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**Supporting information for article:**

# Estimation of the protein–ligand interaction energy for model building and validation

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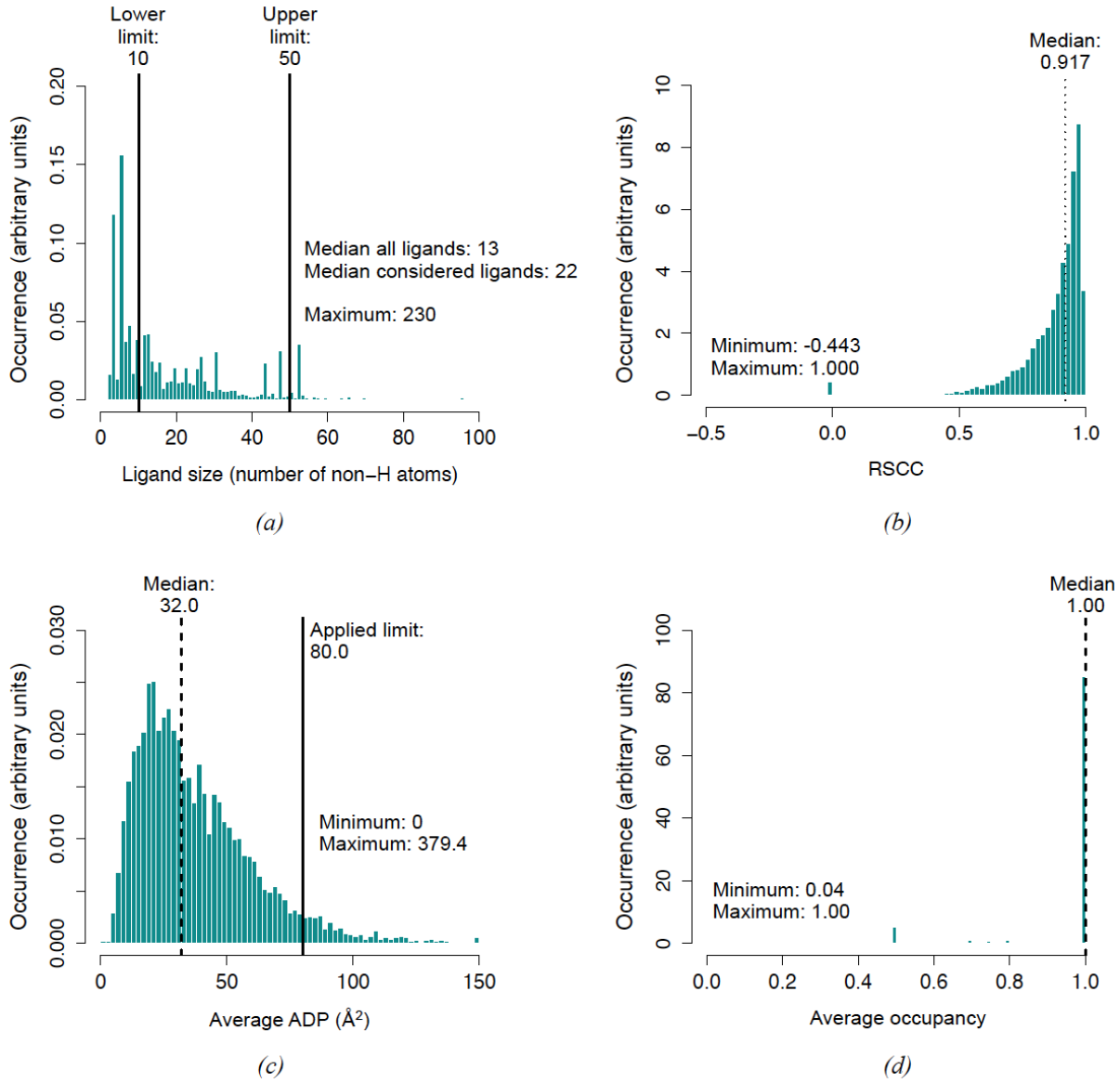


**Figure S1** Distributions of (a) ligand sizes (the number of non-hydrogen atoms), (b) real space correlation coefficients (RSCC), (c) average atomic displacement parameters and (d) average atomic occupancies for the set of 9956 non-covalent protein-ligand complexes collected from the PDB. The median, minimum and maximum values are shown. When the median was not used as the threshold for filtering, the applied limit is indicated. For (a) and (c), only those cases below the applied limit were accepted, while for (b) and (d), those above the median (inclusive) were accepted.

**Table S1** The values of interaction energy for 2,020 ligand-protein structures estimated by LigEnergy approach using equation (1). (See separate Excel file).

