

SUPPORTING INFORMATION

Evidence of Water Molecules – A Statistical Evaluation of Water Molecules Based on Electron Density

Eva Nittinger¹, Nadine Schneider^{1,†}, Gudrun Lange², Matthias Rarey^{1,}*

¹ University of Hamburg, Center for Bioinformatics, Bundesstraße 43, 20146 Hamburg, Germany

² Bayer CropScience AG, Industriepark Hoechst, G836, 65926 Frankfurt am Main, Germany

*rarey@zbh.uni-hamburg.de

SUPPORTING INFORMATION 1: Data set of all PDBids

Table S1: PDBids of the high-resolution data set

1b0b 1b67 1bn6 1bn7 1c1k 1c1n 1c1o 1c1p 1c1q 1c1r 1c1t 1c2h 1c2i 1c2j 1c2l 1c2m 1c5l 1c5n 1c5p 1c5q 1c5r 1c5s 1c5t
1c5u 1c5v 1c7k 1cru 1d3s 1d5t 1dbf 1dg6 1dgi 1djr 1dvj 1dwr 1dws 1dwt 1dxc 1dyq 1dzk 1e19 1e4m 1e5k 1e6s 1e71 1e73
1e85 1e9g 1ea7 1eaj 1eao 1eb6 1eeq 1ehd 1eic 1eid 1eie 1ek0 1ek6 1ekq 1elk 1en2 1eqm 1es5 1es9 1eu5 1euw 1ew4 1f1g
1f1u 1f4l 1f4p 1f8d 1f8e 1f8n 1f9h 1f9i 1f9t 1f9v 1f9z 1fg7 1flm 1fo8 1fo9 1fp2 1fs3 1fw9 1fx2 1fy2 1g2r 1g2y 1g2z
1g39 1g6l 1g67 1g69 1g6c 1g6s 1g6u 1g7a 1g7b 1g7n 1g7p 1g8a 1g8t 1g9o 1ga4 1gd0 1ghz 1gi0 1gi1 1gi2 1gi3 1gi4 1gi6
1gj6 1gj7 1gjn 1gk8 1gk9 1gkl 1gm7 1gmu 1gnt 1goi 1gok 1gp0 1gpi 1gpp 1gq1 1gqi 1gs5 1gut 1gv9 1gvd 1gvo 1gwm 1gwu
1gx4 1gxm 1gxn 1gyx 1gyy 1gz2 1gz8 1gzt 1h05 1h10 1h11 1h13 1h14 1h1n 1h2j 1h32 1h41 1h4a 1h4g 1h50 1h5q 1h61 1h6r
1h91 1h9h 1haz 1hb4 1hbz 1hd2 1hdh 1het 1heu 1hf4 1hf6 1hhc 1hhf 1hhu 1hhy 1hjc 1hk0 1hlq 1hn4 1hq2 1ht6 1hty 1hw1
1hxc 1hyo 1hzc 1hzj 1i0h 1i0v 1i12 1i1j 1i1n 1i24 1i2t 1i4f 1i52 1i5g 1i6w 1i71 1i73 1i76 1i86 1i88 1i8o 1ie9 1ig5
1ijq 1iju 1ijy 1ike 1ikj 1ikp 1inl 1io0 1iom 1iqz 1ir0 1isp 1itx 1iu5 1iua 1iw0 1iw1 1iwx 1iwz 1iyb 1izp 1izr 1j05
1j1m 1j2r 1j2w 1j3f 1j3w 1j77 1j8a 1j8u 1j96 1j97 1j9b 1jbo 1jbx 1jcz 1jcl 1jd0 1jdr 1jf8 1jg1 1jg2 1jg4 1ji7 1jks
1jl0 1jlt 1jnd 1jo8 1jr8 1jub 1jw8 1jx6 1jy2 1jz7 1jz8 1jzl 1k38 1k3i 1k3l 1k55 1k6x 1k9z 1ka1 1kb0 1kcd 1kdv 1kdy
1kdz 1kfc 1kgd 1kgs 1kjq 1kmt 1koi 1kpu 1kq3 1kqp 1kqr 1kr7 1ks8 1kuf 1kug 1kui 1kuk 1kv0 1kv7 1kw3 1kw6 1kwn 1ky3
1kyc 1kyf 1kyp 1kyr 1kys 1kzk 1l0g 1l0z 1l1g 1l6r 1l7l 1l7m 1l9l 1lc0 1lc3 1lc5 1lju 1llf 1llr 1lmi 1ln4 1lo7 1loq
1lq9 1lqp 1lqt 1lqu 1lr7 1lri 1ls9 1lw6 1lw9 1lxz 1ly0 1lyq 1lyv 1lzi 1ljz 1lzl 1mf1 1mq1 1mr1 1m22 1m2x 1m4i 1m5e
1m6j 1m6k 1m70 1m7g 1m7j 1mb3 1md2 1mgo 1mj5 1mk5 1mkk 1moo 1mpl 1mqo 1muw 1mxr 1n0q 1n13 1n1x 1n3l 1n40 1n45 1n7e
1n7o 1n7s 1n8k 1n92 1na5 1ncw 1ney 1nf9 1nki 1nko 1nlq 1nlu 1nn5 1nnf 1nnx 1nof 1nq7 1nqj 1nte 1ntv 1nwa 1nxx 1nyc
1nzi 1nzj 1o04 1o06 1o08 1o0f 1o0h 1o0m 1o0n 1o0o 1o1h 1o2i 1o2n 1o2p 1o2q 1o2r 1o2u 1o2v 1o2w 1o2x 1o2y 1o33 1o34
1o35 1o37 1o38 1o3d 1o3j 1o3k 1o3l 1o3y 1o4y 1o5x 1o6v 1o7i 1o7j 1o7n 1o7u 1o81 1o82 1o85 1o8b 1o8s 1o8x 1o98 1o9g

