**Supplementary Table S6.** The performance of the DeepBindRG\_ele model which uses element as atom type.

|  |  |  |  |
| --- | --- | --- | --- |
| Metrics | Training set(135000) | Test set(1000) | Validation set(925) |
| R value | 0.5715 | 0.5350 | 0.5422 |
| MAE | 1.2788 | 1.2786 | 1.2973 |
| MSE | 2.5463 | 2.5389 | 2.5768 |
| RMSE | 1.5957 | 1.5934 | 1.6052 |