

|    | mol  | receptor | rseq | mseq | S        | rmsd_ref... |
|----|------|----------|------|------|----------|-------------|
| 1  | 1VTQ | DnmA     | 1    | 1    | -71.8782 | 1.0056      |
| 2  | 1VTQ | DnmA     | 1    | 1    | -66.0463 | 0.6606      |
| 3  | 1VTQ | DnmA     | 1    | 1    | -64.6578 | 1.3917      |
| 4  | 1VTQ | DnmA     | 1    | 1    | -62.8473 | 1.5690      |
| 5  | 1VTQ | DnmA     | 1    | 1    | -60.8447 | 0.7948      |
| 6  | 1VTQ | DnmA     | 1    | 1    | -59.9113 | 1.4463      |
| 7  | 1VTQ | DnmA     | 1    | 1    | -59.4673 | 0.4691      |
| 8  | 1VTQ | DnmA     | 1    | 1    | -58.6752 | 0.7458      |
| 9  | 1VTQ | DnmA     | 1    | 1    | -58.3770 | 1.0166      |
| 10 | 1VTQ | DnmA     | 1    | 1    | -58.1916 | 0.7147      |
| 11 | 1VTQ | DnmA     | 1    | 1    | -57.0252 | 0.8195      |
| 12 | 1VTQ | DnmA     | 1    | 1    | -56.8658 | 1.2031      |
| 13 | 1VTQ | DnmA     | 1    | 1    | -56.2346 | 0.5340      |
| 14 | 1VTQ | DnmA     | 1    | 1    | -55.7670 | 1.3767      |
| 15 | 1VTQ | DnmA     | 1    | 1    | -55.0001 | 0.5233      |
| 16 | 1VTQ | DnmA     | 1    | 1    | -54.8181 | 2.2213      |
| 17 | 1VTQ | DnmA     | 1    | 1    | -54.5323 | 3.5133      |
| 18 | 1VTQ | DnmA     | 1    | 1    | -53.9461 | 1.9930      |
| 19 | 1VTQ | DnmA     | 1    | 1    | -52.5316 | 2.9811      |
| 20 | 1VTQ | DnmA     | 1    | 1    | -52.3759 | 1.3800      |
| 21 | 1VTQ | DnmA     | 1    | 1    | -52.1680 | 1.0754      |
| 22 | 1VTQ | DnmA     | 1    | 1    | -51.9997 | 2.2295      |
| 23 | 1VTQ | DnmA     | 1    | 1    | -51.2729 | 1.5826      |
| 24 | 1VTQ | DnmA     | 1    | 1    | -51.1969 | 0.7216      |
| 25 | 1VTQ | DnmA     | 1    | 1    | -51.1037 | 4.5011      |
| 26 | 1VTQ | DnmA     | 1    | 1    | -51.0263 | 1.3018      |
| 27 | 1VTQ | DnmA     | 1    | 1    | -50.8825 | 1.7474      |
| 28 | 1VTQ | DnmA     | 1    | 1    | -50.5497 | 5.3503      |
| 29 | 1VTQ | DnmA     | 1    | 1    | -50.5208 | 2.0858      |
| 30 | 1VTQ | DnmA     | 1    | 1    | -50.2819 | 0.4065      |
| 31 | 1VTQ | DnmA     | 1    | 1    | -50.2752 | 1.7788      |
| 32 | 1VTQ | DnmA     | 1    | 1    | -49.9078 | 1.3712      |
| 33 | 1VTQ | DnmA     | 1    | 1    | -49.6903 | 4.6637      |
