Task	Dataset	Metric	Method	Notes	N	Mean	95% CI	Meidian
Small Molecules	PoseBusters V2	% RMSD < 2 Å	SiteAF3	AF3 MSA & pocket & hotspot	308	**81.2**	76.4-85.1	-
				AF3 MSA	308	80.8	76.1-84.8	-
				pocket & hotspot	308	41.2	35.9-46.8	-
				baseline	308	38.6	33.4-44.2	-
			AF3	AF3 MSA	308	73.1	67.8-77.7	-
		RMSD (Å)	SiteAF3	AF3 MSA & pocket & hotspot	308	**1.68**	-	**0.38**
				AF3 MSA	308	1.78	-	**0.38**
				pocket & hotspot	308	3.41	-	2.29
				baseline	308	3.72	-	2.56
			AF3	AF3 MSA	308	2.42	-	0.55
	FoldBench protein-ligand	% RMSD < 2 Å	SiteAF3	AF3 MSA & pocket & hotspot	558	69.2	65.2-72.9	-
				AF3 MSA	558	**69.7**	65.8-73.4	-
				pocket & hotspot	558	41.6	37.6-45.7	-
				baseline	558	36.9	33.0-41.0	-
			AF3	AF3 MSA	558	62.0	57.9-65.9	-
		RMSD (Å)	SiteAF3	AF3 MSA & pocket & hotspot	558	**4.03**	-	0.79
				AF3 MSA	558	4.07	-	**0.78**
				pocket & hotspot	558	3.87	-	2.56
				baseline	558	4.32	-	3.01
			AF3	AF3 MSA	558	5.29	-	1.20
Peptides	PepPCBench	DockQ	SiteAF3	AF3 MSA & pocket & hotspot	261	**0.79**	-	**0.92**
				AF3 MSA	261	0.78	-	**0.92**
				pocket & hotspot	261	0.49	-	0.45
				baseline	261	0.43	-	0.34
			AF3	AF3 MSA	261	0.71	-	0.86
Nucleic Acids	FoldBench protein-dsDNA	DockQ	SiteAF3	AF3 MSA & pocket & hotspot	214	**0.54**	-	**0.67**
				AF3 MSA	214	**0.54**	-	0.66
				pocket & hotspot	214	0.25	-	0.04
				baseline	214	0.12	-	0.01
			AF3	AF3 MSA	214	0.49	-	0.59
	Alphafold3 protein-RNA	DockQ	SiteAF3	AF3 MSA & pocket & hotspot	25	**0.39**	-	**0.36**
				AF3 MSA	25	**0.39**	-	**0.36**
				pocket & hotspot	25	0.28	-	0.19
				baseline	25	0.27	-	0.17
			AF3	AF3 MSA	25	0.34	-	0.25