Supplementary Information

A Rapid Identification of Hit Molecules for Target Proteins via Physico-Chemical **Descriptors**

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| PDBID | PD | РА | РР | PMR | Volume | DD | DA | Р | MR | W | BE (Expt.) | BE (Pred) |
|-------|----|----|------|--------|--------|----|----|-------|--------|----------|---------------|--------------|
| 1a4w | 5 | 5 | 0.81 | 38.19 | 1122 | 6 | 11 | 2.27 | 165.9 | 4854.69 | -8.1 | -10.2 |
| 1a9m | 8 | 7 | 2.22 | 65.11 | 1228 | 13 | 14 | -2.35 | 157.59 | 6315.12 | -9.4 | -11.1 |
| 1afl | 5 | 3 | 0.49 | 9.71 | 594 | 4 | 18 | -5.76 | 91.49 | 1754.48 | -8.5 | -8.5 |
| 1apv | 7 | 7 | 1.06 | 50.01 | 1204 | 6 | 10 | 0.91 | 130.56 | 3760.75 | -12.4 | -9.6 |
| 1ba8 | 5 | 5 | 0.87 | 30.41 | 1092 | 7 | 11 | -2 | 118.29 | 2829.55 | -12.3 | -8.7 |
| 1bdr | 7 | 6 | 1.9 | 53.56 | 885 | 4 | 8 | 4.97 | 151.87 | 4502.18 | -9.1 | -12 |
| 1bim | 6 | 7 | 0.63 | 48.79 | 1101 | 4 | 11 | 4.03 | 187.69 | 7755.98 | -12.1 | -10.4 |
| 1bra | 5 | 3 | 0 | 4.49 | 1675 | 4 | 2 | -0.33 | 37.85 | 59.09 | -2.5 | -4.8 |
| 1c2t | 5 | 4 | 1.52 | 32.09 | 1309 | 4 | 12 | -3.17 | 113.59 | 3547.35 | -11.1 | -9.7 |
| 1cbs | 7 | 5 | 1.72 | 47.42 | 716 | 0 | 2 | 4.27 | 91.13 | 1021.33 | -9.8 | -9.9 |
| 1d4l | 7 | 7 | 2.3 | 71.32 | 944 | 5 | 10 | 4.57 | 167.93 | 5257.99 | -11.9 | -12 |
| 1dmp | 7 | 6 | 1.28 | 35.18 | 974 | 6 | 7 | 4.23 | 158.07 | 4096.16 | -13 | -12.5 |
| 1dr1 | 3 | 3 | 1.24 | 23.94 | 733 | 6 | 8 | -1.21 | 58.38 | 379.75 | -7.6 | -5.9 |
| 1drf | 4 | 4 | 1 | 19.28 | 1315 | 5 | 13 | -3.38 | 108.15 | 2907.69 | -10.1 | -8.8 |
| 1dwc | 4 | 3 | 0.4 | 16.56 | 1113 | 7 | 11 | -1.47 | 129.3 | 2866.11 | -10.1 | -8.6 |
| 1dwd | 6 | 5 | 1.49 | 49.37 | 1371 | 6 | 9 | 1.92 | 143.1 | 3639.76 | -11.1 | -10.2 |
| 1dy9 | 4 | 3 | 0.95 | 21.44 | 1046 | 3 | 12 | -1.6 | 111.35 | 3507.21 | -10.3 | -9.1 |
| 1ela | 5 | 5 | 0.94 | 34.38 | 1404 | 5 | 7 | 2.2 | 113.49 | 2765.65 | -8.7 | -8.2 |
| 1epo | 5 | 6 | 0.57 | 35.11 | 1242 | 6 | 12 | 1.83 | 165.62 | 7093.18 | -10.9 | -9.7 |
| 1hbv | 7 | 7 | 2.25 | 73.14 | 1225 | 5 | 10 | 2.17 | 164.18 | 5858.58 | -8.7 | -11.6 |
| 1hge | 2 | 2 | 0 | 3.95 | 718 | 5 | 10 | -4.55 | 66.95 | 836.85 | -3.1 | -4.1 |
| 1hgg | 5 | 4 | 0.58 | 29.68 | 1315 | 12 | 20 | -9.56 | 127.42 | 5214.9 | -3.4 | -5.6 |
| 1hgh | 3 | 2 | 0 | 6.7 | 1033 | 5 | 10 | -4.55 | 66.95 | 836.85 | -3.9 | -4.3 |
| 1hgi | 2 | 2 | 0 | 6.21 | 1171 | 4 | 11 | -3.98 | 76.5 | 1155.64 | -3.7 | -4.5 |
| 1hgj | 2 | 2 | 0 | 6.71 | 1217 | 7 | 10 | -5.3 | 67.62 | 838.98 | -2.3 | -3.1 |
| 1hri | 6 | 6 | 2.38 | 79.07 | 790 | 1 | 4 | 3.6 | 82.95 | 1026.72 | -5.9 | -7.2 |
| 1hvi | 8 | 7 | 2.52 | 79.22 | 794 | 6 | 14 | 3.69 | 221.89 | 13644.07 | -13.7 | -13.7 |
| 1hvk | 8 | 8 | 3.48 | 96.5 | 1211 | 6 | 14 | 3.69 | 221.89 | 13644.07 | -13.8 | -14.3 |
| 1hvr | 7 | 6 | 2.71 | 81.53 | 1077 | 2 | 5 | 7.38 | 184.26 | 5902.99 | -13 | -12.4 |
| 1hxw | 8 | 7 | 3.36 | 93.88 | 1230 | 4 | 11 | 5.91 | 196.9 | 9308.03 | -14.5 | -13.5 |
| 1lyb | 8 | 9 | 3.29 | 103.15 | 1432 | 7 | 14 | 0.13 | 179.62 | 9453.34 | -15.6 | -12.2 |
| 1mcb | 4 | 5 | 0.58 | 45.18 | 1294 | 6 | 14 | -2.32 | 142.07 | 5066.32 | -6.6 | -6.8 |
| 1mch | 6 | 6 | 0.49 | 52.92 | 978 | 8 | 18 | -3.31 | 177.33 | 10126.48 | -7 | -7.8 |
| 1mcj | 4 | 4 | 0.31 | 26.33 | 964 | 5 | 10 | -0.34 | 115.9 | 2551.9 | -5.2 | -7.5 |
| 1mtw | 5 | 4 | 0.75 | 37.35 | 1226 | 6 | 7 | 0.44 | 127.15 | 2874.06 | -10.1 | -8.2 |
| 1ola | 7 | 5 | 0.76 | 24.22 | 852 | 8 | 10 | -1.94 | 101.73 | 1956.49 | -9.5 | -9.4 |
| 1pgp | 5 | 2 | 0 | 0 | 1792 | 4 | 10 | -5.97 | 43.97 | 446.94 | -7.8 | -4.5 |
| 1qbr | 9 | 8 | 3.54 | 100.01 | 980 | 4 | 11 | 6.49 | 209.38 | 9537.35 | -14.4 | -14.9 |

Supplementary Table 1. PDBIDs and Physico-Chemical parameters of 63 Protein-ligand complexes (training set)

| 1qbu | 8 | 7 | 2.41 | 76.27 | 720 | 3 | 8 | 4.99 | 166.76 | 5233.91 | -14 | -12.7 |
|------|---|---|------|-------|------|----|----|--------|--------|----------|-------|-------|
| 1rbp | 7 | 7 | 2.76 | 73.41 | 586 | 1 | 1 | 5.51 | 93.21 | 900.25 | -9.2 | -9.9 |
| 1rgk | 3 | 3 | 0.22 | 10.44 | 311 | 5 | 12 | -1.97 | 71.74 | 807.91 | -5.9 | -5.9 |
| 1rgl | 3 | 2 | 0.19 | 7.07 | 670 | 5 | 13 | -3.96 | 71.83 | 887.63 | -6 | -5.4 |
| 1sre | 4 | 3 | 1.03 | 30.4 | 583 | 1 | 5 | 2.17 | 63.06 | 463.42 | -5.5 | -6.3 |
| 1tlc | 6 | 5 | 1.74 | 45.7 | 997 | 2 | 10 | 0.85 | 130.86 | 3901.61 | -11 | -11.6 |
| 1tng | 5 | 3 | 0 | 9.92 | 1262 | 3 | 1 | 0.81 | 34.33 | 63.25 | -4 | -4.3 |
| 1tnj | 4 | 4 | 0 | 13.35 | 558 | 3 | 1 | 0.47 | 37.9 | 75.12 | -2.7 | -4.1 |
| 1tnk | 4 | 4 | 0 | 24.05 | 554 | 3 | 1 | 0.86 | 42.52 | 111.04 | -2 | -3.2 |
| 2acs | 2 | 1 | 0 | 0 | 1088 | 1 | 7 | -5.25 | 29.2 | 213.61 | -2.8 | -2.5 |
| 2cgr | 5 | 4 | 0.36 | 36.6 | 644 | 2 | 6 | 2.26 | 109.12 | 1771.2 | -9.9 | -7.1 |
| 2cmd | 5 | 1 | 0 | 0 | 506 | 1 | 7 | -5.25 | 29.2 | 213.61 | -6.2 | -4.7 |
| 2msb | 1 | 1 | 0 | 0 | 532 | 15 | 25 | -10.59 | 170.17 | 11954.29 | -3.9 | -4.7 |
| 2wea | 5 | 6 | 0.25 | 25.89 | 1609 | 2 | 9 | 2.88 | 145.38 | 3491.12 | -8.4 | -9.8 |
| 2wec | 5 | 6 | 0.7 | 33.99 | 1285 | 2 | 9 | 2.95 | 142.76 | 4124.83 | -6.8 | -9.9 |
| 2урі | 5 | 2 | 0 | 5.16 | 369 | 0 | 6 | -3.42 | 19.94 | 55.82 | -6.6 | -4.4 |
| 4dfr | 6 | 4 | 1.4 | 34.63 | 1003 | 6 | 13 | -2.19 | 113.97 | 2997.15 | -13.2 | -9.9 |
| 4est | 8 | 7 | 1.19 | 64.67 | 1491 | 3 | 9 | 1.97 | 127.54 | 3880.27 | -9.6 | -9 |
| 4phv | 6 | 6 | 1.48 | 51.27 | 1111 | 5 | 7 | 4.16 | 175.65 | 7243.22 | -12.5 | -11.1 |
| 4ts1 | 5 | 5 | 0 | 3.29 | 1335 | 4 | 4 | -1.7 | 43.49 | 218.04 | -7.6 | -5.7 |
| 5hvp | 9 | 8 | 3.48 | 98.69 | 1246 | 7 | 14 | -0.89 | 165.84 | 7848.16 | -10.5 | -13.1 |
| 5tim | 6 | 0 | 0 | 0 | 1117 | 0 | 4 | -0.26 | 10.52 | 5 | -3.1 | -4.7 |
| 7dfr | 6 | 4 | 1.58 | 28.54 | 861 | 5 | 13 | -2.3 | 105.48 | 2830.36 | -10.1 | -10.8 |
| 8gpb | 6 | 3 | 0 | 6.79 | 1187 | 4 | 12 | -3.13 | 70.59 | 842.57 | -4.9 | -7.1 |
| 1a4k | 6 | 4 | 0.94 | 20.21 | 1201 | 2 | 10 | -0.05 | 104.3 | 2232.54 | -6.8 | -10.9 |

| Supplementary Table 2. PD | IDs and Physico-Chemica | l parameters of 352 Protein-ligand |
|---------------------------|-------------------------|------------------------------------|
| complexes (test set) | | |

| | | | | | | | | | | | BE | BE |
|-------|----|----|------|--------|--------|---------|----|----|------|--------|-------|--------|
| PDBID | PD | PA | PP | PMR | Volume | DD | DA | Р | MR | W | (Exp) | (Pred) |
| 1a30 | 4 | 4 | 1.01 | 28.23 | 1009 | 1645.36 | 5 | 11 | 5.97 | 78.86 | -5.8 | -6 |
| 1aaq | 8 | 8 | 3.35 | 92.94 | 970 | 5942.44 | 8 | 12 | 0.56 | 152.83 | -11.4 | -12.4 |
| 1ae8 | 5 | 4 | 0.62 | 19.44 | 1282 | 2374.41 | 7 | 9 | 0.23 | 112.96 | -9 | -8.9 |
| 1afk | 5 | 3 | 0.76 | 15.08 | 1215 | 1754.48 | 4 | 18 | 5.76 | 91.49 | -9 | -8.3 |
| 1ajv | 7 | 7 | 2.63 | 76.24 | 1155 | 3947.5 | 2 | 8 | 4.95 | 156.4 | -10.6 | -12.3 |
| 1ajx | 7 | 6 | 1.26 | 34.64 | 1148 | 4157.84 | 2 | 7 | 4.74 | 152.83 | -10.9 | -12.8 |
| 1anf | 4 | 3 | 0.48 | 18.49 | 1434 | 962.92 | 8 | 11 | 5.4 | 68.62 | -7.4 | -4.3 |
| 1apt | 6 | 7 | 0.68 | 37.42 | 1399 | 3754.35 | 7 | 10 | 0.53 | 133.79 | -12.8 | -9.4 |
| 1apu | 6 | 7 | 0.67 | 36.87 | 1065 | 3424.13 | 4 | 9 | 2.16 | 131.63 | -10.5 | -9.8 |
| 1apw | 6 | 7 | 0.66 | 39.01 | 1385 | 3564.44 | 5 | 9 | 1.59 | 129.4 | -10.9 | -9.1 |
| 1b38 | 6 | 5 | 1.07 | 25.66 | 573 | 1711.54 | 4 | 18 | 4.16 | 89.35 | -9.4 | -9.6 |
| 1b39 | 6 | 5 | 0.86 | 21.75 | 820 | 1711.54 | 4 | 18 | 4.16 | 89.35 | -9 | -9.3 |
| 1b5g | 6 | 6 | 1.12 | 47.62 | 1267 | 4742.12 | 8 | 10 | 0.19 | 154.28 | -10.9 | -10.1 |
| 1b6j | 8 | 7 | 2.91 | 84.59 | 1037 | 8739.9 | 10 | 15 | 2.19 | 179.62 | -10.8 | -12.2 |
| 1b6k | 7 | 7 | 2.73 | 74.58 | 1161 | 8325.84 | 7 | 12 | 1.03 | 184.56 | -11.9 | -13.2 |
| 1b6l | 6 | 6 | 1.75 | 47.94 | 970 | 4426.75 | 7 | 11 | 1.04 | 144.79 | -11.3 | -11.4 |
| 1b6m | 7 | 7 | 2.33 | 70.25 | 1242 | 5888.35 | 6 | 10 | 2.09 | 164.54 | -11.4 | -12 |
| 1bb0 | 5 | 4 | 0.88 | 24.46 | 846 | 3574.22 | 6 | 11 | 0.05 | 130.56 | -11.4 | -10.4 |
| 1bil | 7 | 7 | 0.85 | 52.13 | 1509 | 6649.58 | 5 | 10 | 4.18 | 178.19 | -12.6 | -10.5 |
| 1bmm | 5 | 5 | 1.12 | 43.81 | 1242 | 3389.8 | 8 | 11 | 1.2 | 131.38 | -9.8 | -8.4 |
| 1bmn | 6 | 5 | 1.09 | 42.58 | 1145 | 3794.8 | 7 | 11 | 0.36 | 139.03 | -11.6 | -9.9 |
| 1bv7 | 9 | 8 | 3.95 | 107.59 | 1048 | 9537.35 | 4 | 11 | 6.49 | 209.38 | -12.6 | -15.1 |
| 1c5c | 5 | 3 | 0.67 | 19.03 | 1156 | 557.61 | 1 | 8 | 2.77 | 74.27 | -9.5 | -7.7 |
| 1c83 | 6 | 3 | 0.94 | 30.33 | 1042 | 435.59 | 2 | 7 | 1.78 | 56.27 | -6.6 | -6.7 |
| 1c84 | 6 | 3 | 0.89 | 28.89 | 867 | 506.96 | 1 | 6 | 1.11 | 61.92 | -6.8 | -7.4 |
| 1c86 | 6 | 3 | 0.98 | 23.01 | 815 | 430.1 | 1 | 7 | 2.36 | 54.71 | -7.1 | -7.7 |
| 1c87 | 5 | 3 | 0.99 | 23.07 | 956 | 430.1 | 1 | 7 | 2.36 | 54.71 | -6.6 | -7 |
| 1c88 | 5 | 3 | 0.96 | 31.17 | 846 | 433.69 | 3 | 7 | 3.81 | 55.55 | -8.9 | -5.5 |
| 1c8k | 3 | 3 | 0.34 | 14.04 | 763 | 1462.84 | 4 | 6 | 1.73 | 104.14 | -6.8 | -7.4 |
| 1cf8 | 7 | 6 | 1.28 | 75.66 | 1271 | 3228.77 | 2 | 9 | 1.78 | 121.44 | -8.2 | -7.3 |
| 1com | 4 | 1 | 0 | 0 | 769 | 365.74 | 1 | 6 | 3.08 | 46.36 | -5.4 | -5.3 |
| 1cqp | 3 | 3 | 0.56 | 16.86 | 813 | 2045.71 | 1 | 5 | 4.2 | 110.84 | -6.6 | -8 |
| 1ctr | 2 | 3 | 1 | 20.67 | 1933 | 1676.31 | 0 | 3 | 4.95 | 107.57 | -5.8 | -7.4 |
| 1d3h | 4 | 4 | 1.02 | 31.83 | 821 | 620.83 | 2 | 4 | 2.16 | 60.86 | -6 | -5.9 |
| 1d3p | 7 | 6 | 1.25 | 55.48 | 951 | 4638.36 | 1 | 6 | 6.21 | 158.31 | -10.1 | -10.7 |
| 1d4p | 5 | 5 | 1.11 | 39.06 | 1310 | 1749.21 | 5 | 5 | 1.73 | 107.29 | -8.6 | -8.1 |