2qh7 2qhs 2qht 2qif 2qip 2qj5 2qj7 2qjl 2qjw 2qjz 2ql8 2qmo 2qmt 2qng 2qnl 2qnn 2qnt 2qo4 2qo5 2qo8 2qoc 2qod 2qof
 2qoi 2qok 2qol 2qoo 2qp6 2qp8 2qpx 2qq0 2qr6 2qrf 2qsb 2qsk 2qsw 2qt2 2qt4 2qt6 2qt7 2quz 2qvb 2qvg 2qvk 2quv 2qwx
 2qxf 2qxi 2qxx 2qz0 2qzc 2r01 2r0x 2r14 2r1u 2r2z 2r3f 2r3h 2r3i 2r3q 2r3r 2r5o 2r6j 2r6q 2r6u 2r75 2r80 2r8e 2r8o
 2r8q 2ra3 2ra6 2ra9 2rb2 2rbn 2rbo 2rbp 2rbr 2rbt 2rbv 2rbw 2rbx 2rby 2rc0 2rc2 2rc8 2rcq 2rct 2rdk 2rdr 2rdq 2re2
 2rff 2rfg 2rfr 2rfv 2rgb 2rge 2rgg 2rhf 2ri7 2ril 2rit 2riv 2riz 2rj4 2rj5 2rj6 2rjv 2rjy 2rk1 2rk3 2rk4 2rk5 2rk6
 2rkl 2rkq 2rkl 2ruq 2ruu 2ruv 2ruv 2ruv 2ruv 2ruv 2ruv 2ruv 2ruv 2ruv 2ruv 2ruv 2ruv 2ruv 2ruv 2ruv 2ruv 2ruv 2ruv
 2v1i 2v1j 2v1k 2v1m 2v1q 2v25 2v27 2v2b 2v2h 2v2p 2v2s 2v38 2v3g 2v4v 2v4x 2v52 2v6a 2v6k 2v6v 2v8t 2v8u 2v9n 2v9v
 2vb9 2vba 2vbb 2vbk 2vbp 2vc4 2vc8 2vch 2vcn 2vd8 2ve8 2veb 2vez 2vfd 2vfk 2vfm 2vfn 2vfo 2vfr 2vh3 2vhs 2vi2 2vi3
 2vi4 2vif 2vim 2vji 2vk2 2vk6 2vk7 2vk8 2v1w 2v1x 2vmh 2vn6 2vng 2vno 2vnx 2vnz 2voc 2vov 2vpa 2vpt 2vq4 2vq8 2vqr
 2vr6 2vr8 2vs0 2vu7 2vuc 2vuk 2vuv 2vv6 2vw8 2vws 2vx5 2vxt 2vxx 2vy8 2vyo 2vyx 2vzc 2vzp 2w0o 2w12 2w13 2w14 2w15
 2w1j 2wlp 2wlr 2wls 2wlv 2w20 2w2a 2w2b 2w2e 2w31 2w39 2w3g 2w3p 2w3z 2w40 2w47 2w4j 2w5q 2w6a 2w7a 2w91 2w9h 2wag
 2wbo 2wbq 2wbx 2wcj 2wcm 2wd2 2wd4 2wdc 2wdd 2wds 2wdy 2we2 2we5 2weg 2weo 2wf5 2wf6 2wf7 2wf8 2wf9 2wgy 2wh6 2whl
 2whm 2wi9 2wkl 2wll
 2wra 2ws6 2wsb 2wsn 2wso 2wtg 2wtp 2wts 2wu9 2wu9 2wu9 2wu9 2wu9 2wu9 2wu9 2wu9 2wu9 2wu9 2wu9 2wu9 2wu9 2wu9
 2wzc 2wzx 2x02 2x04 2x18 2x1o 2x1p 2x1q 2x25 2x2o 2x2p 2x3m 2x49 2x4k 2x4l 2x4w 2x5l 2x5o 2x5x 2x6w 2x6y 2x76 2x7k
 2x7m 2x85 2x8s 2x9g 2x9v 2x9x 2xa3 2xbr 2xbs 2xc3 2xde 2xdw 2xep 2xff 2xfy 2xgb 2xgi 2xhf 2xhg 2xio 2xir 2xiu 2xiv
