**Supporting Information**

**REINDEER: A Protein-Ligand Feature Generator Software for Machine Learning Algorithms**

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Table 1- PDBIDs of train, validation, and test sets.

|  |  |
| --- | --- |
| Set | PDBIDs |
| Train | 3nq3, 4b5w, 3uxl, 6eog, 6p89, 1qbs, 4u1b, 4avj, 3acx, 5fut, 3b65, 5xo7, 2dri, 4q4q, 4bt5, 2jdu, 6p87, 4wn5, 3su1, 5fyx, 5ko5, 6hke, 1b8y, 6b4u, 5ad1, 4bj8, 6gl8, 3zhx, 5zyg, 1ndw, 5lz7, 1g2k, 1lee, 3tsk, 4x50, 4r4c, 5hwv, 4ndu, 2i80, 2o4j, 5ult, 3nhi, 6t1m, 4epy, 5nau, 3t2q, 3e5u, 3nu5, 5j3l, 1ajq, 5ka7, 1nl9, 1ogz, 1msn, 1ajp, 2doo, 4kz3, 5aba, 5dgu, 3zi8, 4ynb, 1srg, 3lea, 3o9p, 2fzk, 2q8z, 6jbb, 5cp5, 1aid, 4kwg, 5eqy, 2qdt, 3pb7, 1yvm, 4b6o, 3jup, 3n7o, 2xbw, 2jf4, 4cr5, 1n51, 2jdp, 1f8d, 1olx, 6q4e, 3ljg, 4bt4, 3zi0, 1r9l, 4fxq, 6g29, 4y3j, 2vzr, 3a6t, 5hvt, 3rt8, 4yo8, 4zow, 3tcg, 3pcj, 2clh, 3ui7, 1km3, 4k55, 2f8g, 3gi5, 6gvz, 1hee, 1ecq, 3s45, 2wyj, 4u43, 4hw3, 4f6u, 2yaz, 1pzi, 5fbi, 2jg0, 4qfp, 3t09, 5dxt, 1jmg, 2v2q, 4i8w, 2wyg, 3wjw, 4l51, 3wz7, 1bju, 5o2d, 5mrm, 3pce, 6d1h, 5nvx, 1fzq, 3mv0, 3nu4, 6arn, 6jap, 4bps, 6o5t, 4aia, 4cjp, 5u6j, 4bb9, 4pb2, 5btx, 5zni, 2b4l, 1phw, 4ih5, 3zq9, 2y81, 4css, 5fs5, 3n86, 4u6c, 5yh8, 6fnq, 6f9g, 5fnu, 1x39, 6jay, 3zso, 2zcq, 1a9q, 4bs0, 5igm, 3jrx, 3lq2, 2vl4, 4av4, 6dy7, 2zz2, 1u1w, 6k04, 3ps1, 2hah, 1x8r, 3pck, 3lka, 4tkh, 4m0f, 1uwf, 6qpl, 5m17, 2qbp, 5zg3, 4ufi, 3v2n, 3f37, 5nvw, 1hlk, 5h9r, 4u71, 3f80, 2psu, 3rv8, 6ncn, 4zei, 2qwd, 3rlb, 1f73, 6dil, 5e2o, 3vf7, 6n3w, 4ggz, 5upj, 1xgi, 4n7u, 3o84, 2whp, 1w4o, 6r1d, 3g2z, 6cn5, 1hmt, 4ljh, 3fed, 5w44, 4ly9, 3sue, 5oh4, 6g27, 3su0, 3l0v, 1px4, 5u0z, 6i13, 4cst, 1x38, 6f92, 3p3t, 5i2f, 6ayr, 3suf, 1g74, 4kwo, 4tpw, 1nja, 4i74, 4xaq, 6d5j, 4bqs, 2jfz, 2xb8, 6euw, 2y8c, 3d52, 6jbe, 2qi7, 2i19, 1ws1, 4w9i, 6g24, 2ya6, 5jxq, 3su3, 2vnp, 6qlq, 1rnm, 2nsj, 3ekp, 