

SUPPORTING INFORMATION

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

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SUPPORTING INFORMATION 1: Data set of all PDBids

Table S1: PDBids of the high-resolution data set

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 4e3h 4e3k 4e3l 4e3m 4e3n 4e3u 4e3x 4e46 4e49 4e4a 4e4u 4e6f 4e6u 4e7t 4e97 4e9o 4e9q 4e9r 4e9t 4e9w 4e9x 4e9y 4e9z
 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 4et1 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
 4f51 4f5z 4f60 4f66 4f6j 4f87 4f8d 4f8l 4f8x 4f8z 4f98 4f9t 4fat 4fb7 4fbi 4fcf 4fc8 4fcs 4fee 4feg 4ffl 4fg1 4fh2
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 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 4ii5 4iiy 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
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 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, 3g16, 3giw,
 3gr3, 3gzs, 3hm4, 3hmz, 3hx8, 3i0y, 3mho, 3mst, 3ndo, 3pp1, 3scy, 3u3g, 3v1c, 3v7p, 4efi, 4ici,
 4igv, 4iyj, 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