64.31	48.9	62.42	62.26	58.96	44.97	61.95	64.15
1dt1A	32.75	33.14	25.58	33.91	25.58	31.59	32.36	27.52	27.33	15.7	32.75
1ds7A	51.41	51.92	53.33	50.51	43.33	51.41	51.67	48.08	49.87	49.87	51.67
1dveA	43.93	45.33	39.02	43.69	40.07	43.81	43.69	41.36	37.85	48.25	44.74
1dud_	59.07	59.48	59.27	58.67	48.99	58.47	55.65	51.41	50.4	57.66	58.87
1dxpA	25.86	27.43	21	26.86	21	25.29	24.57	24	23.14	23.43	27
1dw0A	32.81	32.81	32.37	33.71	29.69	31.25	32.37	31.47	30.36	30.58	30.8
1dzrA	45.22	46.86	45.22	46.72	49.04	46.04	45.22	46.04	45.49	46.58	46.17
1e29A	42.22	38.89	35	40.74	37.41	40.37	38.52	38.7	36.11	42.59	42.41
1e20A	51.76	51.49	48.51	52.3	44.59	51.22	50.41	49.46	46.89	53.11	51.89
1ejbA	65.33	66.52	64.58	64.73	60.71	66.37	65.77	63.24	61.46	67.56	67.41
1e6iA	72.05	75.23	72.95	72.27	68.64	73.86	75.23	71.82	63.86	71.59	72.73
1elrA	60.74	62.5	65.04	64.06	62.7	60.74	63.48	67.58	63.48	58.2	61.52
1elkA	58.99	60.46	58.01	59.48	57.52	59.97	59.15	55.56	61.6	58.33	59.31
1elwA	68.59	72.86	72.01	72.01	82.05	71.79	74.79	83.55	83.97	70.73	69.44
1eumA	75.31	73.45	68.63	74.69	65.37	72.36	68.32	69.25	66.3	71.58	74.84
1eqmA	57.28	57.75	56.96	59.97	50.47	57.12	56.8	58.7	46.2	51.74	57.91
1f71A	51.27	54.45	56.99	53.18	51.06	53.18	56.78	52.33	56.78	48.94	51.91
1eyhA	54.34	54.86	53.99	55.03	55.56	53.99	55.73	56.08	53.99	50.52	53.47
1ew4A	59.43	61.56	63.21	59.91	64.15	60.14	60.38	66.75	67.92	66.04	59.43
1ff3A	52.62	49.29	49.17	53.1	42.62	50	46.9	46.9	48.1	52.98	51.19
1fdk_	25.81	25	23.58	25.81	23.78	24.19	22.97	20.53	19.11	22.15	23.58
1g5tA	42.04	42.83	41.56	42.68	36.62	42.04	40.92	41.08	35.51	40.61	42.83
1fim0D	70.67	71.33	68.67	70	66	69.67	66	65	64	68.33	69.67
1goyA	36.57	35.42	27.55	37.73	31.02	35.19	34.49	33.1	31.25	30.09	36.57
1gevb	60.85	62.5	54.04	63.42	56.8	60.66	59.93	56.43	53.49	61.58	61.95
1gy7A	63.84	64.67	65.5	63.64	57.23	63.84	64.26	64.26	64.67	62.6	64.26
1gxuA	58.81	60.23	59.09	61.08	51.99	60.23	62.22	52.84	54.55	58.81	59.66
1gppA	45.28	45.08	43.11	45.28	47.83	44.69	43.11	40.16	45.67	45.87	45.87
1h97A	54.08	54.08	51.53	54.42	47.79	52.89	52.38	54.76	54.42	53.06	54.59
1h4hA	47.82	48.06	43.57	48.54	42.48	47.09	47.45	46.48	40.66	46	46.84
1hbg_	59.86	62.24	55.44	59.86	60.71	60.54	60.37	54.59	52.21	60.2	59.69