3f19, 5zg1, 2hzl, 3f8c, 2pwg, 5e2p, 3djv, 4avh, 6gfs, 3sm2, 1tsy, 1pvn, 4re2, 1qbu, 4fxp, 5yft, 1qaw, 5d1r, 6qgf, 1bq4, 4b6r, 5kh3, 1s39, 5ka1, 4u6w, 1fkg, 5kax, 4y5d, 3t0b, 4qge, 6arm, 1lgt, 5tbm, 3dx2, 6f90, 4l19, 4oc3, 4f6w, 5m7u, 4iif, 3td4, 4z07, 5evb, 5kqy, 1li2, 1elc, 1fkw, 2r38, 4n9c, 5z66, 2bz6, 4qfo, 6d5h, 2h4g, 1v48, 3k37, 6c85, 3f6g, 3alt, 3mjl, 1tcx, 3vf5, 3mxd, 1pgp, 3sug, 6haz, 3c2r, 1ecv, 3pgu, 6t1j, 2vrj, 4dzy, 4x5z, 4x8u, 5e74, 5lli, 3sfg, 4yzu, 5yum, 3b7j, 4uye, 3ejq, 2gvj, 6d17, 4b5t, 5b5f, 2cex, 4lm1, 6jag, 3r6u, 6e1z, 2zwz, 1det, 3n7a, 3zj6, 6dh8, 3gc4, 2uxi, 2ovv, 1os5, 3nx7, 3t2w, 4cd4, 2qci, 2x0y, 6d9x, 3fql, 2i4z, 5yjm, 4ih7, 4dkq, 1lbk, 3acw, 3gst, 5upe, 1v11, 3ao4, 4iie, 6ajr, 4fai, 4r3w, 3f33, 3u90, 6udv, 5wa8, 1hpv, 5ueu, 3kdd, 4lko, 5nap, 1lgw, 4y0a, 4tun, 3v3q, 1uz4, 6dz0, 2xd9, 3f17, 6s4n, 4cc5, 6cbf, 4np3, 3x00, 2ovy, 5g1z, 4b73, 4zyf, 2gst, 3pb8, 6ays, 2r9w, 5a5q, 5mro, 1ogx, 1li6, 3sww, 6mg5, 5jgi, 3pb9, 4djq, 3mf5, 2f2h, 6qqq, 5yfs, 2cet, 3mfv, 2q7q, 5d2r, 2qnq, 2wbg, 5t19, 4b5s, 1pbq, 6nzv, 6j0o, 1no6, 5k1f, 3ip9, 3pbb, 5wuk, 2x91, 2cle, 6ayi, 5edb, 6fhu, 1v1j, 1hi3, 3d50, 1igb, 4bt3, 1bp0, 6iez, 5kr1, 5edl, 6n7b, 2d3u, 2j7b, 6d1g, 1kav, 3ocp, 3g35, 6b1k, 1q1g, 6r18, 3ovn, 1q91, 5ot9, 2flr, 4xtv, 3ddf, 3qbc, 5oht, 4kn1, 6ej2, 3gk1, 6hlx, 4o0y, 5dey, 6ayo, 6dyy, 1e66, 2wvt, 3ddg, 4ayp, 6ny0, 3hcm, 5evk, 2jgs, 6n79, 5ufp, 1uwu, 1e3v, 4lzs, 4gqq, 1m0o, 4hla, 5n0f, 1ctu, 1c83, 1xbo, 3fvl, 4cra, 4x8v, 3hkw, 4cd5, 3veh, 1hms, 4pvx, 3fur, 4tu4, 2mas, 5b25, 1ps3, 2q89, 6e9a, 1ai5, 4kz6, 6cwh, 2vwo, 5m7s, 2pwr, 4u8w, 4buq, 4z0k, 3tkw, 5wqc, 1w4q, 5avf, 3gdt, 3vfa, 1f74, 4k3h, 5fe9, 3su4, 3pgl, 3nyd, 4umb, 4kyh, 2hs1, 4luz, 6ckr, 3ttm, 2qnp, 6g2f, 1o7o, 2qbq, 1uj5, 2v3d, 1fm9, 2xp7, 5fck, 6qlr, 6d50, 5ceq, 5u11, 3ppq, 5l30, 3uw5, 1moq, 4pnu, 3dzt, 1met, 5qqp, 4nra, 1ajx, 2hb1, 5bwc, 3umq, 5tcj, 