 2xiw 2xj3 2xjh 2xji 2xjk 2xjq 2xki 2x18 2xld 2xlm 2xlv 2xm0 2xmf 2xmj 2xmk 2xmt 2xn6 2xn7 2xnq 2xoe 2xon 2xpc 2xpv
 2xpw 2xqo 2xqq 2xr5 2xr6 2xrh 2xrw 2xry 2xt1 2xtp 2xtt 2xu1 2xu3 2xuv 2xw9 2xw1 2xwv 2xxh 2xxu 2xz2 2xza 2zxc 2xzi
 2zxk 2y0g 2y1o 2y1q 2y39 2y3c 2y3f 2y53 2y5a 2y5d 2y60 2y64 2y66 2y68 2y6k 2y6l 2y6n 2y71 2y77 2y7g 2y7l 2y8e 2y8k
 2y9f 2yb6 2yc3 2ycd 2yde 2yef 2yfn 2yfo 2ygi 2yhg 2yih 2yim 2yiv 2yke 2ykg 2y1b 2y1l 2y1n 2y2o 2y2n 2y2a 2y2z
 2yoa 2yog 2yoi 2yod 2yvo 2yve 2yxc 2yxf 2yxw 2yyw 2yz1 2z0j 2z12 2z18 2z19 2z26 2z2f 2z3g 2z3n 2z4u 2z51 2z53 2z6r
 2z6s 2z6t 2z6w 2z79 2z7k 2z8a 2z8r 2z8x 2z98 2zac 2zbn 2zbx 2zcc 2zcm 2zcn 2zde 2zdp 2zew 2zex 2zfd 2zff 2zgw 2zhj
 2zhn 2zib 2zjx 2z15 2z16 2z17 2zm0 2zm9 2zmx 2zmy 2zmz 2znr 2zo6 2zoh 2zou 2zow 2zpb 2zpe 2zpf 2zpg 2zpi 2zpm 2zpt
 2zq7 2zq8 2zq9 2zqa 2zqc 2zqd 2zqt 2zsc 2zsn 2zso 2zsp 2zsq 2zsr 2zss 2zst 2zsx 2zsy 2zsz 2zt0 2zt1 2zt2 2zt3 2zt4
 2zu1 2zui 2zux 2zvp 2zvq 2zvx 2zw0 2zwd 2zwe 2zwf 2zwg 2zws 2zwt 2zww 2zxy 2zyd 2zyp 2zzv 3a02 3a07 3a0n 3a0s 3a1s
 3a2z 3a35 3a38 3a39 3a3v 3a40 3a4j 3a4r 3a55 3a57 3a6q 3a6r 3a71 3a72 3a7i 3a7j 3a7l 3a8a 3a8g 3a8m 3a8o 3a8u 3a8z
 3a90 3a92 3a95 3a9b 3a9j 3a9k 3ab5 3abx 3acg 3ach 3agh 3agi 3agn 3ago 3agt 3ahs 3ahw 3ahz 3aia 3aja 3aj6 3aj7 3aj9
 3ajz 3ak2 3ak3 3ak8 3ak9 3akb 3ake 3al7 3ald 3alf 3alj 3amc 3aok 3ap9 3aqj 3arq 3arv 3arw 3arx 3ary 3ast 3atn 3ato
 3au2 3aub 3aug 3auh 3av8 3aws 3awt 3awv 3aww 3awx 3awz 3ax0 3axi 3ayx 3ayy 3ayz 3az1 3az3 3az6 3azd 3b0f 3b0g 3b0s
 3b0t 3b0x 3b0y 3b12 3b27 3b28 3b2c 3b2x 3b34 3b35 3b36 3b3a 3b3c 3b3r 3b3s 3b3t 3b3v 3b4n 3b4u 3b50 3b51 3b52 3b53
 3b5m 3b5o 3b64 3b6d 3b72 3b79 3b7e 3b7s 3b7v 3b80 3b8z 3b9g 3ba1 3bb0 3bb2 3bb7 3bbb 3bc9 3bdf 3bdg 3bdi 3bed 3ber
