**Supplementary data for "Multi-shelled ECIF: Improved extended connectivity interaction features for accurate binding affinity prediction."**

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# Table S1. Correspondence between protein side atoms in PDB and ECIF atom type.

|  |  |  |
| --- | --- | --- |
| PDB residue | PDB atom | ECIF atom type |
| ALA | C | C;4;3;0;0;0 |
| ALA | CA | C;4;3;1;0;0 |
| ALA | CB | C;4;1;3;0;0 |
| ALA | N | N;3;2;1;0;0 |
| ALA | O | O;2;1;0;0;0 |
| ALA | OXT | O;2;1;0;0;0 |
| ARG | C | C;4;3;0;0;0 |
| ARG | CA | C;4;3;1;0;0 |
| ARG | CB | C;4;2;2;0;0 |
| ARG | CD | C;4;2;2;0;0 |
| ARG | CG | C;4;2;2;0;0 |
| ARG | CZ | C;6;3;0;0;0 |
| ARG | N | N;3;2;1;0;0 |
| ARG | NE | N;4;2;1;0;0 |
| ARG | NH1 | N;4;1;2;0;0 |
| ARG | NH2 | N;4;1;2;0;0 |
| ARG | O | O;2;1;0;0;0 |
| ARG | OXT | O;2;1;0;0;0 |
| ASN | C | C;4;3;0;0;0 |
| ASN | CA | C;4;3;1;0;0 |
| ASN | CB | C;4;2;2;0;0 |
| ASN | CG | C;4;3;0;0;0 |
| ASN | N | N;3;2;1;0;0 |
| ASN | ND2 | N;3;1;2;0;0 |
| ASN | O | O;2;1;0;0;0 |
| ASN | OD1 | O;2;1;0;0;0 |
| ASN | OXT | O;2;1;0;0;0 |
| ASP | C | C;4;3;0;0;0 |
| ASP | CA | C;4;3;1;0;0 |
| ASP | CB | C;4;2;2;0;0 |
| ASP | CG | C;5;3;0;0;0 |
| ASP | N | N;3;2;1;0;0 |
| ASP | O | O;2;1;0;0;0 |
| ASP | OD1 | O;2;1;0;0;0 |
| ASP | OD2 | O;2;1;0;0;0 |
| ASP | OXT | O;2;1;0;0;0 |
| CYS | C | C;4;3;0;0;0 |
| CYS | CA | C;4;3;1;0;0 |
| CYS | CB | C;4;2;2;0;0 |
| CYS | N | N;3;2;1;0;0 |
| CYS | O | O;2;1;0;0;0 |
| CYS | OXT | O;2;1;0;0;0 |
| CYS | SG | S;2;1;1;0;0 |
| GLN | C | C;4;3;0;0;0 |
| GLN | CA | C;4;3;1;0;0 |
| GLN | CB | C;4;2;2;0;0 |
| GLN | CD | C;4;3;0;0;0 |
| GLN | CG | C;4;2;2;0;0 |
| GLN | N | N;3;2;1;0;0 |
| GLN | NE2 | N;3;1;2;0;0 |
| GLN | O | O;2;1;0;0;0 |
| GLN | OE1 | O;2;1;0;0;0 |
| GLN | OXT | O;2;1;0;0;0 |
| GLU | C | C;4;3;0;0;0 |