1h1b_	50.16	50	48.73	51.27	50.32	49.52	51.59	54.46	49.2	52.07	50.32

lhdoA	56.71	58.29	57.8	58.41	61.83	56.59	59.63	63.54	64.76	59.39	59.76
lj3wA	59.51	63.43	56.72	59.7	56.34	61.01	60.82	60.26	59.14	61.57	61.57
li4sA	44.9	43.54	42.01	47.79	40.99	43.54	40.99	42.69	44.05	44.9	45.41
lhn_	28.65	28.27	26.92	29.23	27.31	27.69	29.62	26.92	25.58	28.85	28.08
lkafA	24.77	24.07	22.69	24.54	20.83	23.84	24.31	21.76	21.3	22.45	24.54
lj77A	43.97	45.48	42.59	43.09	41.96	44.22	44.85	43.47	43.47	43.97	45.48
lmn8A	24.74	25.26	25	25.79	27.89	25	25	25	25	26.32	25.53
lmk0A	44.59	45.1	42.53	45.1	38.4	44.33	41.24	40.72	40.46	43.56	44.85
l191A	59.8	62.5	54.39	61.15	65.2	58.78	55.74	55.07	59.8	58.11	57.77
lnlqA	23.1	22.62	20.48	21.9	20.95	22.62	24.52	20.71	18.81	19.29	23.1
loh0A	62.8	64.6	64.8	64.4	62.4	63.8	65.8	64.4	63	67.2	65.6
lo82A	30.36	30.36	30	31.43	21.07	29.29	28.93	27.86	30.71	31.43	29.64
lnwaA	24.11	25.15	23.07	24.4	26.19	24.26	23.51	24.26	26.34	24.85	24.7
lou8A	41.51	42.22	46.46	41.27	36.32	41.27	45.75	46.7	44.34	44.1	42.22
loohA	48.21	48.81	50.2	49.4	52.38	48.61	50.4	51.79	48.61	49.6	48.21
lok0A	18.24	16.22	16.22	18.24	17.23	17.23	16.22	15.54	14.86	12.16	17.57
low4A	54.79	53.96	56.46	53.54	54.17	53.54	53.75	52.71	56.46	53.13	55.21
lq4kA	7.88	8.22	8.11	8.22	7.55	8	8	8.56	8.22	8.22	8.33
lq1fA	62.5	65.2	63.68	63.85	54.9	65.37	64.02	61.49	56.42	62.33	63.18
lrfyA	61.8	62.92	59.27	61.8	49.72	62.08	62.64	60.11	56.18	59.27	61.24
lsz7A	46.86	48.58	45.75	47.48	41.98	47.33	47.33	44.34	42.45	46.38	47.17
lt3yA	62.21	62.79	65.08	63.93	52.86	62.6	63.93	65.65	52.29	63.55	62.79
lt1vA	61.56	62.1	52.96	59.14	50.54	60.75	57.8	50.81	49.46	60.48	59.95
ltkuA	9.44	9.69	9.95	9.69	8.93	9.18	9.31	9.06	9.06	9.57	10.33
lt7dA	4.81	4.69	5.17	4.93	4.69	4.57	4.69	4.93	4.69	4.81	4.81
ltqgA	72.14	72.62	74.05	73.81	64.76	72.14	70.71	71.19	71.43	76.19	72.38
ltp6A	42.06	42.06	42.26	42.86	40.28	42.26	42.86	40.87	38.29	45.63	44.25
ltugB	41.18	39.22	36.27	41.99	37.25	39.54	38.73	38.07	35.62	40.03	41.18
lu2hA	80.21	82.81	74.48	81.25	77.86	83.07	82.55	76.56	74.22	79.43	80.47
ltzvA	51.77	52.66	52.13	51.06	51.95	50.53	52.48	55.14	53.01	53.55	52.84
lufyA	34.17	33.26	36.01	34.86	27.98	33.94	33.72	32.57	33.72	35.09	34.63