 3bf7 3bfo 3bgu 3bh4 3bhd 3bhl 3bhw 3bi1 3bje 3bkr 3bkt 3blb 3bld 3bli 3bln 3bm7 3bmx 3bmz 3bnb 3bne 3bng 3bnj 3bo6
 3bob 3boe 3bog 3boi 3boj 3bok 3bom 3bon 3bpt 3bpv 3bpq 3bpv 3bqx 3br8 3bs2 3bt5 3bu1 3bu9 3bub 3bui 3buu 3buw 3buw
 3bux 3bva 3bv6 3bv7 3bv8 3bv9 3bv9 3bwa 3bwh 3bwx 3bwy 3bwz 3bxq 3bxu 3by8 3bzo 3bzp 3bzq 3bzs 3btz 3bzy 3bzz
 3c00 3c1v 3c22 3c31 3c3y 3c5a 3c6y 3c76 3c77 3c78 3c8b 3c8c 3c8e 3c8l 3c8y 3c9q 3c9u 3c9z 3ca6 3ca7 3cb9 3cbe 3cbp
 3cbw 3cbz 3ccd 3ccg 3cd1 3ce1 3ch0 3chm 3chv 3ci3 3ci7 3cij 3cim 3ciw 3cjm 3cjs 3ckc 3ckf 3ckm 3clm 3cm3 3cn4 3cnj
 3co1 3cov 3cp7 3cpo 3cql 3ct5 3ct6 3ctg 3ctp 3cu4 3cu9 3cui 3cuz 3cv2 3cvb 3cvd 3cwn 3cwr 3cxm 3cxy 3cxz 3cy6 3cyw
 3cyx 3cz1 3cz9 3cza 3czn 3czs 3czt 3czz 3d02 3d06 3d08 3d0y 3d1k 3d1p 3d1x 3d20 3d2q 3d32 3d3b 3d43 3d49 3d4e 3d51
 3d59 3d5p 3d5y 3d6i 3d7j 3d80 3d97 3d9a 3d9q 3d9t 3d9x 3da8 3daq 3db7 3dbk 3dbp 3dcr 3dcw 3dd0 3dda 3ddo 3deo 3dfg
 3dfj 3d9g 3dgd 3dgt 3dha 3dhb 3dhc 3dhp 3dib 3djh 3dke 3dlc 3dmi 3dnj 3dou 3dpv 3dq4 3dq5 3dq7 3dq9 3dqa 3dqo 3dqd
 3dqe 3dqf 3dqh 3dqi 3dqk 3dql 3dqm 3dqn 3dqo 3dqp 3dqu 3dr9 3drf 3drj 3ds2 3ds4 3dsb 3dt2 3dt4 3dt7 3dth 3duw 3dvw
 3dx2 3dx3 3dx4 3dxl 3dxy 3dyb 3dze 3e0x 3e10 3e2d 3e2n 3e2v 3e4g 3e4n 3e4v 3e55 3e5h 3e5i 3e5o 3e6z 3e7r 3e7u 3e8m
 3e8o 3e8t 3eaz 3ebv 3ec1 3ecx 3ecz 3ed9 3eda 3edb 3edn 3edh 3edi 3edn 3edo 3eer 3ef3 3ef4 3ef8 3eg3 3ein 3eix 3e19
 3ejp 3ejq 3ejr 3ejs 3ejt 3eju 3ejv 3elf 3eln 3em1 3emh 3en0 3eo6 3eoj 3epw 3er7 3erx 3esc 3esn 3eso 3esp 3ess 3esu
 3eu3 3eur 3eva 3evd 3evf 3evo 3evp 3ew0 3ew1 3eww 3ewx 3ewy 3ewz 3ex1 3ex3 3ex4 3ex6 3exd 3exv 3exx 3exy 3ey6 3eye
 3ezg 3f00 3f03 3f04 3f05 3f0d 3f0l 3f0m 3f14 3f16 3f17 3f18 3f19 3f1a 3f1l 3f1n 3f1p 3f22 3f40 3f5l 3f5s 3f5v 3f66
 3f6b 3f6c 3f6e 3f6v 3f6y 3f71 3f7e 3f7k 3f7l 3f7x 3f8d 3f8y 3f9b 3f9l 3f9m 3f9x 3f9y 3fa0 3fad 3fas 3fbw 3fci 3fcn