| GLU | CA | C;4;3;1;0;0 |
| GLU | CB | C;4;2;2;0;0 |
| GLU | CD | C;5;3;0;0;0 |
| GLU | CG | C;4;2;2;0;0 |
| GLU | N | N;3;2;1;0;0 |
| GLU | O | O;2;1;0;0;0 |
| GLU | OE1 | O;2;1;0;0;0 |
| GLU | OE2 | O;2;1;0;0;0 |
| GLU | OXT | O;2;1;0;0;0 |
| GLY | C | C;4;3;0;0;0 |
| GLY | CA | C;4;2;2;0;0 |
| GLY | N | N;3;2;1;0;0 |
| GLY | O | O;2;1;0;0;0 |
| GLY | OXT | O;2;1;0;0;0 |
| HIS | C | C;4;3;0;0;0 |
| HIS | CA | C;4;3;1;0;0 |
| HIS | CB | C;4;2;2;0;0 |
| HIS | CD2 | C;4;2;1;1;1 |
| HIS | CE1 | C;4;2;1;1;1 |
| HIS | CG | C;4;3;0;1;1 |
| HIS | N | N;3;2;1;0;0 |
| HIS | ND1 | N;3;2;0;1;1 |
| HIS | NE2 | N;3;2;1;1;1 |
| HIS | O | O;2;1;0;0;0 |
| HIS | OXT | O;2;1;0;0;0 |
| ILE | C | C;4;3;0;0;0 |
| ILE | CA | C;4;3;1;0;0 |
| ILE | CB | C;4;3;1;0;0 |
| ILE | CD1 | C;4;1;3;0;0 |
| ILE | CG1 | C;4;2;2;0;0 |
| ILE | CG2 | C;4;1;3;0;0 |
| ILE | N | N;3;2;1;0;0 |
| ILE | O | O;2;1;0;0;0 |
| ILE | OXT | O;2;1;0;0;0 |
| LEU | C | C;4;3;0;0;0 |
| LEU | CA | C;4;3;1;0;0 |
| LEU | CB | C;4;2;2;0;0 |
| LEU | CD1 | C;4;1;3;0;0 |
| LEU | CD2 | C;4;1;3;0;0 |
| LEU | CG | C;4;3;1;0;0 |
| LEU | N | N;3;2;1;0;0 |
| LEU | O | O;2;1;0;0;0 |
| LEU | OXT | O;2;1;0;0;0 |
| LYS | C | C;4;3;0;0;0 |
| LYS | CA | C;4;3;1;0;0 |
| LYS | CB | C;4;2;2;0;0 |
| LYS | CD | C;4;2;2;0;0 |
| LYS | CE | C;4;2;2;0;0 |
| LYS | CG | C;4;2;2;0;0 |
| LYS | N | N;3;2;1;0;0 |
| LYS | NZ | N;4;1;3;0;0 |
| LYS | O | O;2;1;0;0;0 |
| LYS | OXT | O;2;1;0;0;0 |
| MET | C | C;4;3;0;0;0 |
| MET | CA | C;4;3;1;0;0 |
| MET | CB | C;4;2;2;0;0 |
| MET | CE | C;4;1;3;0;0 |
| MET | CG | C;4;2;2;0;0 |
| MET | N | N;3;2;1;0;0 |
| MET | O | O;2;1;0;0;0 |
| MET | OXT | O;2;1;0;0;0 |
| MET | SD | S;2;2;0;0;0 |
| PHE | C | C;4;3;0;0;0 |
| PHE | CA | C;4;3;1;0;0 |
| PHE | CB | C;4;2;2;0;0 |
| PHE | CD1 | C;4;2;1;1;1 |
| PHE | CD2 | C;4;2;1;1;1 |
