

Model	F1 \uparrow	DAF \uparrow	Prec \uparrow	Acc \uparrow	TPR \uparrow	TNR \uparrow	MAE \downarrow	RMSE \downarrow	R ² \uparrow	Training Set	Model Params	Targets	Date Added
eqV2 DeNS	0.815	5.042	0.771	0.941	0.864	0.953	0.036	0.085	0.788	146K (1.6M) (MPtrj)	31.2M	EFS _D	2024-10-18
ORB MPtrj	0.765	4.702	0.719	0.922	0.817	0.941	0.045	0.091	0.756	146K (1.6M) (MPtrj)	25.2M	EFS _D	2024-10-14
SevenNet	0.724	4.252	0.650	0.904	0.818	0.919	0.048	0.092	0.750	146K (1.6M) (MPtrj)	842.4K	EFS _C	2024-07-13
MACE	0.669	3.777	0.577	0.878	0.796	0.893	0.057	0.101	0.697	146K (1.6M) (MPtrj)	4.7M	EFS _C	2023-07-14
CHGNet	0.613	3.361	0.514	0.851	0.758	0.868	0.063	0.103	0.689	146K (1.6M) (MPtrj)	412.5K	EFS _C ^M	2023-03-03
M3GNet	0.569	2.882	0.441	0.813	0.803	0.813	0.075	0.118	0.585	63K (188.3K) (MPF)	227.5K	EFS _C	2022-09-20
ALIGNN	0.567	3.206	0.490	0.841	0.672	0.872	0.093	0.154	0.297	155K (MP 2022)	4.0M	E	2023-06-02
MEGNet	0.510	2.959	0.452	0.826	0.585	0.870	0.130	0.206	-0.248	133K (MP Graphs)	167.8K	E	2022-11-14
CGCNN	0.507	2.855	0.436	0.818	0.605	0.857	0.138	0.233	-0.603	155K (MP 2022)	128.4K (N=10)	E	2022-12-28
CGCNN+P	0.500	2.563	0.392	0.786	0.693	0.803	0.113	0.182	0.019	155K (MP 2022)	128.4K (N=10)	E	2023-02-03
Wrenformer	0.466	2.256	0.345	0.745	0.719	0.750	0.110	0.186	-0.018	155K (MP 2022)	5.2M (N=10)	E	2022-11-26
BOWSR	0.423	1.964	0.300	0.712	0.718	0.693	0.118	0.167	0.151	133K (MP Graphs)	167.8K	E	2022-11-17
Voronoi RF	0.333	1.579	0.241	0.668	0.535	0.692	0.148	0.212	-0.329	155K (MP 2022)	26.2M	E	2022-11-26
Dummy	0.185	1	0.154	0.687	0.232	0.769	0.124	0.184	0				