 3fcx 3fdo 3fe0 3fe7 3fea 3fec 3fed 3fev 3ff3 3fg9 3fgd 3fgh 3fgv 3fia 3fk8 3fke 3fkx 3fll 3fm6 3fmu 3fmy 3fn5 3fo3
 3fo7 3fod 3fp6 3fp7 3fp8 3fpc 3fpo 3fq4 3fq9 3frr 3fs6 3fs9 3fsa 3fsj 3fso 3fss 3ftd 3ftk 3fuc 3fv1 3fv2 3fva 3fvg
 3fvk 3fyn 3fvo 3fvp 3fvs 3fvx 3fw8 3fw9 3fwa 3fwh 3fww 3fwn 3fyn 3fz4 3fzw 3g02 3g0k 3g16 3g1a 3g1b 3g1d 3g1p 3g1s
 3g1v 3g1y 3g22 3g24 3g2y 3g2z 3g32 3g34 3g35 3g36 3g3m 3g3p 3g48 3g5f 3g5h 3g5s 3g6k 3g7n 3g7r 3g89 3g8f 3g8h 3ga3
 3ga4 3gah 3gai 3gaj 3gba 3gbw 3gc5 3ge7 3gef 3gfa 3gg7 3ghc 3ghj 3ghv 3ghw 3gip 3giw 3gix 3gj0 3g1y 3gkn 3gkv 3gmg
 3gmx 3gne 3gnl 3gnz 3go5 3gof 3gp2 3gp3 3gp6 3gpi 3gq1 3gr3 3grd 3gt3 3gu4 3gu6 3gui 3gun 3gup 3gve 3gvj 3gvl 3gxh
 3gyi 3gyj 3gyl 3gz2 3gzq 3gzt 3h0n 3h0o 3h0u 3h12 3h1x 3h31 3h4i 3h4n 3h4o 3h4t 3h4w 3h4x 3h56 3h5b 3h5k 3h61 3h62
 3h63 3h68 3h6w 3h74 3h79 3h7c 3h7f 3h7r 3h82 3h8g 3h91 3h99 3h9b 3h9c 3hau 3haw 3hd1 3hd2 3hds 3hdx 3hfs 3hh3 3hh4
 3hh5 3hh6 3hhp 3his 3h10 3h1b 3h1i 3h1w 3h1x 3h1z 3h24 3hmc 3hmd 3hna 3hnb 3hnx 3hny 3hp4 3hpc 3hpw 3hre 3hrv 3hsg
 3hsj 3hsv 3hsz 3ht0 3ht1 3htd 3htg 3htn 3hu5 3hu9 3huh 3huk 3huv 3hup 3huq 3hv2 3hv8 3hvh 3hvi 3hvk 3hwu
 3hx8 3hyd 3hyg 3hz8 3hza 3hzc 3h3p 3i03 3i06 3i07 3i0g 3i0j 3i0y 3i10 3i11 3i19 3i1u 3i24 3i2l 3i2v 3i2y 3i2z 3i30
 3i33 3i34 3i35 3i37 3i39 3i3f 3i3q 3i3s 3i45 3i4g 3i4o 3i4w 3i5o 3i67 3i6c 3i6f 3i6h 3i6j 3i6o 3i7m 3i8r 3i8u 3i95
 3i9q 3ia9 3ib0 3ib4 3ib5 3ibo 3ibu 3ich 3icv 3id7 3ie4 3ifl 3ifn 3igs 3ihs 3iis 3iiu 3iix 3ij8 3ijj 3ijl 3ikw 3ili
 3ilo 3i1r 3im9 3imk 3ims 3imt 3imu 3imv 3imw 3iof 3iog 3ioh 3ioi 3ip0 3ip5 3ip6 3ip8 3ipc 3ipe 3ipn 3iql 3iqo 3iqu
 3iqv 3ir4 3irp 3is3 3isg 3isx 3it3 3itf 3itq 3iu1 3iu7 3iub 3iut 3iv0 3iv4 3ivv 3iww 3ix3 3ixl 3jql 3jqu 3jr3 3jsc