| PHE | CE1 | C;4;2;1;1;1 |
| PHE | CE2 | C;4;2;1;1;1 |
| PHE | CG | C;4;3;0;1;1 |
| PHE | CZ | C;4;2;1;1;1 |
| PHE | N | N;3;2;1;0;0 |
| PHE | O | O;2;1;0;0;0 |
| PHE | OXT | O;2;1;0;0;0 |
| PRO | C | C;4;3;0;0;0 |
| PRO | CA | C;4;3;1;0;1 |
| PRO | CB | C;4;2;2;0;1 |
| PRO | CD | C;4;2;2;0;1 |
| PRO | CG | C;4;2;2;0;1 |
| PRO | N | N;3;3;0;0;1 |
| PRO | O | O;2;1;0;0;0 |
| PRO | OXT | O;2;1;0;0;0 |
| SER | C | C;4;3;0;0;0 |
| SER | CA | C;4;3;1;0;0 |
| SER | CB | C;4;2;2;0;0 |
| SER | N | N;3;2;1;0;0 |
| SER | O | O;2;1;0;0;0 |
| SER | OG | O;2;1;1;0;0 |
| SER | OXT | O;2;1;0;0;0 |
| THR | C | C;4;3;0;0;0 |
| THR | CA | C;4;3;1;0;0 |
| THR | CB | C;4;3;1;0;0 |
| THR | CG2 | C;4;1;3;0;0 |
| THR | N | N;3;2;1;0;0 |
| THR | O | O;2;1;0;0;0 |
| THR | OG1 | O;2;1;1;0;0 |
| THR | OXT | O;2;1;0;0;0 |
| TRP | C | C;4;3;0;0;0 |
| TRP | CA | C;4;3;1;0;0 |
| TRP | CB | C;4;2;2;0;0 |
| TRP | CD1 | C;4;2;1;1;1 |
| TRP | CD2 | C;4;3;0;1;1 |
| TRP | CE2 | C;4;3;0;1;1 |
| TRP | CE3 | C;4;2;1;1;1 |
| TRP | CG | C;4;3;0;1;1 |
| TRP | CH2 | C;4;2;1;1;1 |
| TRP | CZ2 | C;4;2;1;1;1 |
| TRP | CZ3 | C;4;2;1;1;1 |
| TRP | N | N;3;2;1;0;0 |
| TRP | NE1 | N;3;2;1;1;1 |
| TRP | O | O;2;1;0;0;0 |
| TRP | OXT | O;2;1;0;0;0 |
| TYR | C | C;4;3;0;0;0 |
| TYR | CA | C;4;3;1;0;0 |
| TYR | CB | C;4;2;2;0;0 |
| TYR | CD1 | C;4;2;1;1;1 |
| TYR | CD2 | C;4;2;1;1;1 |
| TYR | CE1 | C;4;2;1;1;1 |
| TYR | CE2 | C;4;2;1;1;1 |
| TYR | CG | C;4;3;0;1;1 |
| TYR | CZ | C;4;3;0;1;1 |
| TYR | N | N;3;2;1;0;0 |
| TYR | O | O;2;1;0;0;0 |
| TYR | OH | O;2;1;1;0;0 |
| TYR | OXT | O;2;1;0;0;0 |
| VAL | C | C;4;3;0;0;0 |
| VAL | CA | C;4;3;1;0;0 |
| VAL | CB | C;4;3;1;0;0 |
| VAL | CG1 | C;4;1;3;0;0 |
| VAL | CG2 | C;4;1;3;0;0 |
| VAL | N | N;3;2;1;0;0 |
| VAL | O | O;2;1;0;0;0 |
| VAL | OXT | O;2;1;0;0;0 |