| 1dg5 | 3 | 3 | 0.71 | 13.38 | 1279 | 715.08 | 4 | 7 | 1.26 | 79.76 | -5.5 | -7 |
|------|---|---|------|--------|------|----------|----|----|------|--------|-------|-------|
| 1dhf | 5 | 4 | 1.46 | 27.33 | 1201 | 2886.87 | 5 | 13 | 2.65 | 105.88 | -10.1 | -9.8 |
| 1dog | 2 | 2 | 0 | 0 | 655 | 132.78 | 5 | 5 | 2.97 | 36.9 | -5.5 | -3 |
| 1dwb | 3 | 3 | 0 | 4.49 | 661 | 59.09 | 4 | 2 | 0.33 | 37.85 | -4 | -4 |
| 1eap | 6 | 4 | 0.28 | 29.3 | 960 | 947.42 | 1 | 7 | 0.78 | 81.06 | -8.5 | -7.2 |
| 1elc | 7 | 6 | 0.92 | 46.05 | 1154 | 3722.38 | 6 | 7 | 2.94 | 130.83 | -9.8 | -9 |
| 1epp | 8 | 8 | 1.73 | 73.04 | 1108 | 6161.4 | 8 | 12 | 1.42 | 167.73 | -9.8 | -11 |
| 1etr | 4 | 4 | 0.38 | 15.92 | 1599 | 2866.11 | 7 | 11 | 1.47 | 129.3 | -10.1 | -8.7 |
| 1ets | 7 | 6 | 1.49 | 49.88 | 1452 | 3639.76 | 6 | 9 | 1.92 | 143.1 | -11.2 | -10.9 |
| 1ett | 4 | 4 | 0.37 | 22.21 | 1143 | 1855.31 | 5 | 7 | 1.96 | 117.32 | -8.4 | -7.8 |
| 1fax | 7 | 6 | 1.01 | 45.18 | 996 | 2898.95 | 5 | 7 | 1.35 | 127.26 | -10.1 | -9.9 |
| 1fkg | 3 | 3 | 0.94 | 24.01 | 1060 | 2837.39 | 0 | 5 | 5.29 | 128.47 | -8.8 | -9 |
| 1flr | 6 | 3 | 0.46 | 32.25 | 905 | 930.48 | 1 | 5 | 1.83 | 90.18 | -6.3 | -7.4 |
| 1g2k | 7 | 7 | 2.44 | 75.06 | 1148 | 5122.03 | 3 | 10 | 4.31 | 169.79 | -10.8 | -12.5 |
| 1gno | 7 | 7 | 2.09 | 67.39 | 1076 | 6315.12 | 13 | 14 | 2.35 | 157.59 | -10.6 | -9.9 |
| 1gpy | 5 | 2 | 0 | 0 | 1370 | 325.4 | 4 | 9 | 4.37 | 43.83 | -6.4 | -5 |
| 1hdt | 4 | 4 | 0.36 | 19 | 1442 | 5211.92 | 9 | 12 | 2.08 | 148.14 | -10.7 | -8.4 |
| 1hew | 5 | 3 | 1.18 | 26.76 | 634 | 5289.26 | 11 | 19 | 7.14 | 136.05 | -8.2 | -8.6 |
| 1hih | 7 | 6 | 1.22 | 39.62 | 1043 | 5229.88 | 5 | 10 | 2.31 | 159.26 | -11 | -12.3 |
| 1hii | 6 | 6 | 1.73 | 48.43 | 1035 | 5229.88 | 5 | 10 | 2.31 | 159.26 | -9.9 | -12 |
| 1hiv | 8 | 8 | 3.03 | 86.44 | 1153 | 14528.96 | 6 | 14 | 4.57 | 223.6 | -12.6 | -14 |
| 1hos | 9 | 8 | 3.83 | 107.34 | 1403 | 10442.37 | 4 | 12 | 5.9 | 209.22 | -11.7 | -14.5 |
| 1hpo | 6 | 6 | 1.97 | 53.9 | 933 | 3000.38 | 2 | 7 | 6.84 | 134.12 | -11.8 | -10.8 |
| 1hps | 9 | 8 | 3.33 | 93.6 | 667 | 7648.47 | 4 | 9 | 6 | 181.73 | -12.7 | -14 |
| 1hpv | 7 | 6 | 1.88 | 51.73 | 921 | 2999.86 | 4 | 9 | 3.48 | 133.28 | -12.6 | -11.7 |
| 1hpx | 6 | 6 | 2.05 | 61.83 | 1100 | 7210.7 | 4 | 11 | 2.37 | 181.49 | -12.5 | -12.4 |
| 1hrn | 7 | 6 | 0.96 | 51.17 | 1488 | 4064.21 | 5 | 6 | 3.98 | 142.2 | -10.9 | -9 |
| 1hsg | 7 | 7 | 2.79 | 81.16 | 925 | 6952.26 | 4 | 9 | 2.63 | 173.13 | -12.9 | -12.6 |
| 1hsh | 7 | 7 | 2.67 | 78.93 | 1332 | 6952.26 | 5 | 9 | 1.22 | 172.26 | -11.7 | -12.4 |
| 1hte | 5 | 4 | 1.34 | 35.34 | 1228 | 2336.73 | 4 | 7 | 0.44 | 116.54 | -7.7 | -9.8 |
| 1htg | 8 | 8 | 3.64 | 99.88 | 1261 | 12138.69 | 7 | 12 | 3.51 | 213.39 | -13.2 | -13.9 |
| 1hvh | 7 | 7 | 2.52 | 69.23 | 1249 | 5134.68 | 5 | 8 | 3.07 | 167.87 | -10.8 | -12.9 |
| 1hvj | 7 | 7 | 2.51 | 78.63 | 1237 | 13280.22 | 5 | 13 | 4.71 | 220.5 | -14.3 | -12.8 |
| 1hvl | 8 | 8 | 3.44 | 97.9 | 1510 | 13644.07 | 6 | 14 | 3.69 | 221.89 | -12.3 | -13.9 |
| 1hxb | 7 | 7 | 1.99 | 62.78 | 1148 | 8320.63 | 7 | 11 | 1.68 | 187.34 | -13.5 | -12.6 |
| 1ida | 9 | 8 | 3.03 | 88.49 | 1315 | 9859.17 | 4 | 10 | 5.15 | 207.73 | -11.9 | -14.7 |
| 1mcf | 4 | 4 | 0.56 | 35.23 | 1172 | 10126.48 | 8 | 18 | 3.31 | 177.33 | -7 | -8 |
| 1mcs | 3 | 3 | 0.35 | 21.62 | 1093 | 5066.32 | 6 | 14 | 2.32 | 142.07 | -6.6 | -7.7 |
| 1nnb | 6 | 3 | 0 | 0 | 1029 | 669.06 | 5 | 9 | 4.4 | 60.67 | -5.5 | -6.8 |
| 1nsd | 6 | 3 | 0 | 0 | 1089 | 669.06 | 5 | 9 | 4.4 | 60.67 | -7.2 | -6.8 |
| 1phh | 3 | 2 | 0 | 0 | 610 | 110.1 | 2 | 4 | 0.54 | 34.1 | -4 | -4.5 |
| 1ррс | 5 | 5 | 0.96 | 39.04 | 1013 | 3639.76 | 6 | 9 | 1.92 | 143.1 | -8.4 | -9.5 |

| 1pph | 4 | 3 | 0.38 | 26.81 | 1102 | 1841.37 | 5 | 7 | 1.44 | 116.13 | -8.5 | -7.2 |
|------|----|---|------|--------|------|----------|---|----|------|--------|-------|-------|
| 1qbt | 10 | 9 | 4.82 | 123.22 | 1344 | 14312.69 | 6 | 13 | 7.33 | 237.34 | -14.5 | -16.3 |
| 1tmt | 5 | 5 | 1.4 | 41.06 | 1532 | 2404.24 | 8 | 10 | 3.01 | 107.8 | -8.5 | -7.7 |
| 1tnh | 4 | 3 | 0 | 15.98 | 1156 | 66.49 | 3 | 1 | 0.57 | 32.99 | -4.6 | -3 |
| 1tni | 4 | 3 | 0 | 18.63 | 628 | 156.97 | 3 | 1 | 1.25 | 47.14 | -2.3 | -3.7 |
| 1tnl | 5 | 4 | 0 | 16.4 | 1176 | 97.02 | 3 | 1 | 0.78 | 40.48 | -2.6 | -4.2 |
| 1tph | 4 | 3 | 0.39 | 15.06 | 778 | 72.02 | 1 | 7 | 2.59 | 23.71 | -3.1 | -4 |
| 1ulb | 3 | 2 | 0.43 | 7.88 | 795 | 96.37 | 4 | 6 | 0.9 | 37.34 | -2.8 | -4.5 |
| 1uvs | 3 | 3 | 0.41 | 16.93 | 1350 | 2691.09 | 3 | 9 | 2.71 | 123.55 | -7.4 | -8 |
| 2ifb | 8 | 6 | 1.64 | 51.71 | 826 | 941.19 | 0 | 2 | 4.22 | 75.32 | -7.4 | -9.1 |
| 2upj | 9 | 8 | 3.49 | 96.03 | 958 | 5598.63 | 3 | 8 | 6.48 | 156.88 | -10.1 | -13.1 |
| 2web | 6 | 6 | 0.46 | 40.49 | 583 | 3489.96 | 2 | 9 | 2.95 | 142.74 | -7 | -9.7 |
| 3cla | 2 | 2 | 0 | 0 | 1173 | 702.44 | 3 | 7 | 0.91 | 72.57 | -6 | -5.7 |
| 3ptb | 4 | 4 | 0 | 4.5 | 1231 | 59.09 | 4 | 2 | 0.33 | 37.85 | -6.1 | -4.6 |
| 4hmg | 3 | 2 | 0 | 6.58 | 644 | 750.7 | 6 | 10 | 5.21 | 62.16 | -3.5 | -3.9 |
| 5cna | 3 | 2 | 0 | 3.97 | 592 | 197.84 | 4 | 6 | 2.57 | 40.78 | -2.7 | -3.8 |
| 7gpb | 7 | 3 | 0 | 7.55 | 1435 | 842.57 | 4 | 12 | 3.13 | 70.59 | -7.5 | -7.6 |
| 1a4q | 9 | 6 | 0.38 | 9.07 | 1146 | 1766.51 | 3 | 8 | 0.67 | 100.56 | -11.8 | -12.6 |
| 1ac4 | 2 | 3 | 0 | 0 | 1126 | 38.66 | 0 | 1 | 1.19 | 34.97 | -3.8 | -4.1 |
| 1aco | 8 | 3 | 0 | 0 | 452 | 167.91 | 0 | 6 | 4.45 | 27.72 | -5.2 | -7.3 |
| 1aeb | 2 | 4 | 0 | 0 | 1026 | 14.87 | 0 | 1 | 0.57 | 25.49 | -4.8 | -3.9 |
| 1aee | 2 | 2 | 0 | 0 | 1220 | 29.33 | 2 | 1 | 1.27 | 30.85 | -4 | -3.1 |
| 1ai4 | 2 | 2 | 0 | 0 | 649 | 157.14 | 2 | 4 | 0.61 | 38.48 | -3.5 | -4.1 |
| 1ai5 | 2 | 2 | 0.26 | 5.3 | 1398 | 194.24 | 0 | 5 | 0.11 | 41.81 | -5.1 | -4.6 |
| 1ai6 | 4 | 2 | 0.25 | 11.61 | 1088 | 127.71 | 1 | 3 | 0.32 | 36.82 | -5.5 | -4.6 |
| 1ajn | 3 | 3 | 0.24 | 16.4 | 630 | 207.26 | 0 | 5 | 0.22 | 41.92 | -3.6 | -4.5 |
| 1ajp | 2 | 2 | 0.28 | 5.8 | 642 | 159.64 | 2 | 4 | 0.05 | 39.13 | -3.1 | -4.3 |
| 1apb | 4 | 3 | 0 | 0 | 416 | 122.96 | 4 | 5 | 2.19 | 34.57 | -7.9 | -4.8 |
| 1b9t | 5 | 3 | 0 | 0 | 745 | 846.9 | 7 | 9 | 4.34 | 78.31 | -7 | -7 |
| 1c85 | 5 | 2 | 0.7 | 19.09 | 883 | 283.72 | 1 | 6 | 2.26 | 44.41 | -6.4 | -5.9 |
| 1c9d | 4 | 3 | 0.85 | 22.44 | 713 | 376.31 | 1 | 4 | 1.44 | 61.53 | -8.7 | -6.7 |
| 1cdg | 2 | 1 | 0.5 | 10.55 | 580 | 962.92 | 8 | 11 | 5.4 | 68.62 | -3.3 | -3.9 |
| 1cpi | 7 | 7 | 2.95 | 85.65 | 1005 | 8721.87 | 8 | 15 | 0.56 | 179.5 | -10.1 | -12.3 |
| 1csc | 8 | 7 | 2.27 | 65.96 | 1498 | 9700.65 | 6 | 25 | 5.64 | 165.84 | -9.8 | -11.8 |
| 1ctt | 3 | 3 | 0 | 0 | 670 | 345.76 | 4 | 7 | 2.04 | 52.14 | -6.2 | -5.2 |
| 1cvu | 5 | 4 | 1.51 | 45.25 | 648 | 1517.65 | 0 | 2 | 4.88 | 93.41 | -10.8 | -8 |
| 1cw2 | 5 | 3 | 0.84 | 25.42 | 495 | 371.46 | 1 | 5 | 1.06 | 62.6 | -8.5 | -7.3 |
| 1cx2 | 6 | 4 | 1.29 | 30.27 | 696 | 1105.75 | 2 | 5 | 5.24 | 93.28 | -10.9 | -9.4 |
| 1cx9 | 5 | 3 | 0.82 | 24.65 | 492 | 350.22 | 2 | 4 | 1.05 | 64.66 | -9.3 | -7.2 |
| 1d3t | 6 | 6 | 1.08 | 47.15 | 1309 | 4511.03 | 0 | 6 | 6.55 | 156.03 | -7.8 | -10.4 |
| 1die | 3 | 2 | 0 | 0 | 1115 | 132.78 | 5 | 5 | 2.97 | 36.9 | -2.9 | -3.4 |
| 1elb | 5 | 5 | 0.67 | 24.37 | 1386 | 3056.71 | 5 | 7 | 3.46 | 121.44 | -9.8 | -8.8 |