lu84A	33.64	33.64	33.95	35.49	32.41	33.64	35.19	33.33	33.64	34.88	34.88
lu55A	48.46	49.02	41.9	50.42	44.13	48.04	48.32	49.86	38.83	48.04	48.46
lugiA	16.87	17.17	16.57	17.77	14.76	16.27	15.66	15.96	15.66	16.57	16.27
lusqA	32.91	32.55	31.29	32.73	28.6	32.73	33.27	31.47	32.91	33.27	33.09
lw53A	50.3	47.32	45.54	50.3	41.07	47.32	44.35	44.05	49.7	52.08	49.4
luxzA	61.45	61.83	55.34	61.26	50.19	60.69	59.92	51.72	51.34	59.35	60.69
luuyA	64.91	67.39	67.08	66.15	62.11	67.24	69.41	67.55	63.66	66.3	66.46
lw1zA	36.18	36.18	37.06	36.18	36.18	36.18	37.06	37.35	37.06	36.18	36.18
lwmhB	59.45	60.67	55.79	60.37	70.12	61.28	60.98	68.9	75.3	58.84	60.98
lwmhA	72.89	75.9	71.69	72.29	57.23	72.29	70.48	60.84	64.76	69.88	72.89
lwzdA	46.41	47.37	41.39	46.53	37.68	46.65	46.65	43.42	37.44	49.28	49.16
lwpaA	24.77	23.6	23.36	25.47	23.36	21.96	22.66	23.6	23.6	25.23	25
lx91A	72.32	72.99	71.64	70.3	70.47	71.98	69.3	66.11	62.25	69.13	71.48
lx6iA	53.37	55.9	65.17	54.21	66.29	55.06	61.24	67.42	64.04	52.53	53.93
lxa8A	22.96	24.23	24.11	22.83	21.56	23.09	24.23	22.07	21.43	23.72	22.83



1xmtA	55.79	57.11	56.32	56.58	50	53.42	52.89	58.16	54.74	54.47	55.79
1y3dI	39.06	38.67	41.02	41.41	37.5	38.28	37.89	37.11	37.11	39.06	39.06
1xppA	62.37	63.89	60.1	62.63	47.47	64.39	59.34	57.83	50.25	48.74	63.89
1yd0A	44.94	46.63	41.01	46.91	41.85	45.51	46.35	44.94	43.54	39.04	43.54
1y9tA	20.23	19.55	19.09	19.77	18.18	18.86	18.41	18.18	19.32	20	20.45
1z3eB	66.07	68.75	66.07	65.18	68.75	65.63	69.2	63.84	71.88	70.54	66.07
2bwfA	64.61	67.21	65.26	68.83	58.12	64.94	64.61	58.12	68.18	63.64	63.96
2b5aA	77.6	76.95	69.81	78.9	74.35	77.27	69.81	73.05	69.81	81.17	77.6
2chhA	17.26	17.26	16.15	16.59	15.04	17.04	17.48	16.81	15.04	11.95	16.37
2cb8A	76.74	78.2	77.62	77.62	78.2	76.74	77.33	77.62	79.07	76.16	77.33
2c92A	63.78	67.52	68.88	63.27	63.95	65.99	66.5	69.39	64.46	63.61	63.1
2ev1A	17.97	19.19	20.27	18.92	16.89	18.11	18.65	19.46	20.54	11.89	17.97
2gkgA	70.49	71.31	56.76	71.72	64.55	69.88	68.65	68.24	60.04	68.65	70.29
2fcwA	46.46	46.23	45.28	46.46	42.22	46.46	44.81	43.4	43.63	48.11	47.88
2h7zA	53	55.33	55.67	54.67	51.33	53.33	53.33	53.33	51	49.67	54.33
2grrB	21.02	21.18	22.13	21.02	20.22	21.18	21.18	22.77	19.27	20.54	22.45