# Table S2. PDB IDs used for training set and validation set.

Train set

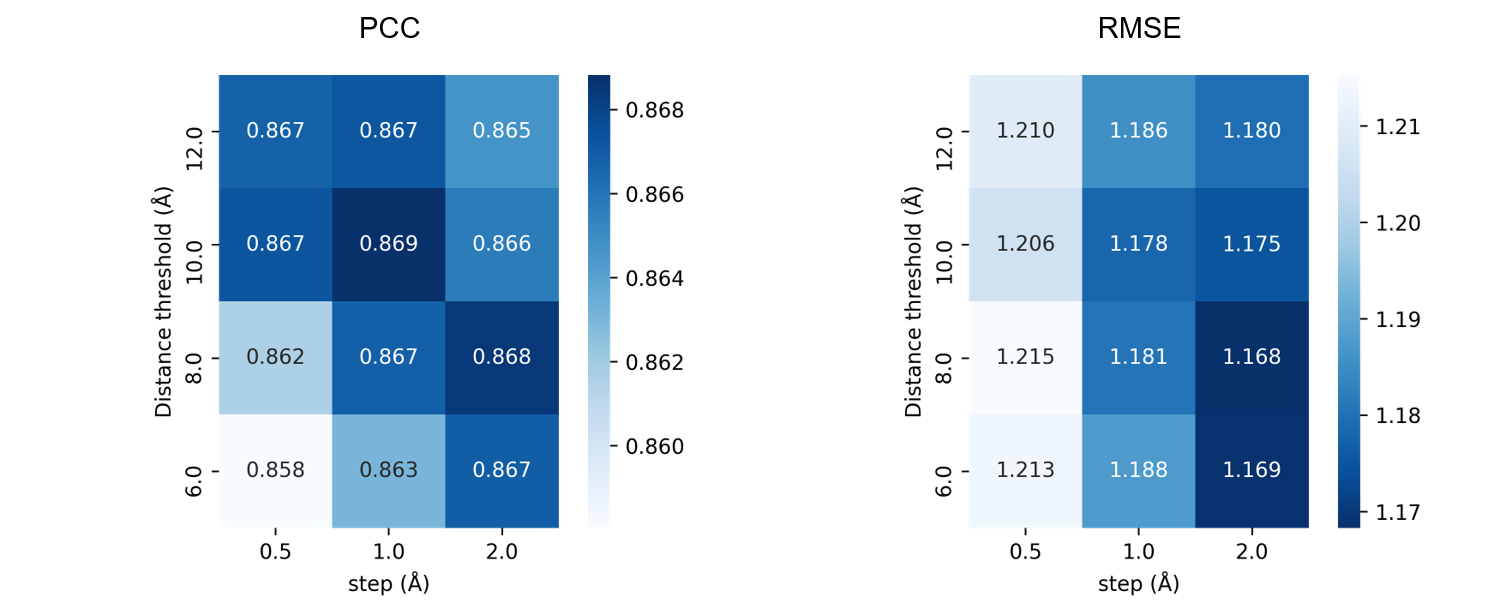
|  |
| --- |
| 10gs, 11gs, 13gs, 16pk, 184l, 185l, 186l, 187l, 188l, 1a07, 1a08, 1a0q, 1a1b, 1a1c, 1a1e, 1a28, 1a3e, 1a42, 1a4h, 1a4k, 1a4r, 1a4w, 1a50, 1a52, 1a5h, 1a69, 1a8i, 1a8t, 1a94, 1a99, 1a9m, 1a9q, 1aaq, 1abf, 1add, 1adl, 1ado, 1af2, 1afk, 1afl, 1ag9, 1agm, 1ahx, 1ahy, 1ai4, 1ai5, 1ai6, 1ai7, 1aid, 1aj6, 1aj7, 1ajn, 1ajp, 1ajq, 1ajv, 1ajx, 1akq, 1akr, 1akt, 1aku, 1akv, 1akw, 1al7, 1al8, 1alw, 1amk, 1amw, 1anf, 1ao0, 1apb, 1apv, 1apw, 1aqc, 1aqi, 1aqj, 1at5, 1at6, 1atl, 1atr, 1avn, 1avp, 1awi, 1ax0, 1ax1, 1ax2, 1axr, 1axs, 1axz, 1azl, 1azm, 1azx, 1b05, 1b0h, 1b11, 1b1h, 1b2h, 1b32, 1b38, 1b39, 1b3f, 1b3g, 1b3h, 1b3l, 1b40, 1b42, 1b46, 1b4d, 1b4h, 1b4z, 1b51, 1b52, 1b55, 1b56, 1b57, 1b58, 1b5h, 1b5i, 1b5j, 1b6h, 1b6j, 1b6k, 1b6l, 1b6m, 1b6p, 1b7h, 1b8n, 1b8o, 1b8y, 1b9j, 1bai, 1bap, 1bbz, 1bcd, 1bcj, 1bdl, 1bdq, 1bdr, 1bgq, 1bhf, 1bhx, 1bju, 1bjv, 1bkj, 1bky, 1bm7, 1bma, 1bmm, 1bmn, 1bn1, 1bn3, 1bn4, 1bnm, 1bnn, 1bnq, 1bnt, 1bnu, 1bnv, 1bnw, 1bp0, 1bq3, 1bq4, 1br6, 1br8, 1bsk, 1bt6, 1btn, 1bty, 1bux, 1bv7, 1bv9, 1bwa, 1bwb, 1bwn, 1bxo, 1bxq, 1bxr, 1bzh, 1bzj, 1bzy, 1c12, 1c1r, 1c1u, 1c1v, 1c2t, 1c3e, 1c3x, 1c4u, 1c4v, 1c4y, 1c5c, 1c5n, 1c5o, 1c5p, 1c5q, 1c5s, 1c5t, 1c5x, 1c5y, 1c6y, 1c70, 1c7e, 1c7f, 1c83, 1c84, 1c85, 1c86, 1c87, 1c88, 1caq, 1cbr, 1cbx, 1ce5, 1cea, 1ceb, 1cet, 1cgl, 1ch8, 1ci7, 1cil, 1cim, 1cin, 1ciz, 1cka, 1ckb, 1clu, 1cnw, 1cnx, 1cny, 1cps, 1cr6, 1csh, 1csi, 1csr, 1css, 1ct8, 1ctr, 1ctt, 1ctu, 1cwb, 1czc, 1cze, 1czk, 1czl, 1czo, 