6py0, 3bkk, 4pqa, 1uvt, 6rnt, 4kif, 3zsy, 2xda, 6j9w, 4c52, 2r43, 1j01, 2yfe, 3b5r, 2fu8, 6ftp, 5evd, 5eq1, 4q0k, 3nuo, 3gvb, 1gpn, 5u13, 1ui0, 2xc0, 4dhl, 4qpd, 6dar, 4us3, 1ado, 6nu1, 3l4w, 6fba, 1o5r, 2j47, 6e1y, 5zym, 4ea2, 5k8s, 6qlt, 2yz3, 3lzs, 6ayt, 5hz5, 6d1b, 3w9k, 6dz2, 4crl, 3o75, 5v79, 2w8j, 2ves, 5ld8, 4kwf, 2zy1, 4xoc, 5d0c, 3wz8, 6s5k, 4g0p, 3d8z, 2zcr, 6pi5, 1bjv, 4ts1, 3cd7, 4tte, 6e5l, 2vb8, 1jmf, 4f3k, 2hjb, 6d1d, 1rql, 5dx4, 5bs4, 4r0a, 5qay, 5y13, 5ost, 1pa9, 4aqh, 4avi, 6i8y, 6g2r, 4y2q, 3bgs, 3s0e, 4ej8, 4kxn, 3u9q, 4ghi, 5om2, 3cyw, 1b6l, 4u0w, 4mpn, 5ovx, 4tjz, 3o9e, 4xar, 4gu6, 3rbu, 4n5d, 5dqf, 2uz9, 6euc, 4mhy, 2vw1, 6pg3, 6b4n, 5vo1, 4dst, 2r9x, 1tq4, 4ymq, 4j45, 4og4, 4lhm, 2sim, 6exs, 3ok9, 6gj6, 3sjf, 4zae, 3fx6, 3f78, 5my8, 2vjx, 2qi5, 3ggu, 4k7o, 6ge7, 4i71, 3vw1, 5ohy, 1lbf, 4ual, 1xap, 3zsq, 4q4p, 5j7q, 2yel, 3p8o, 4dfg, 5hvs, 3hky, 4urz, 2cbv, 2jjb, 5dbm, 2o4l, 3wz6, 2xc4, 6udi, 3uev, 3nzk, 6hgi, 1c86, 5d45, 4wkn, 3ttp, 5epn, 1wcq, 6p88, 6qqv, 5kr0, 5f08, 5ih9, 1kzk, 3zm9, 1g98, 3d4z, 2a4m, 3u5l, 1cbx, 6d1k, 4ceb, 3rf5, 4o0x, 5d47, 5n17, 1nhu, 3ehy, 6g25, 3nht, 3gi4, 6qqu, 3spf, 4rsk, 5t8p, 3b3x, 1wc1, 1oba, 4bkt, 4pv5, 6dyv, 3kdb, 1mes, 3f15, 3st5, 5oei, 2oi2, 1a99, 1jvu, 4ibf, 2y82, 4y4j, 2reg, 2zmm, 6ced, 6upj, 5edd, 1pzp, 1o0f, 6r0v, 3e3c, 4q9o, 4wko, 3s54, 4eb8, 4whs, 3p3r, 2zz1, 2qi6, 2rkm, 3gta, 3k8o, 6d16, 3djq, 2w8w, 3vd4, 6iht, 6p8a, 3cd5, 3own, 6d55, 2gj5, 1k4g, 3ppp, 3nox, 5nn6, 4bqh, 6oqb, 1yqy, 1rpf, 2i0a, 3f34, 6fo5, 4lm3, 1a30, 2qbr, 4wrb, 6nyv, 4yc0, 3g2y, 3b92, 3pwk, 4i7m, 2oym, 5dh5, 5qa8, 1l83, 2vo4, 3o5x, 2gz2, 1rmz, 6qr1, 6j0g, 4kqp, 1k9s, 4dkp, 4jxs, 3n2v, 2bt9, 5mgk, 4l9i, 1mrx, 5cy9, 2ri9, 5lne, 5hrw, 5zyl, 2pqz, 6p3v, 1bdq, 5ufr, 1iy7, 6dh7, 1v1m, 1wdn, 4bc5, 5gj9, 4w9c, 1n46, 1ie9, 4xmr, 3k8q, 5d0r, 3kmc, 5vh0, 4i8n, 5fe7, 5fsc, 5y12, 4yrd, 4gr8, 6ep4, 5vp9, 6r1a, 