2hl0A	51.05	50.7	49.48	52.27	47.73	50.17	50.35	51.75	50.7	51.4	50.17
2ifrA	11.76	12.01	12.38	12.62	11.4	11.64	12.01	11.27	10.66	11.89	11.52
2iu5A	28.91	28.77	28.77	28.35	30.03	29.05	28.77	29.33	29.19	26.54	27.93
2ip6A	73.28	76.72	78.74	75	76.44	75	80.46	84.2	76.15	77.59	74.14
2j8wA	55.47	56.05	55.47	55.86	55.08	55.08	56.05	53.91	52.34	52.73	56.45
2nmlA	20.5	19.5	18.75	21	21	19.75	19	18.5	21.5	20	21
2jekA	14.11	14.29	13.04	14.29	13.04	13.93	13.93	13.75	13.57	14.11	13.93
2o37A	55.56	58.64	60.19	59.88	66.98	57.72	61.42	66.67	66.05	54.32	56.48
2ofcA	22.34	22.7	21.99	21.45	15.43	21.45	21.1	19.15	18.62	21.28	21.81
2pmrA	72.7	71.71	72.7	74.01	62.17	69.41	65.79	67.43	67.76	65.79	72.04
2p6wA	21.24	22.09	22.09	23.3	18.93	21.48	22.33	21.72	17.48	17.96	20.27
2oznA	39.85	39.1	37.03	39.66	35.71	38.53	39.29	36.09	37.03	38.91	38.72
2pvbA	40.42	41.82	40.42	42.06	39.25	40.65	41.82	38.55	41.12	38.79	40.19
2pv2A	68.2	68.2	78.64	70.15	74.51	68.93	67.72	74.76	72.82	69.9	68.69
2rb8A	79.57	83.06	77.42	81.72	76.08	82.53	77.15	80.11	77.69	80.65	79.57
2v2pA	80	77.79	67.06	78.97	66.62	77.65	74.85	69.71	69.85	76.47	80.44
2rk3A	59.63	62.43	62.03	59.76	66.58	61.36	61.5	65.64	65.51	59.89	59.22
2zs0D	67.93	68.97	68.62	69.14	69.66	66.21	62.76	65.17	56.72	61.03	66.38
2vyyA	47.27	46.36	48.86	49.77	47.05	45.91	48.86	50.45	52.5	51.59	48.64
2v33A	19.78	21.15	23.9	21.98	22.25	21.15	21.98	23.08	22.25	23.08	21.7
3bqpA	59.69	62.19	60.62	58.75	57.19	61.25	63.75	57.81	52.5	55.94	60.62
3bfoA	71.18	72.94	70.88	71.47	72.06	70.29	74.41	74.71	73.24	75	71.47
3by4A	39.39	40.26	40.12	40.26	36.63	39.97	41.86	39.24	38.95	39.39	39.83
3bqsA	28.24	28.24	26.47	28.82	27.06	27.65	28.24	25	25.29	25.88	27.35
3c7mA	45.26	45	47.82	44.87	42.18	44.74	43.33	45.38	43.33	44.74	45.9
3d9nA	55.43	58.7	61.96	56.7	60.14	59.42	61.05	61.96	63.59	59.96	58.33
3cjsB	57.29	59.72	71.53	56.6	53.13	57.29	62.5	63.54	68.75	60.42	58.68
<b>Mean</b>	<b>48.9988</b>	<b>49.6353</b>	<b>47.7585</b>	<b>49.5585</b>	<b>45.5671</b>	<b>48.8585</b>	<b>48.6577</b>	<b>47.7868</b>	<b>46.4517</b>	<b>48.1588</b>	<b>49.1479</b>

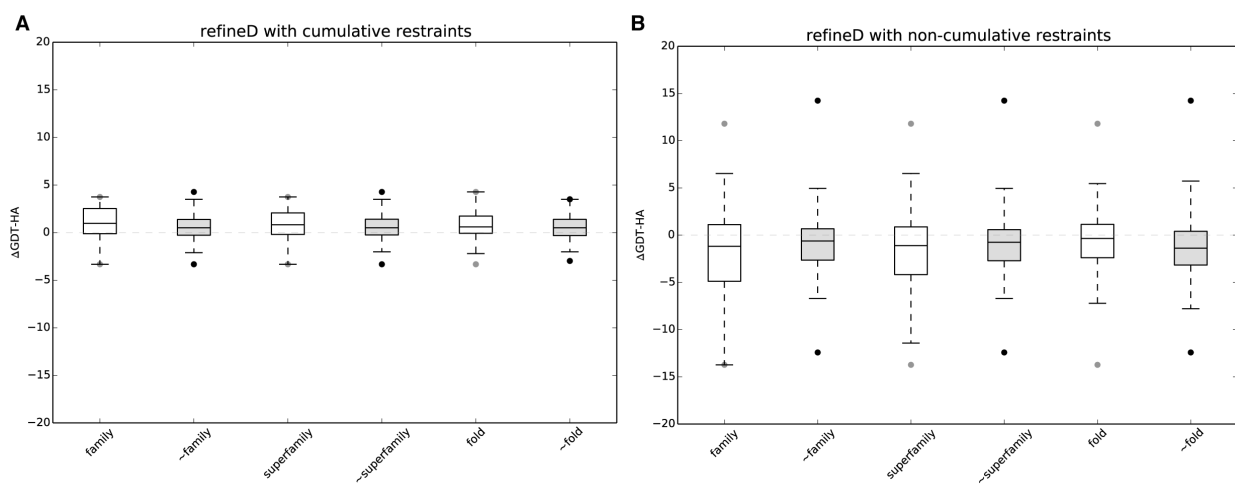
Supplementary Table S3. Refinement performance considering GDT-HA of the best of top five refined structures.