**Table S2** The results of ligand identification in the electron density for 100 test cases with the help of ARP/wARP shape similarity procedure and proposed here the LigEnergy approach.

| PDB ID | Ligand deposited in the PDB | Ligand identified (3-letter ligand identifier) by shape similarity and RSCC | Ligand identified (3-letter ligand identifier) by LigEnergy approach (eq. 2) |
|---|---|---|---|
| 1y89 | 2PE | NAD | 2PE |
| 2yhw | 2PE | 2PE | 2PE |
| 3oa5 | 2PE | P6G | P6G |
| 3vz0 | 2PE | PYR | PEG |
| 1ex7 | 5GP | ADP | 5GP |
| 1hgx | 5GP | THP | 5GP |
| 2qor | 5GP | A3P | 5GP |
| 2xbu | 5GP | 5GP | 5GP |
| 3n1s | 5GP | ATP | 5GP |
| 3tr0 | 5GP | ADP | 5GP |
| 1c9k | 5GP | A3P | AMP |
| 1t8t | A3P | A3P | A3P |
| 3uan | A3P | A3P | A3P |
| 1q1q | A3P | COA | 1PE |
| 2oq2 | A3P | LDA | ORO |
| 3ap1 | A3P | COA | THP |
| 4l0m | ADE | BTB | ADE |
| 2pgf | ADN | NAD | ADN |
| 3oi8 | ADN | ADN | ADN |
| 2q6k | ADN | SAM | NHE |
| 2zbv | ADN | AMP | AMP |
| 3o1c | ADN | SAM | NHE |
| 1ao0 | ADP | SAM | ADP |
| 2c2a | ADP | ATP | ADP |
| 2uyt | ADP | ADP | ADP |
| 4rz3 | ADP | ADP | ADP |
| 1cza | ADP | SAM | COA |
| 1in4 | ADP | TPP | TYD |
| 1um8 | ADP | SAM | CMP |
| 2w58 | ADP | NAD | ATP |
| 2yx6 | ADP | H4B | AMP |
| 3b1n | ADP | ATP | TYD |
| 3bk7 | ADP | AMP | OLA |

| | | | |
|---|---|---|---|
| 3c4n | ADP | IPH | IPH |
| 3cwq | ADP | TYD | TYD |
| 2cfm | AMP | AMP | AMP |
| 2r85 | AMP | TYD | AMP |
| 2v8q | AMP | ATP | AMP |
| 3ber | AMP | 5GP | AMP |
| 3nzt | AMP | ATP | AMP |
| 3o0m | AMP | ADP | AMP |
| 4eei | AMP | AMP | AMP |
| 4eql | AMP | AMP | AMP |
| 4ts5 | AMP | NAD | AMP |
| 4ww7 | AMP | ATP | AMP |
| 1ry2 | AMP | 017 | PLP |
| 1zn8 | AMP | ATP | 5GP |
| 2c5s | AMP | C2E | NHE |
| 2gxq | AMP | ORO | ORO |
| 2i4i | AMP | MLT | MLT |
| 2qga | AMP | TYD | TYD |
| 3ddj | AMP | 5GP | 5GP |
| 3fwz | AMP | ADP | ADP |
| 3glv | AMP | TPP | TPP |
| 1jjv | ATP | ATP | ATP |
| 2e5y | ATP | ATP | ATP |
| 3a8t | ATP | NAP | ATP |
| 3lgx | ATP | ATP | ATP |
| 3rk1 | ATP | ATP | ATP |
| 2f02 | ATP | FPP | FPP |
| 2fgh | ATP | NAD | NAD |
| 2pze | ATP | NAP | NAP |
| 3h1q | ATP | ADP | PYR |
| 3h39 | ATP | BCL | MYR |
| 3ikh | ATP | NAD | 1PE |
| 3lkk | ATP | LDA | CIT |
| 3ll3 | ATP | TYD | TYD |
| 2ooq | B3P | B3P | B3P |
| 3l6g | B3P | B3P | B3P |
| 3q4o | B3P | B3P | B3P |

| | | | |
|---|---|---|---|
| 3q4o | B3P | B3P | B3P |
| 2xsg | B3P | SIA | BTB |
| 3lnl | B3P | PYR | IPH |
| 3ib7 | BTB | BTB | BTB |
| 1y55 | BTN | BTN | BTN |
| 2c4i | BTN | BTN | BTN |
| 4gda | BTN | BTN | BTN |
| 1y55 | BTN | BTN | BTN |
| 2c4i | BTN | BTN | BTN |
| 3ew2 | BTN | ATP | AKG |
| 4bj8 | BTN | MLT | PEP |
| 4z28 | BTN | TAM | HED |
| 2rde | C2E | C2E | C2E |
| 4eu0 | C2E | C2E | C2E |
| 4foj | C2E | C2E | C2E |
| 4urg | C2E | C2E | C2E |
| 5euh | C2E | C2E | C2E |
| 2f6u | CIT | CIT | CIT |
| 3bhd | CIT | CIT | CIT |
| 2r4i | CIT | CIT | CIT |
| 3f7c | CIT | TAM | CIT |
| 3gm5 | CIT | P6G | CIT |
| 3lmz | CIT | BTB | BTB |
| 3nnb | CIT | MLT | MLT |
| 3pko | CIT | ATP | TLA |
| 3qsl | CIT | 2GP | 2GP |
| 3rju | CIT | TAM | TAM |
| 4hfv | CIT | GSH | PEP |
| 4k7g | CIT | TAM | TAM |
| 5kbf | CMP | ADP | ADP |