| 1eld 4 3 0.75 20.37 997 3010.99 3 6 3.44 105.81 -9.1 1ele 4 4 0.98 24.78 903 2161.15 3 6 2.85 90.5 -9.3 1enu 3 3 0.41 19.92 702 159.39 2 5 0.78 43.44 -7 1exq 7 6 0.93 49.11 899 3264.65 7 7 1.43 132.57 -12.5 1f0r 5 4 0.82 29.43 811 1824.27 6 9 0.63 112.14 -8.3 1f0u 6 6 0.96 45.68 854 3264.65 7 7 1.43 132.57 -9.9 1htf 7 7 2.17 63.75 1088 530.51 5 8 2.56 161.91 -11 1mb 4 4 0 0 | -7.9 -7.7 -11.7 -4.2 -9.1 -8.9 -8.2 -9 -12.4 -4.6 -7 -8.5 |
|---|--|
| lele 4 4 0.98 24.78 903 2161.15 3 6 2.85 90.5 -9.3 lent 8 8 2.31 84.17 1437 6808.41 5 13 2.86 174.54 -9.6 lenu 3 3 0.41 19.92 702 159.39 2 5 0.78 43.44 -7 leaq 7 6 0.93 49.11 899 3264.65 7 7 1.43 132.57 -9.9 lff0r 4 4 0.82 29.43 811 1824.27 6 9 0.63 112.14 -8.3 lf0u 6 6 0.96 45.68 854 3264.65 7 7 1.43 132.57 -9.9 lhff 7 7 2.17 63.75 1088 530.51 5 8 2.55 161.91 -11 limb 4 4 0 0 < | -7.7 -11.7 -4.2 -9.1 -8.9 -8.2 -9 -12.4 -4.6 -7 -8.5 |
| lent 8 8 2.31 84.17 1437 6808.41 5 13 2.86 174.54 -9.6 lenu 3 3 0.41 19.92 702 159.39 2 5 0.78 43.44 -77 lezq 7 6 0.93 49.11 899 3264.65 7 7 1.43 132.57 -12.5 1f0r 5 4 0.82 29.43 811 1824.27 6 9 0.63 112.14 -8.3 1f0r 6 0.96 0.56 854 3264.65 7 7 1.43 132.57 -9.91 1mf 7 7 2.17 63.75 1088 530.51 5 8 2.56 161.91 -11 1imb 4 4 0 0 1289 305.72 25 9 4.4 60.67 -6.7 1k1 4 4 0 19.21 55 <t></t> | -11.7 -4.2 -9.1 -8.9 -8.2 -9 -12.4 -4.6 -7 -8.5 |
| lenu 3 3 0.41 19.92 702 159.39 2 5 0.78 43.44 7 lezq 7 6 0.93 49.11 899 3264.65 7 7 1.43 132.57 -1.2.5 lf0r 5 4 0.85 32.77 925 1995.97 3 8 3.59 119.96 -10.6 lf0r 6 0.96 45.68 854 3264.65 7 7 1.43 132.57 -9.9 lhtf 7 7 2.17 63.75 1088 530.51 5 8 2.56 161.91 -111 limb 4 4 0 0 1289 305.72 5 9 4.48 60.67 -6.7 lk1 4 5 0.84 36.83 753 2285.09 6 8 1.23 129.11 -9.6 lk1 4 4 0 19.21 567 < | -4.2 -9.1 -8.9 -8.2 -9 -12.4 -4.6 -7 -7 -8.5 |
| lezq 7 6 0.93 49.11 899 3264.65 7 7 1.43 132.57 -12.5 1f0r 5 4 0.85 32.77 925 1995.97 3 8 3.59 119.96 -10.6 1f0t 4 4 0.82 29.43 811 1824.27 6 9 0.63 112.14 -8.3 1f0u 6 6 0.96 45.68 854 3264.65 7 7 1.43 132.57 -9.9 1htf 7 7 2.17 63.75 1088 530.51 5 8 2.56 161.91 -111 1mb 4 4 0 0 1289 305.72 5 9 4.44 6.67 -6.7 1k11 4 5 0.84 36.83 753 2285.09 6 8 1.23 129.11 -9.6 1k11 4 4 0 19.21 < | -9.1 -8.9 -9 -12.4 -4.6 -7 -8.5 |
| 1f0r 5 4 0.85 32.77 925 1995.97 3 8 3.59 119.96 -10.6 1f0t 4 4 0.82 29.43 811 1824.27 6 9 0.63 112.14 -8.3 1f0u 6 6 0.96 45.68 854 3264.65 7 7 1.43 132.57 -9.9 1htf 7 7 2.17 63.75 1088 5303.51 5 8 2.56 161.91 -11 1mb 4 4 0 0 1289 305.72 5 9 4.48 60.67 -6.7 1k1n 5 5 0.72 31.84 1410 4783.73 6 12 0.21 154.9 -8.8 1mrk 4 4 0 19.21 557 512.62 6 9 1.91 62.81 -6.2 1pbk 8 8 1.49.38 1516 | -8.9 -8.2 -9 -12.4 -4.6 -7 -7 -8.5 |
| 1f0t440.8229.438111824.27690.63112.14-8.31f0u660.9645.688543264.65771.43132.57-9.91htf772.1763.7510885303.51582.56161.91-111imb44001289305.72594.9843.89-5.71ivf6300691669.06594.460.67-6.71k11450.8436.837532285.09681.23129.11-9.61k1n550.7231.8414104783.736120.21154.9-8.81mrk440019.2155751.26691.9162.81-6.21pdz5100106655.82063.4219.94-51pk88149.3815163329.683102134.17-10.41pso882.2480.2859932.475115.98201.44-11.91snc52015.727191062.891133.3871.2-9.22ak3530.3515.61324842.574123.1370.59-5.32er79 <td>-8.2 -9 -12.4 -4.6 -7 -8.5</td> | -8.2 -9 -12.4 -4.6 -7 -8.5 |
| 1f0u 6 6 0.96 45.68 854 3264.65 7 7 1.43 132.57 -9.9 1htf 7 7 2.17 63.75 1088 5303.51 5 8 2.56 161.91 -11 1imb 4 4 0 0 1289 305.72 5 9 4.98 43.89 -5.7 1ivf 6 3 0 0 691 669.06 5 9 4.4 60.67 -6.7 1k11 4 5 0.84 36.83 753 2285.09 6 8 1.23 129.11 -9.6 1k1n 5 5 0.72 31.84 1410 4783.73 6 12 0.21 154.9 -8.8 1mrk 4 4 0 19.21 567 512.62 6 9 1.91 62.81 -6.2 1pdz 5 1 0 0 1066 55.82 0 6 3.42 19.94 -5 1pdz 8 | -9 -12.4 -4.6 -7 -8.5 |
| 1htf772.17 63.75 1088 5303.51 582.56 161.91 -11 1imb44001289 305.72 59 4.98 43.89 -5.7 1ivf6300691 669.06 59 4.4 60.67 -6.7 1k11450.84 36.83 753 2285.09 68 1.23 129.11 -9.6 1k1n550.72 31.84 1410 4783.73 612 0.21 154.9 -8.8 1mrk44019.21567 512.62 69 1.91 62.81 -6.2 1pdz51001066 55.82 06 3.42 19.94 -55 1pk881 49.38 1516 3329.68 3102 134.17 -10.4 1pso88 2.24 80.2 859 932.47 511 5.98 201.44 -11.9 1snc52015.72 719 1062.89 113 3.38 71.2 -9.2 2ak353 0.35 15.6 1324 842.57 412 3.13 70.59 -5.3 2pk320051.46 37.83 -7.1 2ak353 0.55 115.2 417 106.68 33 <t< td=""><td>-12.4 -4.6 -7 -8.5</td></t<> | -12.4 -4.6 -7 -8.5 |
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| livf 6 3 0 0 691 669.06 5 9 4.4 60.67 -6.7 lk1l 4 5 0.84 36.83 753 2285.09 6 8 1.23 129.11 -9.6 lk1n 5 5 0.72 31.84 1410 4783.73 6 12 0.21 154.9 -8.8 1mrk 4 4 0 19.21 567 512.62 6 9 1.91 62.81 -6.2 1pdz 5 1 0 0 1066 55.82 0 6 3.42 19.94 -5 1pbk 8 8 1.49.38 1516 3329.68 3 10 2 134.17 -10.4 1pso 8 8 2.24 80.2 859 9323.47 5 11 5.98 201.44 -11.9 1snc 5 2 0 15.72 719 1062.89 | -7 -8.5 |
| 1k1l 4 5 0.84 36.83 753 2285.09 6 8 1.23 129.11 -9.6 1k1n 5 5 0.72 31.84 1410 4783.73 6 12 0.21 154.9 -8.8 1mrk 4 4 0 19.21 567 512.62 6 9 1.91 62.81 -6.2 1pdz 5 1 0 0 1066 55.82 0 6 3.42 19.94 -5 1ppk 8 8 1 49.38 1516 3329.68 3 10 2 134.17 -10.4 1pso 8 8 2.24 80.2 859 9323.47 5 11 5.98 201.44 -11.9 1snc 5 2 0 15.72 719 1062.89 1 13 3.38 71.2 -9.2 2ak3 5 3 0.35 15.6 1324 842.57 4 12 3.13 70.59 -5.3 2er7 9 | -8.5 |
| Ikin 5 5 0.72 31.84 1410 4783.73 6 12 0.21 154.9 -8.8 1mrk 4 4 0 19.21 567 512.62 6 9 1.91 62.81 -6.2 1pdz 5 1 0 0 1066 55.82 0 6 3.42 19.94 -5 1ppk 8 8 1 49.38 1516 3329.68 3 10 2 134.17 -10.4 1pso 8 8 2.84 94.61 1216 9453.34 7 14 0.13 179.62 -14.1 1rne 8 8 2.24 80.2 859 9323.47 5 11 5.98 201.44 -11.9 1snc 5 2 0 15.72 719 1062.89 1 13 3.38 71.2 -9.2 2ak3 5 3 0.35 15.6 1324< | |
| 1mrk44019.21567512.62691.9162.81-6.21pdz5100106655.82063.4219.94-51ppk88149.3815163329.683102134.17-10.41pso882.8494.6112169453.347140.13179.62-14.11rne882.2480.28599323.475115.98201.44-11.91snc52015.727191062.891133.3871.2-9.22ak3530.3515.61324842.574123.1370.59-5.32er79114.13127.04188532981.5110240.78287.86-12.32mcp3200835119.54051.4637.83-7.12pk4320.5511.52417106.68331.4631.23-5.92r04882.7688.548841805.75054.3397.32-8.52sim6200814669.06594.460.67-8.83er513135.33162.81142750659.0517293.232.92-12.44er2< | -10.3 |
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| 1ppk88149.3815163329.683102134.17-10.41pso882.8494.6112169453.347140.13179.62-14.11rne882.2480.28599323.475115.98201.44-11.91snc52015.727191062.891133.3871.2-9.22ak3530.3515.61324842.574123.1370.59-5.32er79114.13127.04188532981.5110240.78287.86-12.32mcp3200835119.54051.4637.83-7.12pk4320.5511.52417106.68331.4631.23-5.92r04882.7688.548841805.75054.3397.32-8.52sim6200814669.06594.460.67-8.83er513135.33162.81142750659.0517293.2329.2-12.44er2881.9473.4621279453.347140.13179.62-115enl6200133153.49063.4219.94-4.1< | -4.4 |
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| 2mcp3200835119.54051.4637.83-7.12pk4320.5511.52417106.68331.4631.23-5.92r04882.7688.548841805.75054.3397.32-8.52sim6200814669.06594.460.67-8.83er513135.33162.81142750659.0517293.2329.2-12.44er2881.9473.4621279453.347140.13179.62-115enl6200107698.26174.0625.95-5.26enl6200557772.444123.1370.59-3.26tim540.4815.9292885.39262.8228.02-4.4 | -12.8 |
| 2pk4320.5511.52417106.68331.4631.23-5.92r04882.7688.548841805.75054.3397.32-8.52sim6200814669.06594.460.67-8.83er513135.33162.81142750659.0517293.2329.2-12.44er2881.9473.4621279453.347140.13179.62-115enl6200107698.26174.0625.95-5.26enl6200557772.444123.1370.59-3.26tim540.4815.9292885.39262.8228.02-4.4 | -4.9 |
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| 3er5 13 13 5.33 162.81 1427 50659.05 17 29 3.2 329.2 -12.4 4er2 8 8 1.94 73.46 2127 9453.34 7 14 0.13 179.62 -11 5enl 6 2 0 0 1076 98.26 1 7 4.06 25.95 -5.2 6enl 6 2 0 0 1331 53.49 0 6 3.42 19.94 -4.1 6rnt 3 3 0 0 557 772.44 4 12 3.13 70.59 -3.2 6tim 5 4 0.48 15.92 928 85.39 2 6 2.82 28.02 -4.4 | -6.7 |
| 4er2881.9473.4621279453.347140.13179.62-115enl6200107698.26174.0625.95-5.26enl6200133153.49063.4219.94-4.16rnt3300557772.444123.1370.59-3.26tim540.4815.9292885.39262.8228.02-4.4 | -11.5 |
| 5enl 6 2 0 0 1076 98.26 1 7 4.06 25.95 -5.2 6enl 6 2 0 0 1331 53.49 0 6 3.42 19.94 -4.1 6rnt 3 3 0 0 557 772.44 4 12 3.13 70.59 -3.2 6tim 5 4 0.48 15.92 928 85.39 2 6 2.82 28.02 -4.4 | -11.4 |
| 6enl 6 2 0 0 1331 53.49 0 6 3.42 19.94 -4.1 6rnt 3 3 0 0 557 772.44 4 12 3.13 70.59 -3.2 6tim 5 4 0.48 15.92 928 85.39 2 6 2.82 28.02 -4.4 | -5.3 |
| 6rnt 3 3 0 0 557 772.44 4 12 3.13 70.59 -3.2 6tim 5 4 0.48 15.92 928 85.39 2 6 2.82 28.02 -4.4 | -5.1 |
| 6tim 5 4 0.48 15.92 928 85.39 2 6 2.82 28.02 -4.4 | -6.3 |
| | -4.9 |
| 9hvp 9 8 3.83 107.25 1089 11116.46 5 11 5.7 206.94 -11.4 | -14.2 |
| 1E2J 3 2 0 9.62 674 411.95 3 7 1.09 55.51 -7.2 | -4.5 |
| 1G6N 5 4 1.02 24.27 984 695.92 3 11 1.45 68.77 -10.3 | -7.9 |
| 1HXD 6 5 1.31 38.79 553 444.81 2 5 0.54 58.96 -9.9 | -7.8 |
| 1K1J 4 5 0.76 33.35 1325 3366.96 5 9 1.69 139.79 -10.4 | -8.9 |
| 2EWN 9 7 1.62 48.29 596 4216.07 6 15 0.74 129.81 -14 | -12.9 |
| 2IKG 4 3 0.87 21.42 1095 1133.01 1 5 2.3 87.22 -8.5 | -8 |
| 2IKH 3 0.82 20.95 598 420.73 0 9 0.3 53.06 -7.5 | -6.3 |
| 2IKJ 4 3 2.11 46.45 1134 1296.24 1 8 1.31 86.22 -10 | -8.6 |
| 1ECM 5 2 0 0 538 334.32 1 6 3.05 45.49 -7.6 | -6.2 |
| 10GS 5 4 1.08 39.53 1331 2884.28 5 9 1.85 117.78 -8.7 | |