4b2i 4b2l 4b32 4b33 4b35 4b3b 4b41 4b4d 4b4i 4b4j 4b4u 4b5n 4b62 4b6g 4b78 4b7h 4b89 4b8x 4b97 4b9c 4b9f 4b9g 4b9i
4b9p 4ba6 4bad 4bal 4bap 4bar 4bat 4baz 4bb3 4bb9 4bcd 4bct 4bcw 4bcy 4beg 4beq 4beu 4bfl 4bf5 4bfh 4bfn 4bfo 4bgb
4bgc 4bi6 4bji 4bkd 4blk 4bli 4bln 4blx 4bm1 4bm2 4bmh 4bn4 4bnd 4boq 4bps 4bpz 4bq1 4br4 4brc 4brd 4brg 4brk 4brq
4bs5 4bt2 4bt3 4bt7 4bte 4bu0 4buh 4bw1 4bw3 4bx5 4c0x 4c45 4c4c 4c4d 4c6a 4c6c 4c72 4c80 4cay 4cb5 4cdj 4cdp 4cfl
4d8b 4d8e 4d8i 4d9w 4dat 4dbc 4dc5 4dc6 4dc7 4dc8 4dd5 4dds 4ddy 4de0 4de1 4de2 4de3 4df0 4df7 4dfa 4dfg 4dfx 4dga
4dgd 4dgz 4dhr 4di9 4dja 4djc 4djp 4djQ 4djx 4dk2 4dkn 4dlr 4dm5 4dm7 4dmi 4dmk 4dmt 4dmv 4dn2 4dnd 4do2 4dp0 4dp1
4dp8 4dp9 4dpb 4dpc 4dq5 4dq6 4dq7 4dqa 4dqB 4dqe 4dqj 4dri 4drk 4drm 4drn 4dro 4drr 4dt4 4dt5 4dty 4duh 4dui 4duq
4dwd 4dwo 4dwr 4dww 4dxk 4dxm 4dxu 4dz7 4dz9 4e15 4e19 4e1h 4e2b 4e2v 4e2w 4e2x 4e2z 4e30 4e32 4e34 4e35 4e3b 4e3f
4e3h 4e3k 4e3l 4e3m 4e3n 4e3u 4e3x 4e46 4e49 4e4a 4e4u 4e6f 4e6u 4e7t 4e97 4e9o 4e9q 4e9r 4e9t 4e9w 4e9x 4e9y 4ea7
4eaa 4eab 4ead 4eae 4eb0 4ede 4ee6 4ee9 4eet 4eeu 4eeW 4ef0 4efi 4efp 4egu 4eid 4eif 4eih 4eiv 4ek3 4ek4 4ekr 4el4
4emn 4emt 4enp 4eo7 4eod 4ep4 4epv 4eq8 4eqi 4eqp 4eqs 4eqw 4erc 4ery 4es1 4es2 4esa 4ese 4esp 4etl 4etn 4eu9 4eul
4euo 4ev4 4evz 4exy 4ey1 4ey2 4eyb 4eza 4ezf 4ezg 4ezi 4f06 4f0b 4f0j 4f18 4f19 4f1u 4f1v 4f2c 4f2e 4f2f 4f2l 4f3i
4f5l 4f5z 4f60 4f66 4f6j 4f87 4f8d 4f8l 4f8x 4f8z 4f98 4f9t 4fat 4fb7 4fbi 4fcf 4fch 4fcs 4fee 4feg 4ffl 4fgl 4fh2
4fh4 4fh6 4fi6 4fi7 4fi8 4fio 4fk9 4fkb 4fkl 4fku 4fl8 4flg 4flk 4fl1 4fm6 4fn7 4fo2 4fon 4fp5 4fps 4fpt 4fra 4fru
4frv 4ftf 4fvn 4fvo 4fwb 4fyo 4fzo 4fzp 4g13 4g14 4g1s 4g1x 4g3b 4g3n 4g41 4g44 4g47 4g48 4g4m 4g4p 4g6c 4g7x 4g8b
4g8d 4g9e 4g9g 4gai 4gc3 4gc4 4gci 4gcj 4gcx 4gcy 4gd0 4gd9 4ge6 4gei 4gek 4ges 4gg1 4gg9 4ggc 4gge 4gh0 4gh1 4ghg
4ghi 4gie 4gjy 4gjz 4gkb 4gkc 4gl1 4gm0 4gm1 4gm4 4gm5 4gmQ 4gmu 4gnb 4gne 4gnm 4gno 4gnq 4gnu 4gnv 4gnw 4gog 4gp9
4gpe 4gpq 4gql 4gqq 4gqr 4gr0 4gr3 4gr8 4grj 4grr 4grz 4gs3 4gt9 4gta 4gv1 4gvf 4gvh 4gvq 4gxw 4gy1 4gy7 4gyq 4gyx