1czr, 1d04, 1d09, 1d1p, 1d2e, 1d2s, 1d3d, 1d3p, 1d3q, 1d4h, 1d4i, 1d4j, 1d4k, 1d4l, 1d4p, 1d4t, 1d4w, 1d4y, 1d6n, 1d6s, 1d6v, 1d6w, 1d7i, 1d7j, 1d9i, 1dar, 1db1, 1dbb, 1det, 1df8, 1dfo, 1dg9, 1dgm, 1dhi, 1dhj, 1dif, 1dkd, 1dl7, 1dmb, 1dmp, 1dqn, 1dqx, 1drj, 1drk, 1drv, 1dub, 1dud, 1duv, 1dva, 1dwc, 1dwd, 1dxp, 1dy4, 1dzk, 1e03, 1e1v, 1e1x, 1e2k, 1e2l, 1e3g, 1e3v, 1e4h, 1e5a, 1e5j, 1e6q, 1e6s, 1e72, 1e8h, 1eb1, 1eb2, 1ebg, 1ebw, 1ebz, 1ec0, 1ec1, 1ec2, 1ec3, 1ec9, 1ecq, 1ecv, 1eed, 1efy, 1egh, 1eix, 1ej4, 1ejn, 1ek2, 1ela, 1elb, 1elc, 1eld, 1ele, 1elr, 1els, 1ent, 1enu, 1eoc, 1epo, 1epp, 1erb, 1ets, 1ett, 1etz, 1evh, 1ew8, 1ew9, 1ewj, 1ex8, 1ez9, 1ezq, 1f0r, 1f0s, 1f0t, 1f0u, 1f28, 1f3e, 1f47, 1f4e, 1f4f, 1f4g, 1f4x, 1f4y, 1f57, 1f5k, 1f5l, 1f73, 1f74, 1f8a, 1f8b, 1f8c, 1f8d, 1f8e, 1f90, 1f92, 1fao, 1fax, 1fbm, 1fch, 1fcx, 1fcy, 1fcz, 1fd0, 1fdq, 1fe3, 1fh7, 1fh8, 1fh9, 1fhd, 1fig, 1fiv, 1fj4, 1fjs, 1fkb, 1fkf, 1fkg, 1fkh, 1fki, 1fkn, 1fkw, 1fl3, 1fl6, 1flm, 1flr, 1fm9, 1fmb, 1fo0, 1fpc, 1fpp, 1fpy, 1fq4, 1fq5, 1fq6, 1fq7, 1fq8, 1ft7, 1ftm, 1fv0, 1fw0, 1fwe, 1fwu, 1fwv, 1fzj, 1fzk, 1fzm, 1fzo, 1fzq, 1g1d, 1g2l, 1g2o, 1g30, 1g32, 1g35, 1g36, 1g3b, 1g3c, 1g3d, 1g3e, 1g45, 1g46, 1g48, 1g4j, 1g4o, 1g50, 1g52, 1g53, 1g54, 1g5f, 1g6r, 1g6s, 1g74, 1g7f, 1g7g, 1g7p, 1g7q, 1g7v, 1g85, 1g98, 1g9r, 1g9s, 1g9t, 1gaf, 1gag, 1gah, 1gai, 1gar, 1gca, 1gcz, 1gfy, 1gfz, 1ghv, 1ghw, 1ghy, 1ghz, 1gi1, 1gi4, 1gi6, 1gi7, 1gi8, 1gi9, 1gj4, 1gj6, 1gj7, 1gj8, 1gja, 1gjb, 1gjc, 1gjd, 1gni, 1gnj, 1gnm, 1gnn, 1gno, 1gny, 1gpy, 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9abp, 9hvp, 9icd |