| 1AVN | 1 | 2 | 0 | 0 | 1710 | 53.22 | 3 | 3 | 0.09 | 31.35 | -5.3 | -2.4 |
|------|---|---|------|-------|------|---------|---|----|------|--------|-------|-------|
| 1JYS | 2 | 3 | 0 | 0 | 1016 | 65.66 | 3 | 5 | 0.06 | 36.1 | -4.8 | -4 |
| 1P1Q | 4 | 3 | 0 | 0 | 576 | 205.67 | 4 | 6 | 2.41 | 38.29 | -6.7 | -5 |
| 1PB9 | 4 | 3 | 0 | 0 | 416 | 32.94 | 3 | 4 | 1.62 | 22.07 | -4.9 | -4.3 |
| 1UTP | 4 | 4 | 0 | 22.22 | 1022 | 156.97 | 3 | 1 | 1.25 | 47.14 | -2 | -3.4 |
| 1Y1M | 4 | 2 | 0 | 0 | 1119 | 73.62 | 3 | 3 | 1.71 | 29.09 | -2.5 | -4.1 |
| 1GIC | 2 | 2 | 0 | 0 | 573 | 197.84 | 4 | 6 | 2.57 | 40.78 | -5.5 | -3.6 |
| 1FDQ | 5 | 3 | 0.16 | 7.72 | 1091 | 1916.07 | 0 | 2 | 5.21 | 102.46 | -10.1 | -8.5 |
| 1KZN | 6 | 6 | 1.78 | 52.29 | 1165 | 8087.28 | 5 | 13 | 4.88 | 176.46 | -9.8 | -11.6 |
| 1HWI | 5 | 4 | 0.6 | 13.48 | 584 | 2087.67 | 2 | 5 | 3.21 | 112.29 | -9 | -10.2 |
| 1HWL | 6 | 5 | 0.71 | 15.91 | 1845 | 2594.65 | 2 | 9 | 2.07 | 119.38 | -12.3 | -11.1 |
| 1RD4 | 5 | 5 | 2.97 | 65.07 | 1177 | 2710.55 | 0 | 8 | 4.88 | 132.53 | -10.7 | -11.9 |
| 214Q | 5 | 5 | 1.13 | 49.26 | 1006 | 2763.06 | 4 | 8 | 3.83 | 128.85 | -9.3 | -8.1 |
| 2IKO | 4 | 5 | 0.93 | 42.38 | 1389 | 1443.25 | 5 | 5 | 3.38 | 100.58 | -7.5 | -5.9 |
| 2IKU | 5 | 5 | 1.14 | 45.88 | 1244 | 2094.54 | 4 | 6 | 4.02 | 128.24 | -9.8 | -8.5 |
| 21L2 | 6 | 6 | 1.16 | 54.84 | 1134 | 5566.93 | 4 | 11 | 5.45 | 172.48 | -9.8 | -10.2 |
| 1A69 | 5 | 3 | 0.36 | 12.45 | 724 | 528.84 | 5 | 9 | 2.03 | 60.92 | -7.2 | -6.4 |
| 1BCU | 3 | 4 | 0.18 | 20.37 | 1382 | 272.85 | 4 | 3 | 2.55 | 68.07 | -4.5 | -4.1 |
| 1F5K | 3 | 3 | 0 | 10.59 | 906 | 59.09 | 4 | 2 | 0.33 | 37.85 | -5.1 | -3.3 |
| 1FCX | 5 | 5 | 2.91 | 68.63 | 661 | 1822.62 | 1 | 3 | 4.4 | 113.14 | -9.8 | -10.3 |
| 1J17 | 5 | 6 | 0.99 | 52.16 | 1208 | 3035.02 | 0 | 7 | 4.72 | 133.52 | -7.1 | -8.4 |
| 1JQD | 5 | 5 | 1.03 | 37.73 | 828 | 1375.71 | 7 | 11 | 3.49 | 89.28 | -7 | -6.7 |
| 1NC1 | 4 | 4 | 1.23 | 29.33 | 668 | 567.62 | 4 | 7 | 0 | 76.25 | -8.4 | -7.9 |
| 1PR5 | 4 | 3 | 0.33 | 11.42 | 1084 | 496.3 | 5 | 8 | 1.38 | 64.95 | -5.3 | -6 |
| 1ZS0 | 6 | 6 | 2.07 | 59.46 | 815 | 1153.5 | 2 | 7 | 3.25 | 97.93 | -8.4 | -9.4 |
| 2B1V | 2 | 2 | 0.51 | 9.34 | 556 | 561.7 | 2 | 3 | 2.8 | 72.8 | -7.8 | -6 |
| 2BRB | 4 | 5 | 1.02 | 32.35 | 879 | 1020.03 | 2 | 5 | 3.96 | 98.25 | -6.6 | -8 |
| 2GSS | 4 | 3 | 0.88 | 31.32 | 792 | 564.31 | 0 | 4 | 2.27 | 70.73 | -6.7 | -6.4 |
| 3GSS | 2 | 2 | 0 | 7.62 | 945 | 564.31 | 0 | 4 | 2.27 | 70.73 | -7.9 | -5.1 |
| 1J16 | 4 | 4 | 0.28 | 10.23 | 1051 | 59.09 | 4 | 2 | 0.33 | 37.85 | -5.2 | -4.8 |
| 1KV5 | 4 | 2 | 0 | 5.19 | 717 | 55.82 | 0 | 6 | 3.42 | 19.94 | -5.8 | -3.6 |
| 1XPO | 5 | 4 | 0 | 0 | 894 | 680.64 | 6 | 9 | 3.3 | 67.39 | -6 | -6.9 |
| 1YV5 | 6 | 3 | 0 | 0 | 1079 | 290.27 | 1 | 8 | 2.9 | 50.85 | -8.8 | -7.3 |
| 2FLB | 6 | 6 | 0.54 | 39.62 | 1068 | 1023.04 | 7 | 7 | 0.46 | 88.25 | -7.8 | -6.5 |
| 2FQW | 4 | 4 | 0.84 | 20.22 | 629 | 510.18 | 4 | 9 | 2.1 | 60.85 | -8.9 | -6.6 |
| 2FQY | 5 | 4 | 1 | 23.46 | 540 | 493.96 | 5 | 9 | 1.98 | 62.74 | -8.8 | -7.3 |
| 1bma | 6 | 5 | 0.99 | 41.24 | 1025 | 3874.24 | 3 | 7 | 4.52 | 135.94 | -6.3 | -9.5 |
| 1d3d | 7 | 6 | 1.09 | 50.55 | 1220 | 4118.82 | 1 | 4 | 7.7 | 161.55 | -12.4 | -10.7 |
| 1hdc | 6 | 5 | 1.54 | 58.54 | 1409 | 4958.57 | 0 | 7 | 4.16 | 148.56 | -8.2 | -9.9 |
| 1nis | 7 | 3 | 0 | 0 | 433 | 207.51 | 1 | 8 | 4.12 | 31.44 | -4.1 | -6.8 |
| 1nsc | 6 | 3 | 0 | 0 | 1617 | 750.7 | 6 | 10 | 5.21 | 62.16 | -4.1 | -6.3 |
| 2abh | 8 | 2 | 0 | 0 | 141 | 5.68 | 1 | 4 | 0.05 | 11.2 | -8.9 | -6.8 |

| 7tim540.4615.4875181.51272.7625.011LOQ530.4113.641134709.053113.6660.121TRD540.4615.2657778.89272.7625.011U88420.6514.2820192230.8491.71102.862AB2431.3825.516611674.55044.85112.211FPU662.967.6411041859.44274.24111.912G2H761.8757.68631702.57264.54115.421G3B440.4334.341003453.12662.9259.641G36550.7530.827952476.98572.87129.461GHZ450.4135.251457494.47660.4372.761GI1550.4135.281252482.78650.7373.941G16550.6627.260.76483.79650.7373.94 | -7.4 | -4.8 |
|--|-------|-------|
| 1LOQ 5 3 0.41 13.64 1134 709.05 3 11 3.66 60.12 1TRD 5 4 0.46 15.26 577 78.89 2 7 2.76 25.01 1U88 4 2 0.65 14.28 2019 2230.8 4 9 1.71 102.86 2AB2 4 3 1.38 25.51 661 1674.55 0 4 4.85 112.21 1FPU 6 6 2.9 67.64 1104 1859.44 2 7 4.24 111.91 2G2H 7 6 1.87 57.6 863 1702.57 2 6 4.54 115.42 1G3B 4 4 0.43 34.34 1003 453.12 6 6 2.92 59.64 1G36 5 5 0.75 30.82 795 2476.98 5 7 2.87 129.46 1GHZ 4 5 0.41 35.25 1457 494.47 6 6 | -5 | |
| 1TRD 5 4 0.46 15.26 577 78.89 2 7 2.76 25.01 1U88 4 2 0.65 14.28 2019 2230.8 4 9 1.71 102.86 2AB2 4 3 1.38 25.51 661 1674.55 0 4 4.85 112.21 1FPU 6 6 2.9 67.64 1104 1859.44 2 7 4.24 111.91 2G2H 7 6 1.87 57.6 863 1702.57 2 6 4.54 115.42 1G3B 4 4 0.43 34.34 1003 453.12 6 6 2.92 59.64 1G36 5 5 0.75 30.82 795 2476.98 5 7 2.87 129.46 1GHZ 4 5 0.41 35.25 1457 494.47 6 6 0.43 72.76 1GI1 5 5 0.41 35.28 1252 482.78 6 5 | 5 | -6.3 |
| 1U88 4 2 0.65 14.28 2019 2230.8 4 9 1.71 102.86 2AB2 4 3 1.38 25.51 661 1674.55 0 4 4.85 112.21 1FPU 6 6 2.9 67.64 1104 1859.44 2 7 4.24 111.91 2G2H 7 6 1.87 57.6 863 1702.57 2 6 4.54 115.42 1G3B 4 4 0.43 34.34 1003 453.12 6 6 2.92 59.64 1G36 5 5 0.75 30.82 795 2476.98 5 7 2.87 129.46 1GHZ 4 5 0.41 35.25 1457 494.47 6 6 0.43 72.76 1GI1 5 5 0.41 35.28 1252 482.78 6 5 0.73 73.94 1G16 5 0.66 27.26 0.76 482.78 6 5 0.73 | -7.4 | -4.9 |
| 2AB2 4 3 1.38 25.51 661 1674.55 0 4 4.85 112.21 1FPU 6 6 2.9 67.64 1104 1859.44 2 7 4.24 111.91 2G2H 7 6 1.87 57.6 863 1702.57 2 6 4.54 115.42 1G3B 4 4 0.43 34.34 1003 453.12 6 6 2.92 59.64 1G36 5 5 0.75 30.82 795 2476.98 5 7 2.87 129.46 1GHZ 4 5 0.41 35.25 1457 494.47 6 6 0.43 72.76 1GI1 5 5 0.41 35.28 1252 482.78 6 5 0.73 73.94 1G16 5 0.66 27.26 0.76 482.78 6 5 0.73 73.94 | -7.8 | -7.8 |
| 1FPU 6 6 2.9 67.64 1104 1859.44 2 7 4.24 111.91 2G2H 7 6 1.87 57.6 863 1702.57 2 6 4.54 115.42 1G3B 4 4 0.43 34.34 1003 453.12 6 6 2.92 59.64 1G36 5 5 0.75 30.82 795 2476.98 5 7 2.87 129.46 1GHZ 4 5 0.41 35.25 1457 494.47 6 6 0.43 72.76 1GI1 5 5 0.41 35.28 1252 482.78 6 5 0.73 73.94 1G16 5 5 0.66 27.26 0.76 482.78 6 5 0.73 73.94 | -11.8 | -10.1 |
| 2G2H 7 6 1.87 57.6 863 1702.57 2 6 4.54 115.42 1G3B 4 4 0.43 34.34 1003 453.12 6 6 2.92 59.64 1G36 5 5 0.75 30.82 795 2476.98 5 7 2.87 129.46 1GHZ 4 5 0.41 35.25 1457 494.47 6 6 0.43 72.76 1GI1 5 5 0.41 35.28 1252 482.78 6 5 0.73 73.94 1GI6 5 5 0.66 27.26 0.76 4.82.78 6 5 0.73 73.94 | -10.1 | -11 |
| 1G3B 4 4 0.43 34.34 1003 453.12 6 6 2.92 59.64 1G36 5 5 0.75 30.82 795 2476.98 5 7 2.87 129.46 1GHZ 4 5 0.41 35.25 1457 494.47 6 6 0.43 72.76 1GI1 5 5 0.41 35.28 1252 482.78 6 5 0.73 73.94 1GI6 5 5 0.66 27.26 0.76 4.82.78 6 5 0.73 73.94 | -8.2 | -10.3 |
| 1G36 5 5 0.75 30.82 795 2476.98 5 7 2.87 129.46 1GHZ 4 5 0.41 35.25 1457 494.47 6 6 0.43 72.76 1GHZ 5 5 0.41 35.25 1457 494.47 6 6 0.43 72.76 1GHZ 5 5 0.41 35.28 1252 482.78 6 5 0.73 73.94 1GHE 5 5 0.66 27.26 0.76 482.78 6 5 0.73 73.94 | -6.4 | -3.1 |
| 1GHZ 4 5 0.41 35.25 1457 494.47 6 6 0.43 72.76 1GI1 5 5 0.41 35.28 1252 482.78 6 5 0.73 73.94 1GI6 5 5 0.66 27.26 0.76 482.78 6 5 0.73 73.94 | -8.7 | -9.3 |
| 1GI1 5 5 0.41 35.28 1252 482.78 6 5 0.73 73.94 1GI6 5 5 0.66 27.26 076 482.78 6 5 0.73 73.94 | -6.5 | -4.3 |
| | -7.4 | -5 |
| 13.94 5/ 10,00 5/ 10,00 5/ 10,00 5 13.94 13.94 | -7.4 | -5.5 |
| 1K1I 4 4 0.53 30.22 1386 2876.65 5 9 0.92 134.01 | -9 | -8.3 |
| 1CE5 4 4 0 10.6 658 59.09 4 2 0.33 37.85 | -6.5 | -4.3 |
| 1C5P 3 3 0 10.59 614 59.09 4 2 0.33 37.85 | -6.4 | -3.4 |
| 1NHB 2 2 0.26 5.42 315 49.08 0 0 2.25 35.82 | -5.8 | -4.1 |
| 182L 1 1 0.3 6.31 375 50.67 0 1 2.43 36.21 | -5.5 | -3.3 |
| 184L 1 2 0.24 4.89 536 105.18 0 0 2.89 44.98 | -6.5 | -3.8 |
| 2QWC 5 3 0 0 817 669.06 5 9 4.4 60.67 | -4.9 | -6.3 |
| 2QWD 5 3 0 0 1122 670.98 6 9 4.43 62.64 | -6.6 | -6.1 |
| 1DI8 5 5 1.73 34.41 554 747.97 2 6 3.1 84.03 | -8.3 | -9.7 |
| 1E1V 5 5 1.38 24.45 1159 491.64 3 6 1.89 68.17 | -6.8 | -8.7 |
| 1E1X 5 5 1.37 26.83 891 506.81 4 7 2 68.38 | -8.1 | -8.4 |
| 1GIH 4 5 1.89 37.45 1167 943.36 2 6 2.78 85.4 | -9.7 | -9 |
| 1NVR 4 5 0.84 24.74 1258 2025.94 2 7 4.12 134.71 | -11.2 | -10.2 |
| 1A50 5 3 0.8 27.07 654 495.83 1 5 1.08 61.51 | -8.6 | -6.8 |
| 1ABE 5 3 0 0 541 95.16 4 5 2.58 29.98 | -8.9 | -5.1 |
| 1ADD 4 4 0.53 12.64 621 496.3 5 8 1.38 64.95 | -9.2 | -6.8 |
| 1ADL 4 3 0.7 14.36 1139 1517.65 0 2 4.88 93.41 | -9.2 | -8.1 |
| 1BIR 4 3 0 0 609 887.63 5 13 3.96 71.83 | -7.2 | -6.6 |
| 1CLA 1 0 0 1293 702.44 3 7 0.91 72.57 | -7.2 | -4.7 |
| 1CSC 3 1 0 0 418 84.39 3 5 3.2 23.86 | -2.2 | -3.1 |
| 1D3Q 6 5 1.3 51.36 1438 4443.38 0 4 7.11 158.85 | -7.4 | -10.2 |
| 1FBC 6 2 0 0 943 527.66 2 11 4.83 50.54 | -8.5 | -6.6 |
| 1FBF 5 2 0 0 1072 527.66 2 11 4.83 50.54 | -8.2 | -5.9 |
| 1FEL 8 7 3.05 82.59 760 2291.34 2 3 6.86 122.86 | -9.2 | -11.3 |
| 1FKF 3 3 1.13 31.99 1432 11326.58 3 13 4.64 212.59 | -12.8 | -11.2 |
| 1HBP 7 7 2.78 73.82 641 900.25 1 1 5.51 93.21 | -9.8 | -9.9 |
| 1HNL 4 3 0.91 22.38 552 852.96 5 9 5.59 64.72 | -5.1 | -5.7 |
| 1LDM 8 6 2.93 77.97 1237 5384.32 8 21 4.28 136.31 | -7.4 | -11.1 |
| 1LGR 5 4 0.34 9.39 1320 842.57 4 12 3.13 70.59 | -4.2 | -7.3 |
| 1MFA 2 1 0 0 855 2509.89 8 14 4.86 103.24 | -5.8 | -5.5 |