| 34 | 1VTQ | DnmA     | 1    | 1    | -49.6401 | 1.3897      |
| 35 | 1VTQ | DnmA     | 1    | 1    | -49.4617 | 3.5366      |
| 36 | 1VTQ | DnmA     | 1    | 1    | -49.3675 | 10.2634     |
| 37 | 1VTQ | DnmA     | 1    | 1    | -49.2100 | 5.0723      |
| 38 | 1VTQ | DnmA     | 1    | 1    | -49.0092 | 0.9179      |
| 39 | 1VTQ | DnmA     | 1    | 1    | -48.3331 | 2.7606      |
| 40 | 1VTQ | DnmA     | 1    | 1    | -48.2409 | 1.3292      |
| 41 | 1VTQ | DnmA     | 1    | 1    | -48.2256 | 3.1740      |
| 42 | 1VTQ | DnmA     | 1    | 1    | -47.5906 | 1.8357      |
| 43 | 1VTQ | DnmA     | 1    | 1    | -47.0855 | 5.9884      |
| 44 | 1VTQ | DnmA     | 1    | 1    | -46.7796 | 1.0441      |
| 45 | 1VTQ | DnmA     | 1    | 1    | -46.5818 | 1.0869      |

|    | E_conf     | E_place  | E_refine | PLIF_raw         | FP:PLIF    | PLIF_ligidx     |
|----|------------|----------|----------|------------------|------------|-----------------|
| 1  | 1407034.00 | -3.9631  | -71.8782 | [[0,0,0,0,0,0,0] | 1 2 3 4 5  | [0,0,0,0,0,0,0] |
| 2  | 1407034.00 | -13.3841 | -66.0463 | [[0,0,0,0,0,0,0] | 10 11 12 1 | [0,0,0,0,0,0,0] |
| 3  | 1407034.00 | -11.4996 | -64.6578 | [[0,0,0,0,0,0,0] | 10 11 17 1 | [0,0,0,0,0,0,0] |
| 4  | 1407034.00 | -12.3780 | -62.8473 | [[0,0,0,0,0,0,0] | 21 11 22 4 | [0,0,0,0,0,0,0] |
| 5  | 1407034.00 | -5.8018  | -60.8447 | [[0,0,0,0,0,0,0] | 11 30 31 3 | [0,0,0,0,0,0,0] |
| 6  | 1407034.00 | -6.7836  | -59.9113 | [[0,0,0,0,0,0,0] | 35 36 37 3 | [0,0,0,0,0,0,0] |
| 7  | 1407034.00 | -10.9754 | -59.4673 | [[0,0,0,0,0,0,0] | 42 20 12 4 | [0,0,0,0,0,0,0] |
| 8  | 1407034.00 | -4.3853  | -58.6752 | [[0,0,0,0,0,0,0] | 45 35 40 4 | [0,0,0,0]       |
| 9  | 1407034.00 | -6.1024  | -58.3770 | [[0,0,0,0,0,0,0] | 46 47 48 4 | [0,0,0,0,0,0,0] |
| 10 | 1407034.00 | -9.2628  | -58.1916 | [[0,0,0,0,0,0,0] | 58 30 59 6 | [0,0,0,0,0,0,0] |
| 11 | 1407034.00 | -10.3880 | -57.0252 | [[0,0,0,0,0,0,0] | 67 68 69 7 | [0,0,0,0,0,0,0] |
| 12 | 1407034.00 | -4.8750  | -56.8658 | [[0,0,0,0,0,0,0] | 30 73 74 7 | [0,0,0,0,0,0,0] |
| 13 | 1407034.00 | -6.5199  | -56.2346 | [[0,0,0,0,0,0,0] | 10 11 17 4 | [0,0,0,0,0,0,0] |
| 14 | 1407034.00 | -6.9776  | -55.7670 | [[0,0,0,0,0,0,0] | 87 21 30 3 | [0,0,0,0,0,0,0] |