Test set

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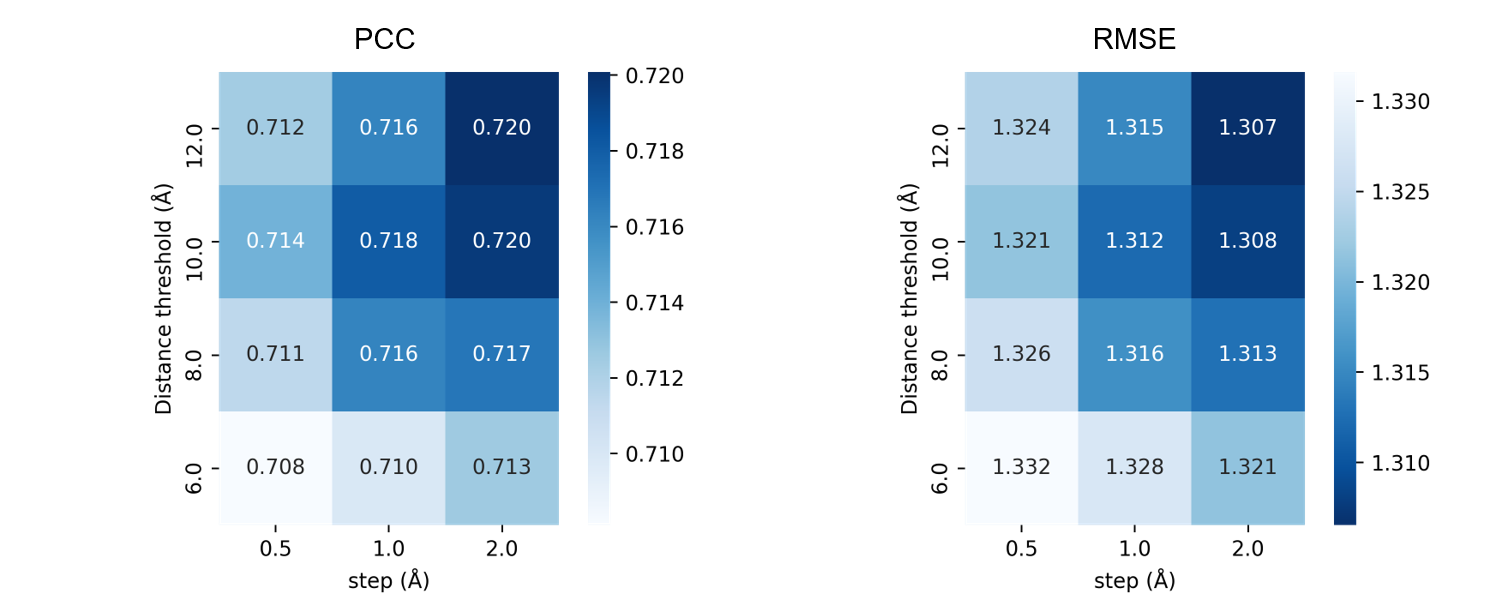
# Table S3. RDkit ligand descriptors used to train with multi-shelled ECIF and weighted ECIF.