3wzn, 5c28, 185l, 2r3t, 4b6p, 6nco, 1cet, 5eyr, 5g5f, 4leq, 4ra1, 3th9, 3usx, 5ehv, 2ceq, 3el5, 2i4j, 186l, 5zg0, 5ovr, 5mby, 2wc3, 1kmy, 2glp, 2za0, 1c84, 4s1g, 5var, 5otc, 1fcy, 2zcs, 5h1t, 3w5n, 6e5t, 1uz1, 6dpy, 6e23, 3m3z, 4ai5, 3nq9, 5cep, 6o0o, 6n78, 4wov, 1yq7, 2yb0, 4ipi, 6dif, 4q1x, 6pg5, 1eld, 4ibd, 1add, 2aac, 3pwm, 4i7k, 2f9k, 6ma2, 6p85, 4fht, 2o8h, 3g3r, 1qk4, 6ht1, 3cj4, 4a95, 5x74, 4sga, 4e9u, 5nw1, 4p5d, 1njc, 4kz4, 3f16, 3g30, 2aj8, 1m2x, 3uxd, 5exn, 3i6o, 3t1m, 5fog, 6fa4, 6a87, 2buv, 3f3c, 5edc, 2j7e, 4c6u, 5kej, 4cfl, 5dnu, 2yek, 3cm2, 6epa, 5od1, 4k7i, 2ot1, 3p8p, 1hwr, 1e6q, 5jfu, 4cig, 1d7i, 2y5f, 2qzr, 5a81, 3b67, 4crb, 6pi6, 6dak, 5lsg, 1rr6, 5eqp, 3lk8, 1jys, 4ovf, 1dmp, 6t1o, 6mll, 1ndz, 2pyn, 2i3i, 4pvy, 2ogy, 3t0x, 4iuo, 2jdm, 5j1r, 6jaw, 1bzc, 6dyz, 2qtn, 4bcs, 6ezq, 4ciw, 6e22, 1kui, 5jhb, 6oqc, 3zqe, 5uf0, 5om7, 6n5x, 3t64, 6eqp, 6h8s, 6pg7, 1ws4, 2gvv, 3jdw, 6ooy, 5mz8, 6ce6, 4l50, 6ios, 6g2b, 4zt8, 2a5c, 4gq4, 6gvf, 5nvv, 3hp9, 4mjp, 4rpo, 2x09, 3v78, 3bgb, 6jaq, 6t1l, 2j7h, 2i4u, 4oc0, 1f4g, 1w96, 5ioz, 2zx7, 6eux, 6dpt, 4lov, 1f4e, 6nv7, 4n7m, 4l4z, 4xt2, 4jym, 6d1j, 4jfs, 6qi4, 4n9a, 5elw, 4h81, 4r4t, 3vw2, 2vwl, 2pym, 2qwc, 6gwr, 3i3b, 4de1, 2v2v, 5yhg, 4i7p, 4ysl, 3f7i, 6nv9, 5vsf, 3dk1, 2fqw, 2q64, 2v00, 4phu, 2pwc, 2ces, 3ewc, 5yl2, 1rnt, 4hdp, 6aro, 2i4d, 4xas, 2z4o, 2vot, 1br6, 6gue, 6dyr, 5iyy, 5kab, 4euo, 4ll3, 6jtc, 3g1v, 6ouv, 3zln, 2h6b, 5wl0, 4d4d, 6szp, 3dx1, 6as8, 2wc4, 2v54, 3pfp, 1hpx, 2qhy, 4dko, 1w3k, 4i7j, 3b68, 1mrw, 4fp1, 5tcy, 6ghj, 1ndv, 4g90, 6pgc, 6cdl, 3c2f, 3hb4, 2xbx, 3tb6, 2f81, 3tfu, 5nw0, 4cg9, 1oe8, 3hk1, 6hpw, 5kbe, 6efj, 5lz4, 3g19, 6mnc, 6cbg, 3lpl, 5f8y, 2y7z, 4ffs, 5er4, 4lk7, 188l, 2x8z, 1sbg, 1vyf, 6qr9, 6jb0, 6fuj, 4ad6, 4mme, 3tz0, 3re4, 3aid, 5khm, 3uex, 3rdq, 3r1v, 2c97, 6d19, 4mrg, 4cgi, 1lvu, 4j47, 6otg, 1k4h, 6eol, 1tjp, 1elb, 4l4v, 6kjd, 