4gzc 4gzg 4h0d 4h1a 4h1b 4h30 4h48 4h4d 4h4i 4h4r 4h4t 4h4v 4h4x 4h53 4h5i 4h6e 4h76 4h7p 4h7w 4h8e 4h8r 4h8x 4h8y
4h8z 4h90 4h91 4h92 4h93 4h94 4h9a 4h9b 4h9c 4h9e 4h9f 4h9h 4h9i 4ha3 4ha4 4hak 4hal 4hbt 4hbu 4hct 4hcu 4hdb 4hdd
4hde 4hdf 4hdk 4hdp 4hdr 4he9 4heg 4heq 4hey 4hfg 4hgh 4hgi 4hgu 4hhp 4hi7 4hil 4hjp 4hjt 4hk2 4hkg 4hl1 4hl2 4hls
4hm6 4hm7 4hmj 4hp0 4hp8 4hpa 4hpc 4hpd 4hpi 4hpi 4hpk 4hpy 4hqs 4hro 4hrr 4hrt 4hry 4hs5 4hsw 4hsx 4ht2 4ht3 4htg
4htk 4htn 4htq 4hu2 4hu7 4hua 4hwm 4hww 4hxm 4hxn 4hxs 4hy4 4hy7 4hyi 4hz6 4hz8 4hzf 4hzm 4hzt 4i0b 4i1i 4i2t 4i2u
4i3b 4i3g 4i4o 4i4p 4i4s 4i4v 4i56 4i5r 4i5u 4i62 4i6r 4i6x 4i6y 4i71 4i7m 4i7v 4i7w 4i84 4i8i 4i93 4iav 4iby 4ic4
4ici 4idc 4idd 4ied 4iej 4ifx 4ig1 4igt 4igv 4ihm 4ihz 4iix 4iyy 4ij5 4ijh 4iji 4ik2 4iku 4imq 4inc 4ine 4inw 4ioo
4ioq 4ior 4ipp 4ips 4ipu 4ipv 4ipw 4iq9 4iqb 4irx 4is5 4isv 4it8 4ita 4itb 4ium 4iva 4ix3 4iyj 4j20 4j2s 4j3y 4j44
4j45 4j46 4j47 4j4z 4j55 4j5q 4j74 4j7a 4j7d 4j7n 4j86 4j8a 4j8p 4j9t 4jb3 4jb7 4jbd 4jc1 4jcc 4jck 4jd5 4jd7 4je1
4jff 4jff 4jfl 4jfm 4jgi 4jgl 4jh2 4jh8 4jht 4jiu 4jje 4jk9 4jl7 4jll 4jml 4jm5 4jm9 4jmb 4jmi 4jmw 4jn7 4jn8 4joe
4jof 4jog 4joh 4joj 4jok 4jor 4jos 4jp6 4jpl 4jpm 4jpt 4jpu 4jqk 4jqm 4jqv 4jsa 4jss 4jtm 4ju8 4jv8 4jvo 4jvu 4jwx
4jx9 4jxc 4jxh 4jyf 4jym 4jzz 4k3l 4k45 4k4o 4k60 4k69 4k6b 4k6f 4k6y 4k75 4k7t 4k8g 4k93 4k9c 4k9k 4kae 4kal 4kap
4kb9 4kc1 4kdy 4kee 4kf0 4kg7 4kgd 4kh7 4kjj 4kjk 4kjl 4kl9 4klw 4klx 4km0 4km2 4kn9 4knn 4kor 4kow 4koy 4kp5 4kr5
4ks7 4ktf 4ktj 4ktk 4kua 4kv1 4kvp 4kxu 4kxy 4ky2 4ky5 4kzk 4kzv 4l1i 4l1t 4l2h 4l4e 4l5e 4l6d 4l9p 4lbg 4lc6 4lc8
4ldn 4ler 4lfo 4lfx 4lhs 4ljl 4ljh 4lls 4low 4lp9 4lr6 4lrt 4lvf 4lwq 4lx2 4lxq 4lxt 4lxu 4lxx 4lyi 4lz5 4m0k 4mlv
4m2o 4m2p 4m3s 4m4l 4m4m 4m8u 4m9k 4mam 4maq 4max 4mb1 4mby 4mdg 4mij 4mje 4mkn 4mlu 4mq1 4mth 4muz 4mzb 4mzi 4mzj
4n13 4n1i 4n30 4n4b 4n5m 4n6p 4n8z 4n9o 4n9p 4nbu 4ndx 4ni3 4ni6 4nin 4nio 4njj 4nkp 4nmw 4np5 4npo 4nvb 4nvf 4nvl
4nvn 4nzc 4o0a 4o0k 4o5o 7atj