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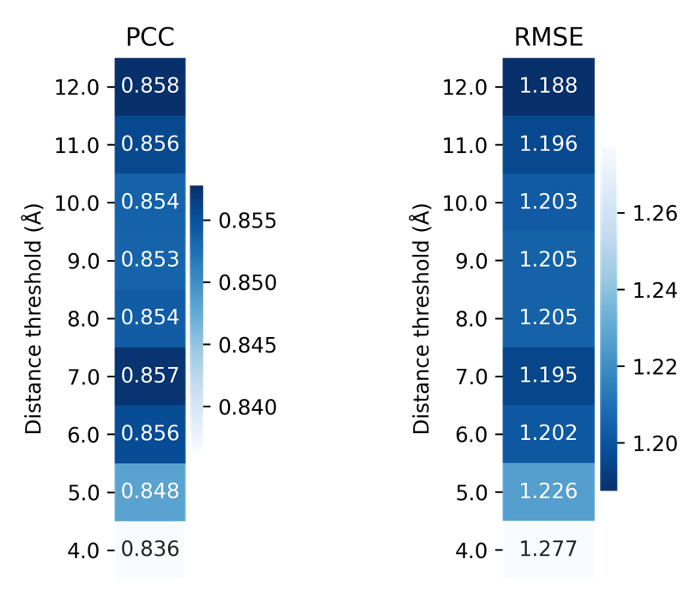
# Supplementary Figure 1. Result of the Multi-shelled ECIF hyper parameter exploration result.

Each cell of the heatmap represents the average PCC (left) and average RMSE (right) of 100 models trained in each condition with different random seeds and evaluated with CASF2016 coreset. The horizontal axis of the heat map shows step width, and the vertical axis shows distance threshold.



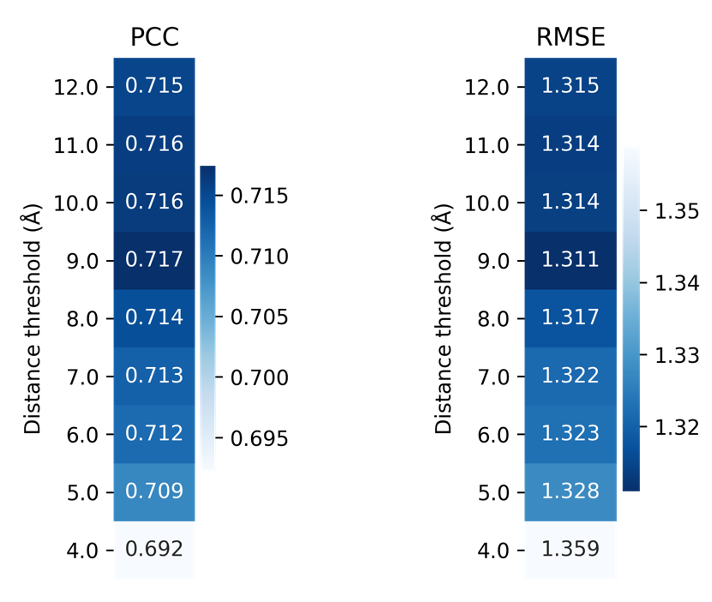
# Supplementary Figure 2. 10-fold cross-validation result of the Multi-shelled ECIF.

Each cell in the heatmap represents the average PCC (left) and average RMSE (right) of the 10-fold cross-validation trained in each condition. The horizontal axis of the heat map shows step width, and the vertical axis shows distance threshold.



# Supplementary Figure 3. Heat map of the Weighted ECIF hyper parameter exploration result.

Each cell in the heatmap represents the average PCC (left) and average RMSE (right) of 100 models trained in each condition with different random seeds and evaluated with CASF2016 coreset. The vertical axis shows distance threshold.



# Supplementary Figure 4. 10-fold cross-validation result of the Weighted ECIF

Each cell in the heatmap represents the average PCC (left) and average RMSE (right) of the 10-fold cross-validation trained in each condition. The vertical axis indicates the distance threshold.