| 1MFE | 2 | 2 | 0.8 | 21.87 | 1038 | 2345.6 | 9 | 14 | 5.52 | 98.45 | -7.2 | -4.8 |
|------|---|---|------|--------|------|---------|----|----|------|--------|-------|-------|
| 1RNT | 4 | 3 | 0 | 0 | 611 | 887.63 | 5 | 13 | 3.96 | 71.83 | -7.1 | -6.6 |
| 1RUS | 4 | 1 | 0 | 0 | 1173 | 110.28 | 1 | 7 | 4.06 | 25.95 | -4.2 | -3.8 |
| 1XIG | 3 | 2 | 0 | 0 | 633 | 115.19 | 5 | 5 | 2.95 | 32.19 | -4.5 | -3.4 |
| 1XLI | 2 | 2 | 0 | 0 | 1545 | 143.46 | 5 | 5 | 2.5 | 42.49 | -2 | -3 |
| 2CSC | 4 | 2 | 0 | 0 | 332 | 81.39 | 2 | 5 | 2.43 | 23.27 | -4.6 | -4.3 |
| 2DBL | 5 | 4 | 1.21 | 45.82 | 1418 | 2414.44 | 0 | 5 | 3.68 | 110.02 | -11.9 | -7.9 |
| 2PHH | 3 | 2 | 0 | 0 | 753 | 86.77 | 1 | 3 | 0.24 | 32.44 | -6.3 | -4.5 |
| 2QWF | 6 | 4 | 0 | 0 | 978 | 1067.67 | 6 | 10 | 4.89 | 81.63 | -7.7 | -8 |
| 2RNT | 5 | 6 | 0.85 | 40.46 | 735 | 4924.06 | 10 | 22 | 5.1 | 134 | -5.2 | -7.7 |
| 2XIM | 3 | 2 | 0.62 | 13.1 | 468 | 115.19 | 5 | 5 | 2.95 | 32.19 | -3.1 | -3.6 |
| 3PGM | 5 | 2 | 0 | 0 | 668 | 110.28 | 1 | 7 | 4.06 | 25.95 | -4.4 | -4.9 |
| 4CLA | 2 | 2 | 0 | 0 | 1324 | 702.44 | 3 | 7 | 0.91 | 72.57 | -7.5 | -5.6 |
| 4TIM | 4 | 2 | 0 | 0 | 979 | 98.26 | 1 | 7 | 4.06 | 25.95 | -2.9 | -4.1 |
| 5YAS | 2 | 2 | 0 | 0 | 549 | 111.58 | 2 | 2 | 0.79 | 19.28 | -4.4 | -2.9 |
| 8RSA | 4 | 2 | 0 | 0 | 404 | 674.21 | 3 | 8 | 0.95 | 67.1 | -5.9 | -7 |
| 8XIA | 3 | 1 | 0 | 0 | 607 | 111.81 | 4 | 5 | 2.74 | 31.17 | -4 | -3.3 |
| 9LDT | 4 | 0 | 0 | 0 | 714 | 21.71 | 2 | 4 | 2.78 | 14.2 | -6.5 | -3 |
| 9RUB | 4 | 2 | 0 | 4.59 | 1360 | 490.47 | 2 | 11 | 5.03 | 46.88 | -6.4 | -4.4 |
| 2AYR | 5 | 5 | 3.08 | 66.88 | 887 | 3574.83 | 1 | 6 | 7.35 | 146.5 | -12.7 | -12 |
| 2R6W | 6 | 6 | 3.36 | 71.46 | 788 | 3292.56 | 2 | 5 | 6.32 | 140.8 | -12.8 | -12.8 |
| 2R6Y | 6 | 6 | 3.09 | 68.47 | 709 | 2668.67 | 2 | 5 | 5.69 | 131.63 | -12.9 | -12.2 |
| 1FKH | 3 | 3 | 0.89 | 22.99 | 1189 | 2927.53 | 0 | 5 | 5.5 | 129.65 | -11.1 | -8.9 |
| 1FM9 | 5 | 4 | 1.87 | 48.27 | 833 | 5707.22 | 1 | 7 | 5.28 | 154.76 | -12.3 | -11.1 |
| 1KSN | 6 | 6 | 1.02 | 41.11 | 1116 | 2974.33 | 5 | 8 | 0.6 | 123.64 | -12.8 | -9.6 |
| 1PRO | 7 | 6 | 1.59 | 42.11 | 965 | 4971.3 | 3 | 9 | 4.94 | 162.59 | -15.4 | -13.1 |
| 2SIM | 6 | 3 | 0 | 0 | 1491 | 669.06 | 5 | 9 | 4.4 | 60.67 | -4.7 | -6.6 |
| 1SBG | 6 | 6 | 1.41 | 42.26 | 1080 | 4502.18 | 4 | 8 | 4.97 | 151.87 | -10.6 | -11.2 |
| 1XKA | 6 | 5 | 0.58 | 33.89 | 1116 | 2119.02 | 5 | 6 | 0.94 | 111.81 | -9.4 | -8.4 |
| 1FKI | 0 | 0 | 0 | 0 | 593 | 2482.34 | 0 | 7 | 3.96 | 116.23 | -9.5 | -6.4 |
| 1J4R | 4 | 4 | 2.25 | 55.79 | 1255 | 6871.84 | 0 | 8 | 6.54 | 165.78 | -10.5 | -10.8 |
| 1G2L | 7 | 5 | 0.9 | 41.29 | 1438 | 4281.02 | 5 | 10 | 2.58 | 150.16 | -9.9 | -10.5 |
| 1XKB | 5 | 5 | 0.58 | 33.7 | 870 | 2119.02 | 5 | 6 | 0.94 | 111.81 | -9.4 | -7.9 |
| 1acj | 3 | 3 | 1.03 | 21.36 | 804 | 239.19 | 2 | 2 | 2.7 | 62.8 | -10.1 | -6.2 |
| 1f3e | 3 | 3 | 0.41 | 20.14 | 971 | 193.08 | 4 | 6 | 0.36 | 47.85 | -9.2 | -4 |
| 2gbp | 5 | 3 | 0.65 | 13.75 | 411 | 159.27 | 5 | 6 | 3.22 | 35.99 | -10.1 | -5.4 |
| 1acm | 6 | 3 | 0 | 0 | 1233 | 340.63 | 2 | 9 | 6.8 | 40.86 | -10.3 | -5.7 |
| 1L83 | 0 | 1 | 0 | 0 | 336 | 18.03 | 0 | 0 | 1.69 | 26.44 | -5.3 | -2.1 |
| 1ABF | 4 | 3 | 0 | 0 | 456 | 122.96 | 4 | 5 | 2.19 | 34.57 | -7.4 | -4.8 |
| 1bv9 | 9 | 8 | 3.52 | 100.31 | 901 | 9537.35 | 4 | 11 | 6.49 | 209.38 | -12.2 | -14.8 |
| 2FVD | 5 | 5 | 1.6 | 31.7 | 1126 | 2067.46 | 3 | 9 | 2.49 | 105.89 | -11.6 | -10.4 |
| 3LFS | 5 | 4 | 1.9 | 35.15 | 995 | 804.13 | 2 | 4 | 4.62 | 90.08 | -7.6 | -9.6 |