PDB	Starting GDT-HA	Refined GDT-HA									
		refined-C	refined-NC	FG-MD	FastRelax	FastRelax-0.5	FastRelax-1.0	FastRelax-2.0	FastRelax-4.0	ModRefiner-0	ModRefiner-100
1a07A	74.05	76.19	73.81	77.38	70.95	74.05	73.33	72.86	73.33	71.19	73.57
1a00A	64.18	65.78	59.93	64.18	64.54	64.01	63.12	62.94	61.17	62.77	64.36
101m_	66.56	71.27	65.26	69.32	52.11	69.16	67.37	66.4	60.39	68.67	67.86
1a5v_	55.82	59.42	58.05	54.62	45.55	56.51	55.99	53.6	51.37	55.48	56.51
1atlA	64	68.25	68.12	64.38	63	66.75	65.25	67.37	65.25	63.88	64.13
1afqC	55.73	57.55	57.81	55.73	45.31	55.99	55.47	53.65	47.66	44.79	56.25
1awqA	57.32	58.54	59.3	56.86	57.32	57.62	59.6	59.3	58.23	57.77	57.47
1b0b_	62.94	62.94	63.48	63.12	57.62	62.23	60.82	60.46	61.52	59.93	63.48
1b11A	54.2	52.88	52.43	52.88	47.12	51.99	51.33	48.45	47.12	50.22	52.88
1b66A	57.07	58.51	56.16	57.97	57.07	56.7	57.25	55.8	55.8	56.16	57.07
1b1cA	66.27	68.83	67.47	64.31	63.25	66.72	66.42	67.17	64.61	66.57	66.87
1bs4A	59.23	60.71	59.82	59.08	57.14	60.12	59.23	59.67	59.23	56.4	58.93
1bh5A	53.1	52.12	45.75	50.33	48.86	50	49.84	46.57	48.86	47.71	50.65
1be9A	58.56	58.56	57.87	59.26	52.31	57.64	58.33	58.33	59.95	53.01	57.41
1bzsA	41.52	40.3	41.36	42.88	41.06	40	40.91	41.21	39.39	39.24	41.36
1bvqA	59.53	61.87	62.05	60.07	60.97	60.97	61.69	62.59	58.81	56.83	57.55
1c9kB	20.56	20.83	22.08	20.56	22.78	20.28	20.83	21.94	21.39	19.31	21.81
1cfvH	63.66	63.03	62.18	63.45	61.55	62.39	61.76	61.55	61.55	65.13	64.08
1ccwA	60.04	60.22	61.31	61.86	61.5	59.31	60.4	58.39	60.04	60.77	60.22
1cv8_	36.13	35.84	36.27	35.69	28.61	35.69	35.98	32.95	32.95	34.83	35.26
1cpq_	66.47	67.25	64.34	65.89	55.04	66.28	67.44	62.21	61.05	67.64	64.53
1d0iA	38.83	39.67	42.5	40.17	41.67	38.67	40.17	41.17	37.5	37.17	38.33
1d01D	56.85	56.55	57.29	56.85	50.3	55.8	54.61	51.79	51.49	56.7	55.8
1d2uA	32.61	32.74	32.47	32.2	29.89	32.2	31.66	30.98	30.84	33.02	32.07
1dljC	53.28	56.2	56.39	54.56	57.3	54.01	54.38	55.66	56.39	51.09	52.55
1d8uA	48.48	50.15	49.55	48.64	36.21	48.64	48.48	43.33	39.85	44.39	47.42
1d7bA	10.41	10.68	10.14	10.14	10.81	9.86	10.27	10.41	11.22	9.86	10
1df8A	62.29	62.29	60.17	62.08	49.15	61.02	59.75	55.93	51.27	60.81	62.29
1ddrA	63.68	64.47	62.74	64.31	55.19	62.58	62.42	58.96	53.46	61.95	64.15
1dt1A	32.75	33.14	32.56	33.91	27.52	32.17	33.72	29.84	29.65	15.7	32.75
1ds7A	51.41	52.44	53.33	50.51	50.64	51.54	51.79	53.85	49.87	49.87	51.67
1dveA	43.93	45.33	44.51	43.69	42.87	43.81	44.74	43.34	43.34	48.25	44.74
1dud_	59.07	61.09	59.27	58.67	54.03	59.07	56.65	54.44	53.02	57.66	58.87
1dxaA	25.86	27.43	24.29	26.86	22	25.29	27.14	25.29	23.29	23.43	27
1dw0A	32.81	33.48	32.59	33.71	29.69	31.47	33.71	32.59	32.59	30.58	30.8
1dzrA	45.22	46.99	48.5	46.72	52.32	46.04	47.27	52.19	47.27	46.58	46.17
1e29A	42.22	41.67	40	40.74	41.85	40.37	41.3	39.81	41.67	42.59	42.41