2vvv, 1vyg, 6cdj, 4asj, 6r13, 4cr9, 3zdv, 4ibc, 5etb, 2ha3, 4y3y, 6gxg, 5fol, 5sym, 4ck3, 6e7j, 1fh8, 4bks, 5ko1, 6b7a, 1zc9, 6nxz, 1o0m, 2wyf, 4rpn, 3vvy, 1kug, 3exh, 1gfy, 6plf, 2p3i, 5hva, 6gf9, 1mq6, 3dyo, 5g46, 2v58, 6g2e, 3ehx, 2vuk, 5ha1, 2wk6, 4trc, 4crf, 4cjr, 2vmd, 3tay, 4b6s, 3ppm, 4llj, 5kad, 4fnn, 4u69, 4m6u, 3kdc, 1r5y, 3ikg, 1w3j, 6chp, 2hxm, 3g31, 4ury, 3lvw, 1qxl, 3su2, 4j46, 1grp, 3qaa, 3g0i, 2j7f, 2ole, 3ljz, 4w9j, 5ov8, 1onz, 1nwl, 6d56, 6gfz, 2fzc, 4de2, 4cjq, 5f0f, 4jkw, 1bma, 4b0b, 5his, 1x8d, 4hws, 3oyw, 5upf, 6ekq, 2bet, 1loq, 1ctt, 2c80, 3elc, 5u0w, 6rtw, 3juo, 4x5p, 3b66, 4oc5, 1c3x, 3ao5, 2e91, 5ka9, 1m5w, 3ao2, 2ca8, 3o5n, 6aqs, 4tz2, 2vpo, 4aq6, 4jh0, 4dkr, 3zyf, 4h7q, 6d1i, 3cd0, 3wvm, 2p53, 2zx6, 5e7n, 5zkc, 1z95, 5eqe, 1s38, 6pg9, 1g85, 4h85, 5chk, 3g32, 4att, 4kb9, 2ha6, 2o4n, 2xii, 6ej3, 5mge, 4avs, 5cso, 6hzy, 2ydw, 5u12, 1b3l, 2bvd, 3d91, 1ajv, 3c2o, 5o5a, 5e73, 4u73, 2uyn, 1nw4, 5hz9, 6q4g, 5lyr, 1fd0, 5mek, 3tf6, 4eo6, 3zsx, 5u0y, 4ufl, 2a8g, 5hwu, 6g2o, 1qbq, 2we3, 6i12, 4msc, 1dar, 6n3x, 4psb, 2y5h, 3f18, 4ty7, 4x5r, 2usn, 3mfw, 1c87, 1zhy, 5dw2, 1nq7, 3tt4, 3eb1, 3lir, 1n1m, 4ad2, 3s0b, 4qsu, 1alw, 3gr2, 4umc, 6d15, 1ikt, 4da5, 4v27, 1atl, 3nu6, 1rp7, 3tfn, 1njd, 2izl, 4zbi, 1e2l, 4z2b, 1ajn, 4ks1, 4zv2, 5k0m, 6ayq, 6dyw, 4j28, 1t7j, 3g1d, 1yc1, 4llx, 1j37, 5e13, 3ekv, 5ehr, 6h5x, 5c2h, 4mc9, 2yfa, 2b9a, 2p4s, 1nje, 3o99, 3d6o, 4llk, 3ebl, 6qqz, 2wzs, 6f05, 2x4z, 4gny, 1drj, 6n3v, 3p5o, 4zek, 2afx, 1d4l, 5ogb, 1t5f, 1dzk, 4ara, 3su6, 6dgl, 4ucc, 4hf4, 1o0n, 5ew0, 4m0e, 4ovg, 4xo8, 3acl, 1yfz, 6ud2, 2y80, 1eoc, 1q65, 4msn, 2q63, 5fns, 6n7a, 3n8k, 7upj, 2oag, 1u0g, 1msm, 4w9k, 1y6q, 2ha2, 1pro, 6m8q, 3t60, 5jsg, 5h1v, 5ndf, 1hdq, 4myd, 1qy1, 2v59, 3ga5, 1c88, 4lbu, 2py4, 1b46, 5ime, 5hz8, 1j36, 3t08, 5lom, 1d7j, 2oax, 4dsu, 4pop, 4nbl, 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