| 2xhw 7 6 1.7.2 3.4.7.3 6.7.3 1741.41 2 9 3.7.1 112.21 1.3.6 -1.3.6 lwb 6 3 0 0 1834 367.01 2 8 0.3.8 53.4 4.7.4 star 9 10 3.66 12.35 1742 125.89 10 3.3.8 53.44 4.7.3 lbby 6 3 0 0 1216 796.71 2 6 0.3 89.74 -0.5 4.44 4.7.5 lbbw 9 9 4.3 15.83 1073 4327.5 2 5 0.04 6.6.61 -1.7.7 lbm 9 9 2.2.8 75.05 1308 49.1 11 2.4.5 10.8.8 4.6.1 -1.7.7 lbm 9 7 1.4 54.12 178.8 2.1 4.28 18.63 -1.4.1 lbm 7 5 3.1 10 | | | | | | | | | | | | | |
|---|------|---|----|------|--------|------|----------|----|----|-------|--------|-------|-------|
| 1vb 6 3 0 1834 367.01 2 8 0.38 53.4 4.1 7.43 Bers 7 3 0.0 0 1216 766.71 2 6 0.33 214.84 4.9.5 1by 6 3 0.0 0 1387 1169.88 3 7 0.43 89.74 1.5.5 1bw 9 9 4.3 115.82 1037 11431.69 6 1.3 75.37 2.73 5 0.44 64.61 1.7.7 6.41 1pm 9 7 0.18 157.47 74.71 5 1.11 1.6.49 209.34 -0.35 1.01 1.3.5 1.03 1.0.5 1.01 1.0.5 1.03 1.0.5 1.01 1.0.5 1.0.3 1.0.3 1.0.3 1.2.5 1.03.6 1.0.3 1.0.3 1.0.3 1.0.3 1.0.3 1.0.3 1.0.3 1.0.3 1.0.3 1.0.3 1.0.3 1.0.3 | 2XMY | 7 | 6 | 1.72 | 34.73 | 673 | 1741.41 | 2 | 9 | 3.71 | 112.21 | -13.6 | -12.6 |
| 3er3 9 10 3.86 112.35 1742 12658.9 10 14 3.33 17.48 -9.7 -1.3 1bby 6 3 0 0 1216 79.71 2 6 0.13 21.82 -4.4 -9.51 1bw 6 3 0.0 1387 1169.8 3 7 0.43 89.74 0.5 9.41 1bw 9 9 4.33 115.82 1037 14312.69 6 13 7.33 237.34 -1.01 -1.51 1pm 9 9 9.28 8.70.5 1130 495.37 2 15 15.4 7.47.17 15 111 2.75 16.88 65 10.33 2PHH 9 7 1.4 54.12 17.84 27.75 11.1 2.75 16.86 6.5 10.3 2PHH 9 7 1.4 50.3 11.3 13.84.32 8.12 14.53 | 1ivb | 6 | 3 | 0 | 0 | 1834 | 367.01 | 2 | 8 | 0.38 | 53.4 | -4.1 | -7.4 |
| 1bbs 7 3 0 0 1216 796.71 2 6 0.13 77. 0.43 89.74 -5. 1bbw 9 9 4.3. 115.82 1037 1431.269 6 10.3 7.33 237.34 -10.10 -15.33 1ghb 5 5 0 16.15 1103 495.37 2 5 0.04 64.61 -1.7 -6.64 1pm 9 9 2.8 8.05 1.574 774.17 5 1.574 774.17 5 1.574 774.17 5 1.57 4.44 -0.5 -1.03 2PHH 9 7 1.4 54.12 1.788 271.88 21 4.55 10.31 4.46 -0.5 -1.03 4SHH 6 4 0 0.93 13.02 54.642 3.8 21 4.52 13.8 7.12 4SH 7 5 1.5 3.58 1123 21 | 3er3 | 9 | 10 | 3.66 | 112.35 | 1742 | 12658.9 | 10 | 14 | 3.33 | 214.84 | -9.7 | -13 |
| 1bbv 6 3 0 0 1387 1169.88 3 7 0.43 89.73,44 -10.1 -10.13 lbwb 9 43 115.8 1103 14312.69 6 13 7.33 237.34 -10.1 -10.13 lpmb 9 8 3.91 107.43 662 953.73.5 4 11 6.40 20.35 -10.1 11.17 lbwa 9 7 1.4 54.12 175.4 77.7 1.5 16.64 10.3 -1.6.1 2PHH 9 7 1.4 54.12 175.4 77.7 1.9 4.55 10.33 4.4.6 9.33 4MDH 7 6 2.39 76.3 3130 541642 78 12.1 4.53 1.4.5 4.4.6 4MDH 7 6 2.39 76.3 1332 541642 73 12.1 4.53 4.57 4.1.7 51011 513.5 1 | 1b9s | 7 | 3 | 0 | 0 | 1216 | 796.71 | 2 | 6 | 0.13 | 75.29 | -4.4 | -9.5 |
| 1bwb 9 9 4.3 115.82 107 1431.269 6 13 7.33 227.34 -1.01 -1.5.3 1ghb 9 9 2.2.8 87.05 1308 5669.08 3 12 2.65 153.54 -7.9 -1.1.7 1bwa 9 9 9 2.2.8 87.05 137.4 774.7.7 5 11 2.7.5 166.68 -6.5 -10.8 2PHH 9 7 1.4 57.1 157.4 7747.17 5 11 2.7.5 168.68 -6.5 -10.8 2PHH 9 7.5 3.2.1 87.03 1328 297.18 7 9 3.5.8 74.75 -4.1 -3.8 4MDH 7 5 3.2.1 80.85 1131 238.42 8 13 3.3.8 2.1 44.2 16.5 6.1 -1.7.7 1DKT 7 5 3.13 91.23 91.04 3 10 | 1b9v | 6 | 3 | 0 | 0 | 1387 | 1169.88 | 3 | 7 | 0.43 | 89.74 | -5 | -9.4 |
| lghb 55 55 0 16.15 1103 495.37 2 55 0.04 64.61 1.7.7 1.6.47 lpmm 9 8 3.91 107.43 6692 93.35 4 11 65.49 209.38 -10.33 -15.11 leed 8 8 1.83 75.1 1574 7747.17 5 11 2.75 168.68 -6.65 -10.33 2PHH 9 7 1.4.4 54.12 1788 2971.86 7 11 2.75 168.68 -6.5 -10.33 4MDH 7 5 3.21 80.85 1134 538432 8 21 44.58 133.35 4.21 44.58 133.35 4.10 10.7 101K 7 6 2.93 100.45 11.87 21.89.56 11 8.15 11.28 10.29 10.7 14.4 101K 7 6 2.94 4.93 10.4 16.40 | 1bwb | 9 | 9 | 4.3 | 115.82 | 1037 | 14312.69 | 6 | 13 | 7.33 | 237.34 | -10.1 | -15.3 |
| 1ppm992.2887.0513085669.083122.65153.44-7.99-11.71bwa983.91107.436929537.354116.492038.3-7.51158.68-6.55-10.82PHH971.454.121778777.175.112.75158.68-6.55-10.82PHH971.454.121778277.177.5182.1513.83-7.45-4.1-3.834SUI64.41.000.0948959.35.9.93.5874.75-4.1-3.834MDH762.3376.0313025416.4282144.25138.65-5.7-10.75ER2762.9376.031302514.621382144.25138.65-5.7-10.75ER2751.1844.6611104460.0882144.25138.65-5.7-10.73UKM75551.1844.6611104460.0881010.14143.06-7.841.171MAG75555.246.155446.249213.42138.8-11.514.81AF2371.259.829.89.934.3131515.829.84.315.11AF666 <t< td=""><td>1ghb</td><td>5</td><td>5</td><td>0</td><td>16.15</td><td>1103</td><td>495.37</td><td>2</td><td>5</td><td>0.04</td><td>64.61</td><td>-1.7</td><td>-6.4</td></t<> | 1ghb | 5 | 5 | 0 | 16.15 | 1103 | 495.37 | 2 | 5 | 0.04 | 64.61 | -1.7 | -6.4 |
| 1bwa983.94107.436929537.3541116.49209.38-10.3-15.11eed87.87.5.1774.751142.75168.68-6.5-10.82PH971.454.1217882971.867194.55108.134.69.34MUH6400948959.3593.5874.754.1-84MDH753.2180.8511145384.328214.52136.51-4.4-10.72DB762.9376.031120541.6428214.52138.65-7.7-10.75ER2897.5312.970.03173314.02374.42116.5-6.1-10.93LFN762.4849.496731534.833.355.36112.9-7.5-12.71A46551.1844.661110446.088100.44143.06-7.8-9.111A5661.2752.421515544.6249213.42138.58-11.5-11.81A5661.427.952.42615544.6249213.42138.69-11.5-11.81A5661.427.07.74.06.054182.5152.8414.5-11.81 | 1ppm | 9 | 9 | 2.28 | 87.05 | 1308 | 5669.08 | 3 | 12 | 2.65 | 153.54 | -7.9 | -11.7 |
| 1eed881.8375.11574774.7451112.75168.68.66.5.10.832PHH971.454.1217882971.867194.55108.13-4.6-9.34SLI640.09489593593.5874.754.418.84MDH762.3.2180.8511345384.328214.28136.31-4.410.72LDB762.9376.0313025416.4218214.28136.5114.434.4810.75ER2892.5310.45118.721.89.5611180.29254.65.9.912.71V1K762.4849.496731534.83355.36112.9.7.712.41A66551.1844.66110446.0081010.14143.06.7.8.9.11A66789.29553.61.1844.60110450.8881010.41143.06.7.8.9.11A677762.4849.99673544.62492.13.433.551.6811.9.1.241A66782.998.524654546.2492.13.4313.551.28.4.2.1.241A673331.22.5284.2 | 1bwa | 9 | 8 | 3.91 | 107.43 | 692 | 9537.35 | 4 | 11 | 6.49 | 209.38 | -10.3 | -15.1 |
| PHH 9 7 1.4 54.12 1788 2971.86 7 19 4.55 108.13 4.66 -9.3 4SU 6 4 0 0 948 558.93 55 9 3.58 74.75 4.41 7.8 4MDH 7 6 2.33 7.03 1302 541.642 8 21 4.28 136.55 5.7 10.7 5ER2 8 9 2.93 10.045 1187 2189.56 11 18 0.02 254.65 1.0.9 11.7 1V1K 7 6 2.28 10.05 11.87 218.97 301.02 3 7 4.42 11.65 6.7 1.0.9 3U1K 7 5.5 1.15 35.89 12.93 301.02 3 7 4.42 13.88 11.65 6.7 1.0.9 3U1K 7 2.5 3.5 3.5 3.5 3.5 3.5 3.5 3.5 | 1eed | 8 | 8 | 1.83 | 75.1 | 1574 | 7747.17 | 5 | 11 | 2.75 | 168.68 | -6.5 | -10.8 |
| 4SLI6400948959.3593.5874.754.4.14MDH753.2180.851134538.428214.28136.31-4.410.72LDB762.9376.031302538.628214.28136.51-4.410.72LDR7592.9810.0411872118.95611180.29254.65-90.12.71V1K751.1535.8912393014.02374.42116.5-6.61-10.93LFN762.4849.496731534.83355.36111.9-7.5-12.41A46551.1844.661110460.088100.14143.06-7.80.121A56655.24544.2492.13.4215.84.130.1311.511.61A57375546.2492.13.4213.811.511.811.511.811.511 | 2PHH | 9 | 7 | 1.4 | 54.12 | 1788 | 2971.86 | 7 | 19 | 4.55 | 108.13 | -4.6 | -9.3 |
| MMDH753.2180.851134538.428214.28136.314.44-10.7210B762.9376.0310025416.428214.52138.65-5.7-10.75ER2892.98100.45118721189.5611180.02254.65-0.9-12.71V1K751.1535.5812399014.02374.42116.5-6.1-0.193LFN762.4849.496.63153.48.33.355.36112.9-7.5-12.41A66555.46.2159.42100122.51158.04-7.8-9.11A67661.2752.421510598.3110122.51158.04-13.8-91A683200778406.05482.5152.84.12-4.91A683200778406.0544.513.8514.5-4.91A683200778406.0544.513.8514.5-4.91A696881011512709.54152.584.15-7.9-7.51B67688101512.84165.66145.26.614.5-7.51B7677.57.5 | 4SLI | 6 | 4 | 0 | 0 | 948 | 959.3 | 5 | 9 | 3.58 | 74.75 | -4.1 | -8 |
| 10B762.9376.0313025416.4282.14.52138.65.5.7.1.075ER2892.9810.045118721189.5011180.29254.65.9.9.1.2.71V1K751.535.81233010.02374.42116.5.6.61.1.0.73LFN755.1.834.661101446.088100.14143.06.7.8.1.2.41A46555515.21510598.3110122.5.115.8.4.1.3.8.1.1.51A4661.0252.421510598.3110102.1.213.4.213.8.5.1.1.5.1.1.81A4675.2.421510598.3110101.2.113.4.213.8.5.1.1.5.1.1.81A4675.2.421510598.31101.01.3.415.2.1.1.5.1.1.8.1.1.5.1.1.81A473778.61.2.21.5.28.4.1.5.2.8.2.1.5.1 | 4MDH | 7 | 5 | 3.21 | 80.85 | 1134 | 5384.32 | 8 | 21 | 4.28 | 136.31 | -4.4 | -10.7 |
| SER2892.98100.45118721189.5611180.29254.65912.71V1K751.5535.8912393014.02374.42116.5-6.1-10.93LFN762.4849.49673153.83355.36112.97.7.5-12.41A46551.1844.6611104460.088100.12133.04143.06-7.7.8-9.11A56661.1.844.661110544.02910.1213.24133.85-11.5-11.81A50982.9.58.5.4615544.62492.13.2.813.18-11.5-11.81A62982.9.58.5.4615544.62492.52.5.82.9.8-4.2-4.91B84433.00.07.78406.054.45.52.5.82.9.8-4.2-4.91B87640.993.3.81162709.454.415.514.5-4.6-7.71B8777.51.5.814.114.95.514.514.514.514.5-1.61B844.57.51.9.11.9.11.9.114.115.814.514.514.514.51B846.71.5.81.9.11.9.11.9.11.9.114.115.514.514.5 | 2LDB | 7 | 6 | 2.93 | 76.03 | 1302 | 5416.42 | 8 | 21 | 4.52 | 138.65 | -5.7 | -10.7 |
| 1V1K751.535.8912393014.02374.42116.5-6.1-1.093LFN762.4849.496731534.83355.36112.97.55-12.41A46551.1844.6611104460.0881010.14143.067.78-9.11A56661.1252.4215105983.110122.51158.04-1.18-1.181A673200778406.05482.5152.284.42-4.91BAP430.0044995.16482.5152.28-4.2-4.91BAP430.0044995.16482.5152.88-7.9-10.51BBT640.9933.4811627094.964165.66145.2-6.6-9.71BW771.5457.871191551.9841351.66145.2-6.6-9.71BW661.1852.2412961915.238191.1155.99-7.1-7.71BW772.544.1291915.238191.4145.99-7.1-7.71BW661.1852.2412931738.373146.1824.14-1.18-6.41FW <td>5ER2</td> <td>8</td> <td>9</td> <td>2.98</td> <td>100.45</td> <td>1187</td> <td>21189.56</td> <td>11</td> <td>18</td> <td>0.29</td> <td>254.65</td> <td>-9</td> <td>-12.7</td> | 5ER2 | 8 | 9 | 2.98 | 100.45 | 1187 | 21189.56 | 11 | 18 | 0.29 | 254.65 | -9 | -12.7 |
| 31FN762.4849.49673153.48355.5611297.754.1241A46551.1844.6611104460.088100.14143.067.789.911A5G661.2752.4215105983.1101222.51158.04-13.89.911AD8982.9985.246155446.2492.113.253.2524.427.491AP732.007.78406.054.482.5152.284.93-1.181BAP430044995.164.752.582.594.42-7.99-1.051BB76640.993.3481162709.564.41381.524.64-7.99-1.051BK7677.71.5457.871.19551.294.41.531.12-7.99-1.051BK077.71.5457.871.19551.294.41.131.524.64-1.18-1.181BK077.71.5457.871.19551.291.41.531.1455.9-7.531.641BK1641.093.884.933.31.05041.2648.27-7.63-1.641BK23472.557.51.53.54.81.91.4159.99-7.14< | 1V1K | 7 | 5 | 1.5 | 35.89 | 1239 | 3014.02 | 3 | 7 | 4.42 | 116.5 | -6.1 | -10.9 |
| 1A46551.1844.6611104460.088100.14143.06-7.89.911A5G661.2752.421510598.110122.51158.04-13.8-91ADB982.2585.24615544.249213.42138.58-11.5-11.81AF233120.0044995.16452.5152.282.9.3-4.2-4.21BAP430.0044995.16452.552.582.9.3-0.3-4.21BBZ882.91100.38137629741.51724.441258.47-7.9-10.51BBF640.9933.4811622974.5541654.412-6.64.52-6-9.71BK0777715.5417.915.1516.1315.1516.1315.1516.1315.16-11.81BK142730.46.841016142.9131.5161.3314.6-11.81BK1640.9933.481015119.53.81.15161.3314.614.51BK2541.05.2.4129.6131.5516.415.216.1311.615.615.516.1311.61DK2430.01.2.3119.515.2 <td>3LFN</td> <td>7</td> <td>6</td> <td>2.48</td> <td>49.49</td> <td>673</td> <td>1534.83</td> <td>3</td> <td>5</td> <td>5.36</td> <td>112.9</td> <td>-7.5</td> <td>-12.4</td> | 3LFN | 7 | 6 | 2.48 | 49.49 | 673 | 1534.83 | 3 | 5 | 5.36 | 112.9 | -7.5 | -12.4 |
| 1A5G661.2752.4215105983.110122.51158.04.13.8.13.81ADB982.9585.246155446.249213.42138.58.11.5.11.81AF2320.00.0778406.054482.5152.28.4.2.4.91BAP430.00.044995.16452.5829.98.9.3.4.51BBZ882.91100.38137629741.51725.4.41258.47.7.9.10.51BHF640.933.4811627094.9641656.66145.2.6.6.9.71BW77.71.5157.871191551.29.8410.5161.33.13.6.11.81BW707.71.5157.871191551.29.841.05161.33.13.6.11.81BW707.71.511.141.121.151.14.11.14.11.1< | 1A46 | 5 | 5 | 1.18 | 44.66 | 1110 | 4460.08 | 8 | 10 | 0.14 | 143.06 | -7.8 | -9.1 |
| 1ADB9882.9985.246f155446.249213.42138.58-11.5-11.81AF23200778406.054482.5152.284.42-4.91BAP430044995.164452.5829.980.9.3-4.51BBZ882.91100.38137629741.517254.41258.477.9-10.51BHF640.9933.4811627094.964165.66145.26.6-9.71BK0771.5457.871191551.29.84131.52161.33-13.6-11.81BZM6.77.71.5457.871191551.29.84131.52161.33-13.6-11.81BZM7.77.33.15141131.52161.33-13.6-11.8-11.81BZM7.77.31.541191551.291.413.51.151.15-11.81CBX7.47.47.41.251.41.42.91.41.531.151.61.151FKB7.37.33.11.61.41.531.151.61.41.121.181.141.41.91.141.121.141.141.41.91.141.121.141.141.41.141.141.14 | 1A5G | 6 | 6 | 1.27 | 52.42 | 1510 | 5983.1 | 10 | 12 | 2.51 | 158.04 | -13.8 | -9 |
| 1AF232.00.00.778406.0548.2.51.52.28.4.2.4.31BAP43.00.00.449.95.16.4.5.2.58.2.93.2.93.4.51BBZ882.91100.38.1376.29741.51.7.2.5.4.41.258.47.7.9.1.051BHF640.99.3.3.48.1162.709.496.4.16.5.66.145.2.6.6.9.71BXO77.1.54.57.87.1191.551.298.4.1.3.1.52.161.33.1.3.6.1.1.81BXD77.1.54.57.87.1.191.551.298.4.1.3.1.52.1.6.3.1.6 | 1ADB | 9 | 8 | 2.95 | 85.24 | 615 | 5446.24 | 9 | 21 | 3.42 | 138.58 | -11.5 | -11.8 |
| IBAP430044995.1644552.582.9.88.9.9.3.4.4.5IBBZ882.9.1100.38137629741.5172.54.4.1258.477.7.9.1.0.5IBHF640.0933.4811627094.9641.65.6.6145.2.6.6.9.7IBXO771.5457.8711915512.9841.05.1.5.6.6.14.5.6.6.1.18IBXO771.5457.8711915512.98.41.0.1.15.5.7.9.6.7.1.1.16IBXO7771.5457.8711915512.98.0.4.1.15.1.15.1.16.1.18IBXO7771.5457.871.9111512.98.0.4.1.15.1.16.1.18IBXO6461.884.93331.05.0.4.1.16.1.18.1.16.1.18IEXW872.6366.481.2.13105.29.0.1.2.1.16.1.16.1.17 | 1AF2 | 3 | 2 | 0 | 0 | 778 | 406.05 | 4 | 8 | 2.51 | 52.28 | -4.2 | -4.9 |
| IBBZ88882.91100.38137629741.517254.41258.47-7.99-1.05IBHF66440.0933.4811627094.964165.66145.26.66.145.2.6.6IBXO777.71.5457.8711915512.9841331.52161.33.13.66.13.63.13.65IBZM22330.046.841016142.913371.7152.59.4.82.6.751CBX544470.98.88493331.05041.2648.27.7.87.6.751CBX544470.08.88493331.05041.2648.27.7.87.6.751CBX544470.08.88493331.05041.2648.27.7.87.6.751CBX666661.1852.241208131.5310811412.6314.1614.2314.1714.17.7.14.7. | 1BAP | 4 | 3 | 0 | 0 | 449 | 95.16 | 4 | 5 | 2.58 | 29.98 | -9.3 | -4.5 |
| 1BHF66440.0933.4811627094.96441665.666145.21.6-6-9.71BXO771.5457.8711915512.9844131.52161.33-1.3.6-1.1.81BZM2330.46.841016142.9133771.7.152.590.8.2-5.51CBX5440.08.88493331.050.0441.2.648.27-8.7-6.41E96661.1.852.2412961915.238.8191.4.195.99-7.1-7.71EXW8772.6.366.4812431065.92102.26.4.384.14-5.3-10.11FKB3331.1226.9112031733.8.73.3146.1.8245.14-13.2-11.81FKB333.1.1226.9112031733.8.73.414.519.86.2.4-13.8-13.11FKB333.1.1226.911733.8.73.414.519.826.9933.97-10.1-13.21FKB441.0.025.2970.8149.34.526.9933.97-11.8-6.41FKB3333.1.21.1.4144.7263.63.9.4-1.1.8-6.41FKD4430.8.120.2140.8140.814 | 1BBZ | 8 | 8 | 2.91 | 100.38 | 1376 | 29741.51 | 7 | 25 | 4.41 | 258.47 | -7.9 | -10.5 |
| 1BXO71.5457.8711915512.98441311.52161.33-1.3.6-1.1.81BZM230.46.8.41016142.91371.7.152.59-8.2-5.51CBX554.40.08.8.8493331.0504.41.2.648.27-8.7-6.41E966.61.1.852.2412961915.238191.4.195.99-7.1-7.71EXW872.6.366.4812431065.92026.4.384.14-5.3-10.11FKB3331.1.22.6.9112031738.3731466.18245.14-13.2-12.11FKM441.0.125.2977.08493.96591.9.862.74-11.8-6.41FKD441.0.025.5652.7135.54452.6.933.97-1.0-4.41NC4430.65.5652.7135.54452.6.933.97-1.0-4.41NC440.021.54144.5144.81.52.6.93.3.871.2.7.3.7.51NNC3331.0.1140.89470.9.293.78.7.2.7.5.7.51TET872.1983.92114956163.26131.1.3 <td< td=""><td>1BHF</td><td>6</td><td>4</td><td>0.99</td><td>33.48</td><td>1162</td><td>7094.96</td><td>4</td><td>16</td><td>5.66</td><td>145.2</td><td>-6</td><td>-9.7</td></td<> | 1BHF | 6 | 4 | 0.99 | 33.48 | 1162 | 7094.96 | 4 | 16 | 5.66 | 145.2 | -6 | -9.7 |
| IBZM230.46.841016142.91371.7152.59.8.2.8.5ICBX5408.88493331.05041.2648.27.8.7.6.4IE9661.61.1852.2412961915.238191.4.195.99.7.1.7.7IEW872.6366.4812431065.92026.4.384.14.5.3.10.1IFKB331.1226.91120317338.373146.1.8245.14.1.3.2.1.12IFMO441.0125.29708493.96591.9.862.74.1.1.8.6.4IFKI430.05.56527135.54452.6933.97.1.1.9.4.4INC440.021.5414151148.7263.6493.46.1.0.9.5.5INNC330.8120.2705140.89470.9293.78.1.2.3.7.6INNC440.015.2110071069.81133.3.871.2.7.3.5.4ITET872.1983.92114956163.26263713.03317.25.4.5.2.5ITET872.1983.921153354.56131.7.4127.05.1.0.3 </td <td>1BXO</td> <td>7</td> <td>7</td> <td>1.54</td> <td>57.87</td> <td>1191</td> <td>5512.98</td> <td>4</td> <td>13</td> <td>1.52</td> <td>161.33</td> <td>-13.6</td> <td>-11.8</td> | 1BXO | 7 | 7 | 1.54 | 57.87 | 1191 | 5512.98 | 4 | 13 | 1.52 | 161.33 | -13.6 | -11.8 |
| 1CBX5408.88493331.05041.2648.27 -8.7 -6.4 1E96661.1852.2412961915.238191.4195.99 -7.1 -7.7 1EXW872.6366.4812431065.92026.4384.14 -5.3 -10.1 1FKB331.122.691120317338.373146.18245.14 -13.2 -12.5 1FMO441.0125.29708493.9659 1.98 62.74 -11.8 -6.4 1HSL4305.56527135.54452.69 33.97 -100 -6.4 1HSL44021.5414151148.726 3.64 93.46 -10.9 -5.8 1MNC44021.5414151148.726 3.64 93.46 -10.9 -5.8 1MNC44021.5414151148.726 3.64 93.46 -10.9 -7.6 1STA44015.211007169.88 11 13 3.38 71.2 -7.3 -5.56 1TLP440.418.3616283544.5613 1.74 127.9 -10.3 -9.4 1TMN440.6512.531536349.6053< | 1BZM | 2 | 3 | 0.4 | 6.84 | 1016 | 142.91 | 3 | 7 | 1.71 | 52.59 | -8.2 | -5 |
| 1E9666661.1.1852.2412961915.2388191.4.195.99-7.1.7.71EXW88772.6.366.4812431065.920266.4384.14.5.3.1.0.11FKB33331.1.226.91120317338.3731466.18245.14.1.3.2.1.2.31FMO444.41.0.025.297.08493.96.5.5.91.9.8.6.6.9.1.1.8.6.1.81HSL44330.05.5.65.571.35.54.4.4.52.6.9.3.3.97.1.0.9.6.4.31NC444.40.021.5414151148.7.2.2.63.6.4.93.46.1.0.9.5.61MNC33.30.8.120.27.051400.89.4.4.0.9.93.78.1.2.3.7.51MNC44.20.0.115.2110071069.88.1.1.1.3.3.3.8.7.1.2.7.5.5.51TLP4.47.29.3.915.2110071069.88.1.1.1.3.3.1.3.317.25.4.5.3.5.51TLP4.87.29.3.815.2166.3.2.2.6.3.713.0.3317.25.4.5.3.5.51TLP4.40.40.6.515.533496.5.6.6.1.1.1.7.910.4.1.6.9.5.61TMN4.44.40.3.934.39 <td>1CBX</td> <td>5</td> <td>4</td> <td>0</td> <td>8.88</td> <td>493</td> <td>331.05</td> <td>0</td> <td>4</td> <td>1.26</td> <td>48.27</td> <td>-8.7</td> <td>-6.4</td> | 1CBX | 5 | 4 | 0 | 8.88 | 493 | 331.05 | 0 | 4 | 1.26 | 48.27 | -8.7 | -6.4 |
| IEXW872.6366.4812431065.92026.4384.14-5.3-10.1IFKB331.1226.91120317338.373146.18245.14-13.2-12IFMO441.0125.29708493.96591.9862.74-11.8-6.41HSL430.05.56527135.544452.6933.97-100-41NC440.021.5414151148.7263.6493.46-10.9-5.81MNC330.8120.27051400.894470.9293.78-10.9-5.81MNC440.8120.27051400.894470.9293.78-10.9-5.81MNC330.8120.27051400.89470.9293.78-10.9-5.81MNC440.8115.2110071069.881133.3871.2-7.3-5.41TET872.1983.92114956163.26263713.03317.25-8.5-2.51TLP440.6512.5315363496.05380.7128.88-10.2-10.41YY440.3934.398641991.526111.79100.41-7.5< | 1E96 | 6 | 6 | 1.18 | 52.24 | 1296 | 1915.23 | 8 | 19 | 1.41 | 95.99 | -7.1 | -7 |
| 1FKB3331.1226.91120317338.3731466.18245.14-13.2-121FMO441.0125.29708493.96591.9862.74-11.8-6.41HSL4305.56527135.54452.6933.97-10.0-41INC44021.5414151148.7263.6493.46-10.9-5.81MNC3330.8120.27051400.89470.9293.78-12.3-7.61STA42015.2110071069.881133.3871.2-7.3-5.41TET872.1983.92114956163.26263713.03317.25-8.5-2.51TLP440.418.3616283544.56131.149127.05-10.3-9.41TMN440.6512.5315363496.05380.7128.88-10.2-10.41YY440.3934.318611991.526111.79100.41-6.9-5.51ZZZ440.3934.318011991.526111.79100.41-7.5-5.72CTC43208.32570750.76105.2162.16-3.7 <td>1EXW</td> <td>8</td> <td>7</td> <td>2.63</td> <td>66.48</td> <td>1243</td> <td>1065.92</td> <td>0</td> <td>2</td> <td>6.43</td> <td>84.14</td> <td>-5.3</td> <td>-10.1</td> | 1EXW | 8 | 7 | 2.63 | 66.48 | 1243 | 1065.92 | 0 | 2 | 6.43 | 84.14 | -5.3 | -10.1 |
| 1FMO441.0125.29708493.96591.9862.74-11.8-6.41HSL43005.56527135.54452.6933.97-10-41INC440021.5414151148.7263.6493.46-10.9-5.81MNC330.8120.27051400.89470.9293.78-12.3-7.61STA42015.2110071069.881133.3871.2-7.3-5.41TET872.1983.92114956163.26263713.03317.25-8.5-21TLP440.418.3616283544.56131.74127.05-10.3-9.41TMN440.6512.5315363496.05380.7128.88-10.2-10.41YY440.6934.318641991.526111.79100.41-6.9-5.72CTC430.00711173.67130.6641.16-5.3-5.92QWB3208.32570750.76105.2162.16-3.7-3.8 | 1FKB | 3 | 3 | 1.12 | 26.91 | 1203 | 17338.37 | 3 | 14 | 6.18 | 245.14 | -13.2 | -12 |
| 1HSL43005.56527135.54452.6933.97-10-41INC440021.5414151148.7263.6493.46-10.9-5.81MNC330.8120.27051400.89470.9293.78-12.3-7.61STA420015.2110071069.881133.3871.2-7.3-5.41TET872.1983.92114956163.26263713.03317.25-8.5-2.11TLP440.418.3616283544.56131.74127.05-10.3-9.41TMN440.6512.5315363496.05380.7128.88-10.2-10.41YY440.3934.398641991.526111.79100.41-6.9-5.61ZZZ440.3934.318011991.526111.79100.41-7-5.72CTC4300711173.67130.6641.16-5.3-5.92QWB3208.32570750.76105.2162.16-3.7-3.8 | 1FMO | 4 | 4 | 1.01 | 25.29 | 708 | 493.96 | 5 | 9 | 1.98 | 62.74 | -11.8 | -6.4 |
| 1INC44021.5414151148.7263.6493.46-10.9-5.81MNC330.8120.27051400.89470.9293.78-12.3-7.61STA42015.2110071069.881133.3871.2-7.3-5.41TET872.1983.92114956163.26263713.03317.25-8.5-21TLP440.418.3616283544.56131.74127.05-10.3-9.41TMN440.6512.5315363496.05380.7128.88-10.2-10.41YYY440.3934.318011991.526111.79100.41-6.9-5.61ZZZ440.3934.318011991.526111.79100.41-7.5-5.72CTC4300711173.67130.6641.16-5.3-5.92QWB3208.32570750.76105.2162.16-3.7-3.8 | 1HSL | 4 | 3 | 0 | 5.56 | 527 | 135.54 | 4 | 5 | 2.69 | 33.97 | -10 | -4 |
| 1MNC330.8120.27051400.89470.9293.78-12.3-7.61STA42015.2110071069.881133.3871.2-7.3-5.41TET872.1983.92114956163.26263713.03317.25-8.5-221TLP440.418.3616283544.56131.74127.05-10.3-9.41TMN440.6512.5315363496.05380.7128.88-10.2-10.41YYY440.3934.398641991.526111.79100.41-6.9-5.61ZZZ440.3934.318011991.526111.79100.41-7-5.72CTC4300711173.67130.6641.16-5.3-5.92QWB3208.32570750.76105.2162.16-3.7-3.8 | 1INC | 4 | 4 | 0 | 21.54 | 1415 | 1148.7 | 2 | 6 | 3.64 | 93.46 | -10.9 | -5.8 |
| 1STA42015.2110071069.881133.3871.2.7.3.5.41TET872.1983.92114956163.26263713.03317.25.8.5.21TLP440.418.3616283544.56131.74127.05.10.3.9.41TMN440.6512.5315363496.05380.7128.88.10.2.10.41YYY440.3934.398641991.526111.79100.41.6.9.5.61ZZZ440.3934.318011991.526111.79100.41.77.5.72CTC430.0711173.67130.6641.16.5.3.5.92QWB3208.32570750.76105.2162.16.3.7.3.8 | 1MNC | 3 | 3 | 0.81 | 20.2 | 705 | 1400.89 | 4 | 7 | 0.92 | 93.78 | -12.3 | -7.6 |
| 1TET872.1983.92114956163.26263713.03317.258.521TLP440.418.3616283544.56131.74127.05-10.39.41TMN440.6512.5315363496.05380.7128.88-10.2-10.41YYY440.3934.398641991.526111.79100.41-6.9-5.61ZZZ440.3934.318011991.526111.79100.41-6.9-5.72CTC430.0711173.67130.6641.16-5.3-5.92QWB3208.32570750.76105.2162.16-3.7-3.8 | 1STA | 4 | 2 | 0 | 15.21 | 1007 | 1069.88 | 1 | 13 | 3.38 | 71.2 | -7.3 | -5.4 |
| 1TLP 4 4 0.41 8.36 1628 3544.5 6 13 1.74 127.05 -10.3 -9.4 1TMN 4 4 0.65 12.53 1536 3496.05 3 8 0.7 128.88 -10.2 -10.4 1YYY 4 4 0.39 34.39 864 1991.52 6 11 1.79 100.41 -6.9 -5.6 1ZZZ 4 4 0.39 34.31 801 1991.52 6 11 1.79 100.41 -6.9 -5.6 1ZZZ 4 4 0.39 34.31 801 1991.52 6 11 1.79 100.41 -77 -5.7 2CTC 4 4 0.39 34.31 801 1991.52 6 11 1.79 100.41 -77 -5.7 2CTC 4 3 0 0 711 173.67 1 3 0.66 41.16 -5.3 -5.9 2QWB 3 2 0 8.32 570 750.7 | 1TET | 8 | 7 | 2.19 | 83.92 | 1149 | 56163.26 | 26 | 37 | 13.03 | 317.25 | -8.5 | -2 |
| 1TMN440.6512.5315363496.05380.7128.88-10.2-10.41YYY440.3934.398641991.526111.79100.41-6.9-5.61ZZZ440.3934.318011991.526111.79100.41-6.9-5.72CTC4300711173.67130.6641.16-5.3-5.92QWB3208.32570750.76105.2162.16-3.7-3.8 | 1TLP | 4 | 4 | 0.41 | 8.36 | 1628 | 3544.5 | 6 | 13 | 1.74 | 127.05 | -10.3 | -9.4 |
| 1YYY 4 4 0.39 34.39 864 1991.52 6 11 1.79 100.41 -6.9 -5.6 1ZZZ 4 4 0.39 34.31 801 1991.52 6 11 1.79 100.41 -6.9 -5.6 1ZZZ 4 4 0.39 34.31 801 1991.52 6 11 1.79 100.41 -7 -5.7 2CTC 4 3 0 0 711 173.67 1 3 0.66 41.16 -5.3 -5.9 2QWB 3 2 0 8.32 570 750.7 6 10 5.21 62.16 -3.7 -3.8 | 1TMN | 4 | 4 | 0.65 | 12.53 | 1536 | 3496.05 | 3 | 8 | 0.7 | 128.88 | -10.2 | -10.4 |
| 1ZZZ 4 4 0.39 34.31 801 1991.52 6 11 1.79 100.41 -7 -5.7 2CTC 4 3 0 0 711 173.67 1 3 0.66 41.16 -5.3 -5.9 2QWB 3 2 0 8.32 570 750.7 6 10 5.21 62.16 -3.7 -3.8 | 1YYY | 4 | 4 | 0.39 | 34.39 | 864 | 1991.52 | 6 | 11 | 1.79 | 100.41 | -6.9 | -5.6 |
| 2CTC 4 3 0 0 711 173.67 1 3 0.66 41.16 -5.3 -5.9 2QWB 3 2 0 8.32 570 750.7 6 10 5.21 62.16 -3.7 -3.8 | 1ZZZ | 4 | 4 | 0.39 | 34.31 | 801 | 1991.52 | 6 | 11 | 1.79 | 100.41 | -7 | -5.7 |
| 2QWB 3 2 0 8.32 570 750.7 6 10 5.21 62.16 -3.7 -3.8 | 2CTC | 4 | 3 | 0 | 0 | 711 | 173.67 | 1 | 3 | 0.66 | 41.16 | -5.3 | -5.9 |
| <u> </u> | 2QWB | 3 | 2 | 0 | 8.32 | 570 | 750.7 | 6 | 10 | 5.21 | 62.16 | -3.7 | -3.8 |