1e20A	51.76	52.84	54.05	52.3	52.57	51.89	51.35	49.46	49.73	53.11	51.89
1ejbA	65.33	67.86	65.92	64.73	65.92	66.37	66.67	65.18	64.88	67.56	67.41
1e6iA	72.05	75.23	76.59	72.27	72.95	73.86	75.45	72.05	72.27	71.59	72.73
1elrA	60.74	62.5	65.04	64.06	64.45	60.74	63.67	75.2	63.48	58.2	61.52
1elkA	58.99	61.6	64.22	59.48	58.99	60.29	59.97	64.38	61.6	58.33	59.31
1elwA	68.59	73.5	82.69	72.01	82.05	72.01	76.28	83.55	83.97	70.73	69.44
1eumA	75.31	74.22	71.89	74.69	70.5	72.52	70.81	71.58	70.96	71.58	74.84

leqmA	57.28	58.7	58.39	59.97	52.69	57.28	57.44	58.7	51.42	51.74	57.91
l171A	51.27	54.66	56.99	53.18	56.57	53.18	56.99	56.14	56.78	48.94	51.91
leyhA	54.34	55.56	56.25	55.03	57.29	53.99	55.73	58.16	55.9	50.52	53.47
lew4A	59.43	61.56	67.92	59.91	66.51	60.14	63.21	67.92	68.16	66.04	59.43
lff3A	52.62	50.6	50	53.1	46.31	50	48.45	46.9	48.57	52.98	51.19
lfdk_	25.81	25.2	25	25.81	23.78	24.39	23.98	22.56	22.97	22.15	23.58
lg5tA	42.04	42.83	41.56	42.68	40.76	42.04	42.36	43.79	41.08	40.61	42.83
lfm0D	70.67	71.33	71.67	70	67	70	70.33	65.67	67.67	68.33	69.67
lgoyA	36.57	35.42	33.56	37.73	31.02	35.19	36.11	33.1	32.18	30.09	36.57
lgevB	60.85	62.68	58.09	63.42	56.8	60.66	59.93	56.8	56.62	61.58	61.95
lgy7A	63.84	65.08	67.15	63.64	63.64	64.26	64.88	65.7	65.08	62.6	64.26
lgxuA	58.81	60.8	62.78	61.08	57.39	60.23	62.22	60.23	59.38	58.81	59.66
lgpqA	45.28	45.67	44.09	45.28	47.83	44.69	44.88	43.9	48.43	45.87	45.87
lh97A	54.08	55.1	54.42	54.42	56.8	53.06	54.08	58.67	54.42	53.06	54.59
lh4hA	47.82	48.06	47.21	48.54	42.72	47.33	47.57	47.94	44.78	46	46.84
lhbq_	59.86	62.24	61.05	59.86	60.71	60.54	60.71	56.97	54.42	60.2	59.69
lh1b_	50.16	50.8	51.59	51.27	50.32	49.68	52.23	54.46	52.55	52.07	50.32
lhdoA	56.71	58.9	63.78	58.41	61.83	56.83	59.63	65.12	64.76	59.39	59.76
lj3wA	59.51	63.62	62.13	59.7	61.57	61.01	63.06	62.13	59.14	61.57	61.57
li4sA	44.9	43.88	45.58	47.79	44.39	43.54	43.54	43.88	44.73	44.9	45.41
lhn1_	28.65	28.65	28.85	29.23	32.31	27.69	30	27.5	33.08	28.85	28.08
lkafA	24.77	24.54	24.07	24.54	26.16	24.07	25.69	24.07	22.22	22.45	24.54
lj77A	43.97	45.98	46.48	43.09	41.96	44.72	45.48	44.1	43.47	43.97	45.48
lmn8A	24.74	26.05	26.58	25.79	30.26	25	26.05	26.32	27.37	26.32	25.53
lmk0A	44.59	45.62	43.56	45.1	38.92	44.59	43.56	44.85	40.98	43.56	44.85
l191A	59.8	63.85	61.15	61.15	65.2	58.78	58.11	55.07	59.8	58.11	57.77
ln1qA	23.1	23.33	23.81	21.9	21.43	22.86	24.52	22.86	23.33	19.29	23.1
loh0A	62.8	67	67.6	64.4	65	64.2	65.8	67	63	67.2	65.6
lo82A	30.36	30.36	30	31.43	32.5	29.64	30	31.43	30.71	31.43	29.64
lnwaA	24.11	25.15	25	24.4	26.19	24.4	25.89	25.45	26.34	24.85	24.7
lou8A	41.51	42.92	48.58	41.27	43.87	41.27	45.75	47.88	49.76	44.1	42.22
loohA	48.21	49.8	52.18	49.4	52.38	48.61	52.18	53.37	52.18	49.6	48.21
lok0A	18.24	17.23	17.57	18.24	17.23	17.23	17.23	17.23	16.89	12.16	17.57
