## Loop Benchmark Report

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## Chapter 1

## Results

#### 1.1 Overall benchmark performance



Model selection	Median rmsd (Å)	$\begin{array}{c} \text{Median score} \\ \text{(REU)} \end{array}$	Median time (sec)	Average time (sec)
Best of top 5 models Lowest scoring models Lowest RMSD models All models	$0.50 \\ 0.72 \\ 0.35 \\ 2.90$	-263.34 -274.85 -247.64 -222.92	$4000 \\ 4000 \\ 4000 \\ 4000$	$4000 \\ 4000 \\ 4000 \\ 4000$

Median fraction of sub-Å models: 15.60%Average fraction of sub-Å models: 23.55%Average number of models per loop: 500.00

#### 1.2 Individual results per loop

		Best	of Top 5	Models	Clos	est Model	
Loop	Models	ID	RMSD	Score	ID	RMSD	Score
1a8d	500	237	0.56	-471.35	14	0.51	-463.34
1arb	500	458	1.00	-166.81	187	0.31	-155.24
1bhe	500	238	0.31	-385.92	159	0.30	-375.35
$1\mathrm{bn8}$	500	81	3.15	-463.54	414	1.05	-455.06
1c5e	500	16	0.38	-343.73	333	0.27	-342.22
1 cb 0	500	324	0.26	-317.82	274	0.18	-317.06
$1 \mathrm{cnv}$	500	1	1.45	-327.95	238	1.18	-321.15
1 cs 6	500	386	0.98	-414.73	246	0.74	-400.49
1 cyo	500	376	0.55	-92.14	204	0.37	-90.98
1 dqz	500	206	0.39	-725.89	292	0.34	-608.26
1dts	500	378	10.94	-209.97	151	0.72	-169.09
1 e c o	500	89	0.35	-153.49	91	0.29	-148.52
1ede	500	318	1.82	-170.18	447	0.46	-165.23
$1 \mathrm{exm}$	500	393	0.45	-492.09	183	0.35	-490.87
1ezm	500	247	0.39	-130.81	295	0.35	-126.29
1f46	500	21	0.53	-369.52	380	0.50	-368.62
1i7p	500	128	0.38	-327.98	308	0.31	-324.79
1 m 3 s	500	497	1.59	-245.22	480	0.50	-217.34
1 ms9	500	406	0.51	-1133.41	298	0.28	-1118.61
$1 \mathrm{msc}$	500	101	1.27	156.86	227	1.04	160.73
1 my 7	500	46	0.56	-225.32	300	0.49	-222.97
1onc	500	482	3.52	-107.95	128	0.61	-104.42
10th	500	324	0.29	-372.81	91	0.25	-368.24
1 oyc	500	274	0.40	1273.20	380	0.25	1377.70
$1 \mathrm{pbe}$	500	186	0.42	-428.85	264	0.32	-419.64
1qlw	500	427	0.64	-371.50	495	0.49	-361.63
1rro	500	15	0.40	-143.17	237	0.33	-139.92
$1 \mathrm{srp}$	500	201	0.32	-291.34	243	0.29	-272.30
1t1d	500	92	0.33	-116.43	339	0.32	-114.57
$1 \mathrm{thg}$	500	486	1.02	-707.49	255	0.54	-628.38
$1 \mathrm{thw}$	500	286	0.38	-188.09	224	0.35	-185.47
1tib	500	200	0.58	-170.30	249	0.33	-167.09
1tml	500	157	0.43	-402.89	435	0.31	-401.84
1xif	500	482	0.35	-384.57	191	0.28	-377.58
2cpl	500	450	0.23	-221.52	373	0.21	-217.78
2ebn	500	308	1.47	-165.97	473	0.62	-164.21
2exo	500	30	0.38	-281.45	302	0.26	-276.58
2pia	500	257	0.49	-286.95	366	0.46	-284.13
2rn2	500	127	0.96	-159.49	436	0.45	-149.71
2sıl	500	123	0.50	209.72	28	0.46	218.35
2tgi	500	81	2.08	-64.07	278	1.07	17.92
3cla	500	266	0.56	-215.36	38	0.32	-212.96
3hsc	500		0.29	-422.69	113	0.23	-409.62
411b	500	436	1.64	-28.07	374	0.79	-25.41





