| 2QWE | 6 | 4 | 0 | 0 | 859 | 945.96 | 9 | 11 | 7.04 | 72.8 | -10.2 | -6.6 |
|------|---|---|------|-------|------|---------|---|----|------|--------|-------|------|
| 2QWG | 6 | 3 | 0 | 0 | 668 | 753.27 | 4 | 8 | 3 | 70.17 | -11.5 | -8 |
| 2SNS | 4 | 2 | 0 | 15.88 | 338 | 1069.88 | 1 | 13 | 3.38 | 71.2 | -9.1 | -5.6 |
| 2TMN | 3 | 2 | 0.2 | 4.05 | 1433 | 191.93 | 3 | 6 | 1.7 | 44.55 | -8 | -4.5 |
| 2XIS | 2 | 2 | 0 | 0 | 933 | 115.19 | 5 | 5 | 2.95 | 32.19 | -7.9 | -2.6 |
| 3CPA | 5 | 4 | 0 | 0 | 1032 | 218.04 | 4 | 4 | 1.7 | 43.49 | -5.5 | -6 |
| 3FX2 | 5 | 5 | 0.38 | 33.85 | 663 | 1978.76 | 4 | 13 | 1.9 | 103.42 | -12.7 | -7.3 |
| 3TMN | 3 | 3 | 0.48 | 8.71 | 1187 | 922.22 | 5 | 6 | 0.79 | 80.45 | -8 | -6.8 |
| 4SGA | 5 | 4 | 0.61 | 42.06 | 677 | 3342.02 | 2 | 10 | 1.03 | 119.83 | -10 | -7.8 |
| 4TLN | 3 | 3 | 0 | 0 | 810 | 118.56 | 5 | 4 | 0.95 | 36.21 | -5.1 | -4.1 |
| 4XIA | 4 | 3 | 0.54 | 11.42 | 1546 | 191.32 | 6 | 6 | 3.59 | 38.2 | -2.1 | -4 |
| 5ABP | 5 | 3 | 0 | 0 | 402 | 159.27 | 5 | 6 | 3.22 | 35.99 | -9.1 | -5.2 |
| 5P21 | 7 | 6 | 1.35 | 44.95 | 1125 | 1925.37 | 9 | 19 | 1.84 | 98.04 | -7.3 | -8.8 |
| 5SGA | 5 | 5 | 0.6 | 41.63 | 847 | 3632.42 | 3 | 11 | 1.32 | 121.5 | -3.9 | -7.8 |
| 5TLN | 4 | 4 | 0.42 | 7.68 | 1049 | 1121.97 | 4 | 8 | 0.93 | 80.39 | -8.7 | -7.9 |
| 6ABP | 4 | 3 | 0 | 0 | 441 | 95.16 | 4 | 5 | 2.58 | 29.98 | -7.7 | -4.5 |
| 7ABP | 4 | 3 | 0 | 0 | 510 | 122.96 | 4 | 5 | 2.19 | 34.57 | -7.6 | -4.8 |
| 7EST | 4 | 3 | 0.77 | 21.01 | 1578 | 2385.13 | 3 | 6 | 3.24 | 95.12 | -10.4 | -7.1 |
| 7TLN | 3 | 2 | 0.21 | 4.42 | 1372 | 266.27 | 1 | 5 | 0.71 | 49.71 | -3.4 | -5.3 |
| 8ABP | 4 | 3 | 0 | 0 | 343 | 159.27 | 5 | 6 | 3.22 | 35.99 | -5.5 | -4.6 |
| 9AAT | 6 | 4 | 0.68 | 26.18 | 663 | 297.27 | 3 | 7 | 1.1 | 52.3 | -11.2 | -6.6 |
| 9ABP | 5 | 3 | 0 | 0 | 391 | 159.27 | 5 | 6 | 3.22 | 35.99 | -10.9 | -5.2 |

| Cutoff for calculating | Cutoff for calculating | Training | Test |
|------------------------|------------------------|----------------|-----------------|
| hydrogen bond | hydrophobicity and | (63 complexes) | (320 complexes) |
| donors and acceptors | polarizability | | |
| MaxD | MaxD | 0.723 | 0.637 |
| MaxD+1 | MaxD+1 | 0.772 | 0.650 |
| MaxD+2 | MaxD+2 | 0.784 | 0.629 |
| MaxD+1 | MaxD | 0.761 | 0.638 |
| MaxD+2 | MaxD | 0.759 | 0.651 |
| MaxD+3 | MaxD | 0.76 | 0.653 |
| MaxD+4 | MaxD | 0.767 | 0.620 |
| MaxD+5 | MaxD | 0.767 | 0.607 |
| MaxD+3 | MaxD+1 | 0.769 | 0.681 |
| MaxD+2.9 | MaxD+1 | 0.78 | 0.676 |
| MaxD+3.1 | MaxD+1 | 0.785 | 0.657 |
| MaxD+3 | MaxD+1.1 | 0.772 | 0.679 |
| MaxD+3 | MaxD+1.5 | 0.772 | 0.668 |
| MaxD+3 | MaxD+0.9 | 0.766 | 0.686 |

Supplementary Table 3: Variation of correlation coefficient between experimental and predicted binding energies on both training and test sets as a function of different sets of distance cut offs.