low4A	54.79	55	56.46	53.54	54.17	53.96	56.67	54.58	56.46	53.13	55.21
lq4kA	7.88	8.33	8.78	8.22	9.12	8	8.45	8.56	8.56	8.22	8.33
lq1fA	62.5	65.54	65.88	63.85	61.49	65.54	64.7	66.72	59.12	62.33	63.18
lrfyA	61.8	62.92	63.48	61.8	61.52	62.08	64.04	62.64	58.99	59.27	61.24
lsz7A	46.86	49.21	49.06	47.48	46.7	47.64	47.8	45.44	47.96	46.38	47.17
lt3yA	62.21	63.55	65.84	63.93	62.6	62.79	64.12	65.65	64.5	63.55	62.79
lt1vA	61.56	62.9	62.37	59.14	57.53	60.75	58.6	56.18	50.54	60.48	59.95
ltkuA	9.44	9.69	9.95	9.69	9.69	9.18	9.31	10.2	10.46	9.57	10.33
lt7dA	4.81	5.29	5.17	4.93	5.05	4.57	4.81	5.29	5.17	4.81	4.81
ltqgA	72.14	74.76	74.29	73.81	67.62	72.14	75	71.19	75.71	76.19	72.38
ltp6A	42.06	43.65	42.66	42.86	41.27	42.66	46.63	43.45	41.67	45.63	44.25
ltugB	41.18	40.36	39.22	41.99	39.22	40.03	40.85	39.54	40.03	40.03	41.18
lu2hA	80.21	84.64	83.33	81.25	77.86	83.33	82.55	78.91	75.26	79.43	80.47

1tzvA	51.77	52.66	53.9	51.06	60.82	50.71	52.48	55.67	60.11	53.55	52.84
1ufyA	34.17	34.63	36.01	34.86	33.49	33.94	33.72	33.94	34.17	35.09	34.63
1u84A	33.64	34.26	36.11	35.49	33.33	33.64	35.8	35.8	35.19	34.88	34.88
1u55A	48.46	49.02	50.14	50.42	57.68	48.18	48.74	49.86	47.77	48.04	48.46
1ugiA	16.87	17.17	16.57	17.77	16.57	16.57	15.66	15.96	17.47	16.57	16.27
1usqA	32.91	33.45	32.73	32.73	30.94	32.73	34.71	32.91	32.91	33.27	33.09
1w53A	50.3	48.81	47.92	50.3	47.92	47.32	46.43	46.43	49.7	52.08	49.4
1uxzA	61.45	62.6	59.35	61.26	50.57	60.88	60.11	56.49	51.34	59.35	60.69
1uuyA	64.91	68.79	68.32	66.15	67.7	67.55	69.41	69.88	68.94	66.3	66.46
1wlzA	36.18	37.06	37.65	36.18	37.06	36.18	37.35	37.94	37.35	36.18	36.18
1wmhB	59.45	62.8	65.85	60.37	70.12	61.28	61.59	68.9	75.3	58.84	60.98
1wmhA	72.89	76.2	76.2	72.29	66.27	72.89	71.99	70.48	68.67	69.88	72.89
1wzdA	46.41	47.85	43.78	46.53	41.75	46.77	47.97	44.86	44.14	49.28	49.16
1wpaA	24.77	23.6	23.83	25.47	24.53	22.43	23.13	24.07	24.77	25.23	25
1x91A	72.32	72.99	73.15	70.3	71.31	71.98	71.48	70.13	66.11	69.13	71.48
1x6iA	53.37	56.18	69.38	54.21	67.42	56.18	62.36	67.42	67.7	52.53	53.93
1xa8A	22.96	24.23	24.49	22.83	24.11	23.09	24.49	24.11	22.32	23.72	22.83
1xmtA	55.79	57.11	57.89	56.58	56.05	54.47	55.79	58.16	54.74	54.47	55.79
1y3dI	39.06	39.06	41.02	41.41	41.02	39.06	38.28	39.84	38.67	39.06	39.06
1xppA	62.37	64.9	60.1	62.63	50.25	64.39	62.37	58.08	53.28	48.74	63.89
1yd0A	44.94	47.47	45.51	46.91	46.91	46.07	48.31	44.94	46.07	39.04	43.54
1y9tA	20.23	19.77	19.09	19.77	18.18	18.86	19.09	19.32	19.32	20	20.45
1z3eB	66.07	69.2	67.86	65.18	70.54	66.07	70.54	72.77	71.88	70.54	66.07
2bwfA	64.61	67.21	65.26	68.83	70.45	64.94	65.91	65.26	70.78	63.64	63.96
2b5aA	77.6	78.25	71.43	78.9	74.35	77.6	74.03	74.68	73.05	81.17	77.6
2chhA	17.26	17.7	17.26	16.59	16.37	17.04	18.36	18.36	15.93	11.95	16.37
2cb8A	76.74	78.78	79.94	77.62	78.78	77.33	82.27	79.94	79.65	76.16	77.33