For the following PDBids the unknown ligands in the PDB files were removed:

1vmg, 1vp8, 2f46, 2fcl, 2ftr, 2oh1, 2ozh, 2peb, 2qe8, 3bog, 3e8o, 3ejv, 3f7x, 3fgv, 3gl6, 3giw,
3gr3, 3gzt, 3hm4, 3hmz, 3hx8, 3i0y, 3mho, 3mst, 3ndo, 3ppl, 3scy, 3u3g, 3v1c, 3v7p, 4efi, 4ici,
4igv, 4iyy, 4j8p, 4jgl

SUPPORTING INFORMATION 2: Tab separated table of captured, PLI, and PPI water molecules with EDIA and hydrogen bond characteristics (csv-file separately available). Surface water characteristics will be provided upon request due to the amount of data.

Header:

1. PDBid

2. Waterid	HOH_'chain identifier'_'reside sequence number from PDB file'
3. EDIA	electron density for individual atoms
4. TotalNofHb	total number of hydrogen bonds formed by the water molecules
5. P_Contact	hydrogen bonds formed with protein
6. L_Contact	hydrogen bonds formed with ligand
7. W_Contact	hydrogen bonds formed with other water molecules
8. Hydrophobicity	proportion of hydrophobic atoms within 4.5 Å radius
9. HydrophobicSurface	proportion of hydrophobic surface pointing to a water molecule
10. WaterClassification	classification into PLI, PPI, or C