MaxD is the maximum distance of the ligand atom (including hydrogen) from its centre of mass. (COM)

| S. No. | Statistical Test Formula |
|--------|--|
| 1. | $\boldsymbol{q}^{2} = 1 - \left(\frac{\sum_{N} (\boldsymbol{y}_{pred} - \boldsymbol{y}_{exp})^{2}}{\sum_{N} (\boldsymbol{y}_{exp} - \overline{\boldsymbol{y}}_{exp})^{2}}\right)$ |
| 2. | $R = \frac{\sum_{N} (y_{exp} - \overline{y}_{exp}) (y_{pred} - \overline{y}_{pred})}{\sqrt{\sum_{N} (y_{exp} - \overline{y}_{exp})^2 \sum (y_{pred} - \overline{y}_{pred})^2}}$ |
| 3. | $\boldsymbol{K} = \frac{\sum_{N} \boldsymbol{y}_{exp} \boldsymbol{y}_{pred}}{\sum_{N} \boldsymbol{y}_{pred}^{2}}$ |
| 4. | $\boldsymbol{K}' = \frac{\sum_{N} \boldsymbol{y}_{\exp} \boldsymbol{y}_{pred}}{\sum_{N} \boldsymbol{y}_{\exp}^{2}}$ |
| 5. | $\boldsymbol{y}_{\mathrm{exp}}^{\boldsymbol{r}_{0}} = \boldsymbol{K} \boldsymbol{y}_{pred}$ |
| 6. | $\boldsymbol{y}_{pred}^{r_{0}}=\boldsymbol{K}^{'}\boldsymbol{y}_{\mathrm{exp}}$ |
| 7. | $\boldsymbol{R}_{0}^{2} = 1 - \frac{\sum_{N} (\boldsymbol{y}_{pred} - \boldsymbol{y}_{exp}^{r_{0}})^{2}}{\sum_{N} (\boldsymbol{y}_{pred} - \overline{\boldsymbol{y}}_{pred})^{2}}$ |
| 8. | $\boldsymbol{R}_{0}^{'2} = 1 - \frac{\sum_{N} (\boldsymbol{y}_{\exp} - \boldsymbol{y}_{pred}^{r_{0}})^{2}}{\sum_{N} (\boldsymbol{y}_{\exp} - \overline{\boldsymbol{y}}_{\exp})^{2}}$ |
| 9. | $RMS \ error = \sqrt{\frac{\sum_{N} (y_{pred} - y_{exp})^2}{N}}$ |
| 10. | $\boldsymbol{S}_{\boldsymbol{PRESS}} = \sqrt{rac{\sum_{N} (\boldsymbol{y}_{pred} - \boldsymbol{y}_{exp})^2}{N - \boldsymbol{c} - 1}}$ |

Supplementary Table 4: Details of Statistical Test Formula performed for the validation of the empirical scoring function.

where, R is the correlation coefficient, y_{pred} is the predicted binding free energy, y_{exp} is the experimental binding free energy, N is the total number of complexes in the training set, c is the number of independent variables.

| Supplementary | Table 5. | Correlation | coefficients | for various | combinations | of the | parameters | in |
|-----------------|----------|-------------|--------------|-------------|--------------|--------|------------|----|
| eq. (2) of main | text. | | | | | | | |

| 1 | WI | 0.592 |
|----|------------------------------|-------|
| 2 | PD | 0.707 |
| 3 | PA | 0.724 |
| 4 | DD | 0.071 |
| 5 | DA | 0.179 |
| 6 | Р | 0.000 |
| 7 | PP | 0.738 |
| 8 | MR | 0.736 |
| 9 | PMR | 0.713 |
| 10 | V | 0.048 |
| 11 | WI+V | 0.595 |
| 12 | PD+PA+DD+DA | 0.784 |
| 13 | P+PP | 0.742 |
| 14 | MR+PMR | 0.772 |
| 15 | WI+MR+PMR+V | 0.789 |
| 16 | WI+P+PP+V | 0.772 |
| 17 | WI+PD+PA+D+A+V | 0.789 |
| 18 | WI+MR+PMR+V | 0.789 |
| 19 | WI+P+PP+V | 0.772 |
| 20 | P+PP+MR+PMR | 0.830 |
| 21 | W+P+PP+MR+PMR+V | 0.842 |
| 22 | W+PD+PA+DD+DA+P+PP+V | 0.806 |
| 23 | W+PD+PA+DD+DA+MR+PMR+V | 0.840 |
| 24 | PD+PA+DD+DA+P+PP+MR+PMR | 0.870 |
| 25 | PD+PA+DD+DA+P+PP+MR+PMR+V | 0.871 |
| 26 | WI+PA+DD+DA+P+PP+MR+PMR+V | 0.860 |
| 27 | WI+PD+DD+DA+P+PP+MR+PMR+V | 0.874 |
| 28 | WI+PD+PA+DA+P+PP+MR+PMR+V | 0.870 |
| 29 | WI+PD+PA+DD+P+PP+MR+PMR+V | 0.875 |
| 30 | WI+PD+PA+DD+DA+PP+MR+PMR+V | 0.870 |
| 31 | WI+PD+PA+DD+DA+P+MR+PMR+V | 0.843 |
| 32 | WI+PD+PA+DD+DA+P+PP+PMR+V | 0.827 |
| 33 | WI+PD+PA+DD+DA+P+PP+MR+V | 0.854 |
| 34 | WI+PD+PA+DD+DA+P+PP+MR+PMR | 0.875 |
| 35 | WI+PD+PA+DD+DA+P+PP+MR+PMR+V | 0.875 |
| | | |

Supplementary Table 6: Experimental and predicted binding energies of 28 HIV 1 Protease complexes.

| PDBID | Expt. | Pred. |
|-------|---------|---------|
| | Energy# | Energy# |
| 1a30 | -5.8 | -6 |
| 1aaq | -11.4 | -12.4 |
| 1ajv | -10.6 | -12.3 |
| 1ajx | -10.9 | -12.8 |
| 1b6j | -10.8 | -12.2 |
| 1b6k | -11.9 | -13.2 |
| 1b6l | -11.3 | -11.4 |
| 1b6m | -11.4 | -12 |
| 1bv7 | -12.6 | -15.1 |
| 1g2k | -10.8 | -12.5 |
| 1gno | -10.6 | -9.9 |
| 1hih | -11 | -12.3 |
| 1hiv | -12.6 | -14 |
| 1hos | -11.7 | -14.5 |
| 1hps | -12.7 | -14 |
| 1hpx | -12.5 | -12.4 |
| 1hsg | -12.9 | -12.6 |
| 1hsh | -11.7 | -12.4 |
| 1hte | -7.7 | -9.8 |
| 1htg | -13.2 | -13.9 |
| 1hvh | -10.8 | -12.9 |
| 1hvj | -14.3 | -12.8 |
| 1hvl | -12.3 | -13.9 |
| 1hxb | -13.5 | -12.6 |
| 1qbt | -14.5 | -16.3 |
| 2upj | -10.1 | -13.1 |
| 1SBG | -10.6 | -11.2 |
| 10HR | -11.8 | -12.1 |

kcal/mol



Computational Flow Chart for Indentifying Hit Molecules for a Target Protein

Supplementary Figure 1. Computational flowchart of RASPD protocol.









scaffolds-094

scaffolds-095



scaffolds-115



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Supplementary Figure 2: 154 most commonly found scaffolds in organic chemistry identified from the million molecule library.



Supplementary Figure 3: Standard errors shown against the predicted binding energies for an assessment of model validation.















1B6K



















1HOS



1HPS



1HPX





1HSH



1HTE



1HVH

1HVJ





Supplementary Figure 4: Structures of 28 ligand molecules for HIV 1 Protease

Supplementary Note 1: An illustrative RASPD Calculation for the protein Glucocorticoid receptor (1NHZ) bound to Mifepristone.

| Physico-Chemical Parameter | Active site | Molecule |
|------------------------------|-------------|----------|
| Hydrogen bond donor | 40 | 1 |
| Hydrogen bond acceptor | 31 | 3 |
| Partition coefficient (logP) | 19.20 | 5.406 |
| Molar refractivity | 417.67 | 129.432 |
| Volume/Wiener Index | 990 | 2219.88 |

Supplementary Table 5. Physico-Chemical Parameters of the drug molecule (Mifepristone) and the active site of the Glucocorticoid receptor (1NHZ) which is bound with Mifepristone

MaxD of the ligand molecule is 7.84 Å.

Regression equation used for estimating the protein-ligand binding energy is given below

$$\Delta E \left(\text{kcal/mol} \right) = a^* \frac{\text{PD}}{\text{MaxD}} + b^* \frac{\text{PA}}{\text{MaxD}} + c^* \frac{\text{PP}}{\text{MaxD}} + d^* \frac{\text{PMR}}{\text{MaxD}} + e^* \text{Volume} + f^* \text{DD} + g^* \text{DA} + h^* |P| + i^* \text{MR} + j^* \text{W} + \text{intercept} + i^* \text{MR} + j^* \text{W} + i^* \text{MR} + j^* \text{W} + j^* \text{W$$

PD: Number of hydrogen bond donor at the active site; PA: Number of hydrogen bond acceptor at the active site; PP: Partition coefficient of the active site residues; PMR: Molar refractivity of the active site residues; Volume: active site volume; DD: Total number of hydrogen bond donor of the ligand/drug molecule; DA: Total number of hydrogen bond acceptor of the ligand/drug molecule; P: Partition coefficient of the ligand/drug molecule; MR: Molar refractivity of the ligand/drug molecule; W: Wiener Index of the ligand/Drug molecule and MaxD is the distance of the farthest atom of the ligand from its COM.

Sample Calculation:

 $\Delta E (kcal/mol) = (-0.62991*40/7.84) + (-0.24581*31/7.84) + (-2.55078*19.2/7.84) + (0.108256*417.67/7.84) + (0.000477*990) + (0.196632*1) + (-0.04004*3) + (0.187565*5.406) + (-0.06165*129.432) + (0.000264*2219.88) + (-0.67154)$

or, $\Delta E (kcal/mol) = -11.1 kcal/mol.$

Predicted binding energy of the 1NHZ- Mifepristone complex is -11.1 kcal/mol.

The corresponding experimental value is -13.63 kcal/mol (source <u>http://www.bindingdb.org/pdb/1nhz</u>)



Calculation of Physico-Chemical Properties at the active site of Glucocorticoid receptor (1NHZ)

Supplementary Table 7. Number of hydrogen bond donors and acceptors at the active site of the protein. Distance cutoff was (MaxD+3) Å.

| Residue | Atom | Residue No. | HBD | HBA |
|------------|------|-------------|-----|-----|
| ASN | OD1 | 35 | 0 | 1 |
| ASN | 1HD2 | 35 | 1 | 0 |
| ASN | 2HD2 | 35 | 1 | 0 |
| GLN | OE1 | 41 | 0 | 1 |
| GLN | 1HE2 | 41 | 1 | 0 |
| GLN | 2HE2 | 41 | 1 | 0 |
| TRP | HE1 | 71 | 1 | 0 |
| ARG | 2HH1 | 82 | 1 | 0 |
| ARG | 1HH2 | 82 | 1 | 0 |
| ARG | 2HH2 | 82 | 1 | 0 |
| GLN | OE1 | 113 | 0 | 1 |
| GLN | 1HE2 | 113 | 1 | 0 |
| GLN | 2HE2 | 113 | 1 | 0 |
| Amide Bond | | | 30 | 28 |
| Total | | | 40 | 31 |

Supplementary Table 8. Hydrophobicity and Molar Refractivity* at the active site of the protein. Cutoff distance was (MaxD+0.9) Å.

| Residue | Residue |
|---------|---------|
| | number |
| MET | 31 |
| LEU | 34 |
| ASN | 35 |
| LEU | 37 |
| GLY | 38 |
| GLY | 39 |
| GLN | 41 |
| TRP | 71 |
| MET | 72 |
| MET | 75 |
| ALA | 76 |
| PHE | 94 |
| GLN | 113 |
| MET | 117 |
| LEU | 203 |

*Hydrophobicity Value: ALA: 1.0262; VAL: 1.6623; LEU: 2.0524; ILE: 2.0524; PRO: 0.3698; MET: 1.7594; TRP: 2.7303; PHE: 2.249.

*Molar Refractivity value: ALA: 21.285; VAL: 30.449; LEU: 35.066; ILE: 35.0662; PRO: 28.660; MET: 38.610; TRP: 57.614; PHE: 45.757; GLY: 16.690; CYS: 29.464; TYR: 47.422; THR: 27.292; SER: 22.697.

Sum of the values of hydrophobic residues is 19.20.

Sum of the values of these residues (except polar one) is 417.67.

Active site volume: 990 $Å^3$.

Supplementary Notes 2: Calculation of the physico-chemical parameters of the ligand.

(a) Wiener Index (W)

The Wiener index value of any molecule is calculated as per literature procedure[29-30]. It is the hydrogen depilated model. Path number between any two pair of atoms is calculated as follow.

$$W_{ij} = \frac{Z_C^2}{B_{ij}Z_iZ_j} = \frac{6^2}{B_{ij}Z_iZ_j}$$

Where W_{ii} is the path number between any two atom i, j respectively. B_{ij} is the bond order between ith and jth pair of atoms. Z_i is the atomic number of the ith atom. Z_c is the atomic number of carbon. A sample calculation between two pair of atoms is tabulated below (Table 1).

| Z_i | Z_j | \mathbf{B}_{ij} | Bond type | \mathbf{W}_{ij} |
|-------|-------|-------------------|-----------|-------------------|
| С | С | 1 | Single | 1.000 |
| С | С | 2 | Double | 0.500 |
| С | С | 3 | Triple | 0.333 |
| С | Ν | 1 | Single | 0.857 |
| С | Ν | 2 | Double | 0.429 |
| С | Ν | 3 | Triple | 0.286 |
| С | 0 | 1 | Single | 0.750 |
| С | Ο | 2 | Double | 0.375 |

Table 1: sample calculation between two pair of atoms

For example the Wiener index value of methyl ether (CH_3-O-CH_3) is 0.75+1.5+0.75=3.

(b) Hydrogen bond donor(s) and acceptor(s)

Hydrogen bond donor is calculated by simple counting OH and NH functional group in a molecule and hydrogen bond acceptor is the total number of nitrogen atoms (N) and oxygen atoms (O) presents in the given molecule.

(c) LogP and Molar Refractivity

Hydrophobicity (logP) and molar refractivity (MR) is calculated as per literature [73].