2c92A	63.78	67.52	69.22	63.27	70.75	66.5	68.2	69.39	66.67	63.61	63.1
2ev1A	17.97	20.27	20.27	18.92	21.49	18.24	19.46	19.46	22.16	11.89	17.97
2gkgA	70.49	71.52	69.26	71.72	64.75	70.08	68.65	68.24	68.65	68.65	70.29
2fewA	46.46	48.11	46.93	46.46	44.58	46.93	46.46	45.99	47.41	48.11	47.88
2h7zA	53	56.67	55.67	54.67	51.33	54	54	54.67	51.33	49.67	54.33
2grrB	21.02	21.82	22.13	21.02	20.22	21.18	22.45	22.77	22.77	20.54	22.45
2hl0A	51.05	51.4	51.22	52.27	55.59	50.17	51.57	51.75	51.75	51.4	50.17
2ifrA	11.76	12.5	12.62	12.62	11.89	11.76	12.99	12.99	11.52	11.89	11.52
2iu5A	28.91	29.33	32.82	28.35	36.31	29.19	29.47	30.31	31.15	26.54	27.93
2ip6A	73.28	77.3	78.74	75	76.44	75.57	80.46	84.2	81.32	77.59	74.14
2j8wA	55.47	56.05	59.57	55.86	55.08	55.66	59.38	58.2	62.89	52.73	56.45
2nmlA	20.5	20.5	20.5	21	22	19.75	21	20.5	21.5	20	21
2jekA	14.11	14.64	14.46	14.29	14.46	14.11	13.93	14.11	14.64	14.11	13.93
2o37A	55.56	58.64	65.74	59.88	67.9	57.72	61.42	67.28	67.9	54.32	56.48
2ofcA	22.34	22.7	22.7	21.45	19.68	21.63	22.34	20.04	20.04	21.28	21.81
2pmrA	72.7	72.37	72.7	74.01	70.72	69.41	68.75	71.38	71.38	65.79	72.04
2p6wA	21.24	22.21	22.21	23.3	22.94	21.48	22.69	22.33	19.9	17.96	20.27
2oznA	39.85	40.04	40.04	39.66	40.79	38.91	39.29	37.97	38.72	38.91	38.72
2pvbA	40.42	41.82	41.59	42.06	39.49	40.89	41.82	42.29	41.12	38.79	40.19

2pv2A	68.2	73.06	78.64	70.15	82.28	69.17	71.36	76.7	73.79	69.9	68.69
2rb8A	79.57	83.33	83.6	81.72	77.42	82.53	79.84	80.11	77.69	80.65	79.57
2v2pA	80	80.15	78.68	78.97	66.62	77.65	74.85	70.59	69.85	76.47	80.44
2rk3A	59.63	62.57	64.57	59.76	66.58	61.76	63.1	65.64	65.64	59.89	59.22
2zs0D	67.93	68.97	68.79	69.14	69.66	66.55	66.21	66.72	66.21	61.03	66.38
2vyyA	47.27	47.05	48.86	49.77	50	46.14	48.86	54.32	52.5	51.59	48.64
2v33A	19.78	21.98	25	21.98	25	21.15	24.45	23.08	25.55	23.08	21.7
3bqpA	59.69	62.81	61.87	58.75	61.56	61.25	65.94	62.19	55.94	55.94	60.62
3bfoA	71.18	72.94	72.65	71.47	81.47	70.88	75.29	74.71	74.12	75	71.47
3by4A	39.39	41.28	41.57	40.26	40.26	40.26	43.02	42.59	44.04	39.39	39.83
3bqsA	28.24	28.24	27.94	28.82	27.65	27.65	28.24	27.35	27.35	25.88	27.35
3c7mA	45.26	45.26	49.36	44.87	45.9	44.87	44.49	45.38	47.31	44.74	45.9
3d9nA	55.43	59.96	61.96	56.7	62.5	59.42	61.05	63.22	66.85	59.96	58.33
3cjsB	57.29	59.72	73.96	56.6	66.32	59.03	62.85	71.88	72.22	60.42	58.68
<b>Mean</b>	<b>48.9988</b>	<b>50.3097</b>	<b>50.5284</b>	<b>49.5585</b>	<b>48.7989</b>	<b>49.0536</b>	<b>49.8799</b>	<b>49.8211</b>	<b>49.0739</b>	<b>48.1588</b>	<b>49.1479</b>



Supplementary Figure S1.  $\Delta$ GDT-HA of refinedD with cumulative and non-cumulative restraints with SCOP family, superfamily, fold class similarity for any of the training proteins. A<sup>-</sup> indicates that none of the test cases belong to the corresponding SCOP classification.