

Model	F1 $\uparrow$	DAF $\uparrow$	Prec $\uparrow$	Acc $\uparrow$	TPR $\uparrow$	TNR $\uparrow$	MAE $\downarrow$	RMSE $\downarrow$	R <sup>2</sup> $\uparrow$	Training Set	Model Params	Targets	Date Added
eqV2 S DeNS	0.815	5.04	0.771	0.941	0.864	0.953	0.036	0.085	0.788	146K (1.6M) ( <a href="#">MPtrj</a> )	31.2M	EFS <sub>D</sub>	2024-10-18
ORB MPtrj	0.765	4.7	0.719	0.922	0.817	0.941	0.045	0.091	0.756	146K (1.6M) ( <a href="#">MPtrj</a> )	25.2M	EFS <sub>D</sub>	2024-10-14
SevenNet	0.724	4.25	0.65	0.904	0.818	0.919	0.048	0.092	0.75	146K (1.6M) ( <a href="#">MPtrj</a> )	842.4K	EFS <sub>C</sub>	2024-07-13
MACE	0.669	3.78	0.577	0.878	0.796	0.893	0.057	0.101	0.697	146K (1.6M) ( <a href="#">MPtrj</a> )	4.7M	EFS <sub>C</sub>	2023-07-14
CHGNet	0.613	3.36	0.514	0.851	0.758	0.868	0.063	0.103	0.689	146K (1.6M) ( <a href="#">MPtrj</a> )	412.5K	EFS <sub>C</sub> <sup>M</sup>	2023-03-03
M3GNet	0.569	2.88	0.441	0.813	0.803	0.813	0.075	0.118	0.585	63K (188.3K) ( <a href="#">MPF</a> )	227.5K	EFS <sub>C</sub>	2022-09-20
ALIGNN	0.567	3.21	0.49	0.841	0.672	0.872	0.093	0.154	0.297	155K ( <a href="#">MP 2022</a> )	4.0M	Energy	2023-06-02
MEGNet	0.51	2.96	0.452	0.826	0.585	0.87	0.13	0.206	-0.248	133K ( <a href="#">MP Graphs</a> )	167.8K	Energy	2022-11-14
CGCNN	0.507	2.85	0.436	0.818	0.605	0.857	0.138	0.233	-0.603	155K ( <a href="#">MP 2022</a> )	128.4K (N=10)	Energy	2022-12-28
CGCNN+P	0.5	2.56	0.392	0.786	0.693	0.803	0.113	0.182	0.019	155K ( <a href="#">MP 2022</a> )	128.4K (N=10)	Energy	2023-02-03
Wrenformer	0.466	2.26	0.345	0.745	0.719	0.75	0.11	0.186	-0.018	155K ( <a href="#">MP 2022</a> )	5.2M (N=10)	Energy	2022-11-26
BOWSR	0.423	1.96	0.3	0.712	0.718	0.693	0.118	0.167	0.151	133K ( <a href="#">MP Graphs</a> )	167.8K	Energy	2022-11-17
Voronoi RF	0.333	1.58	0.241	0.668	0.535	0.692	0.148	0.212	-0.329	155K ( <a href="#">MP 2022</a> )	26.2M	Energy	2022-11-26
Dummy	0.185	1	0.154	0.687	0.232	0.769	0.124	0.184	0				