| 15 | 1407034.00 | -4.9033  | -55.0001 | [[0,0,0,0,0,0,0] | 90 91 92 9 | [0,0,0,0,0,0,0] |
| 16 | 1407034.00 | -4.2625  | -54.8181 | [[0,0,0,0,0,0,0] | 18 97 98 4 | [0,0,0,0,0,0,0] |
| 17 | 1407034.00 | -5.5426  | -54.5323 | [[0,0,0,0,0,0,0] | 3 100 101  | [0,0,0,0,0,0,0] |
| 18 | 1407034.00 | -4.7419  | -53.9461 | [[0,0,0,0,0,0,0] | 47 83 110  | [0,0,0,0,0,0,0] |
| 19 | 1407034.00 | -6.1967  | -52.5316 | [[0,0,0,0,0,0,0] | 113 114 11 | [0,0,0,0,0,0,0] |
| 20 | 1407034.00 | -8.3522  | -52.3759 | [[0,0,0,0,0,0,0] | 42 20 12 7 | [0,0,0,0,0,0,0] |
| 21 | 1407034.00 | -9.4487  | -52.1680 | [[0,0,0,0,0,0,0] | 47 115 51  | [0,0,0,0,0,0,0] |
| 22 | 1407034.00 | -4.1199  | -51.9997 | [[0,0,0,0,0,0,0] | 121 122 12 | [0,0,0,0,0,0,0] |
| 23 | 1407034.00 | -7.9017  | -51.2729 | [[0,0,0,0,0,0,0] | 35 128 129 | [0,0,0,0,0,0,0] |
| 24 | 1407034.00 | -5.3805  | -51.1969 | [[0,0,0,0,0,0,0] | 48 49 51 8 | [0,0,0,0,0,0,0] |
| 25 | 1407034.00 | -5.6234  | -51.1037 | [[0,0,0,0,0,0,0] | 3 134 103  | [0,0,0,0,0,0,0] |
| 26 | 1407034.00 | -7.6916  | -51.0263 | [[0,0,0,0,0,0,0] | 3 100 48 5 | [0,0,0,0,0,0,0] |
| 27 | 1407034.00 | -9.1004  | -50.8825 | [[0,0,0,0,0,0,0] | 46 80 48 4 | [0,0,0,0,0,0,0] |
| 28 | 1407034.00 | -7.4842  | -50.5497 | [[0,0,0,0,0,0,0] | 21 42 20 1 | [0,0,0,0,0,0,0] |
| 29 | 1407034.00 | -6.0277  | -50.5208 | [[0,0,0,0,0,0,0] | 82 134 139 | [0,0,0,0,0,0,0] |
| 30 | 1407034.00 | -4.3184  | -50.2819 | [[0,0,0,0,0,0,0] | 11 17 46 4 | [0,0,0,0,0,0,0] |
| 31 | 1407034.00 | -6.2227  | -50.2752 | [[0,0,0,0,0,0,0] | 145 46 47  | [0,0,0,0,0,0,0] |
| 32 | 1407034.00 | -7.9706  | -49.9078 | [[0,0,0,0,0,0,0] | 67 68 150  | [0,0,0,0,0,0,0] |
| 33 | 1407034.00 | -6.8895  | -49.6903 | [[0,0,0,0,0,0,0] | 3 100 134  | [0,0,0,0,0,0,0] |
| 34 | 1407034.00 | -3.9483  | -49.6401 | [[0,0,0,0,0,0,0] | 152 153 15 | [0,0,0,0,0,0,0] |
| 35 | 1407034.00 | -4.6760  | -49.4617 | [[0,0,0,0,0,0,0] | 87 163 11  | [0,0,0,0,0,0,0] |
| 36 | 1407034.00 | -8.8800  | -49.3675 | [[0,0,0,0,0,0,0] | 101 82 136 | [0,0,0,0,0,0,0] |
| 37 | 1407034.00 | -6.5598  | -49.2100 | [[0,0,0,0,0,0,0] | 31 12 165  | [0,0,0,0,0,0,0] |
| 38 | 1407034.00 | -6.0502  | -49.0092 | [[0,0,0,0,0,0,0] | 42 20 167  | [0,0,0,0,0,0,0] |
| 39 | 1407034.00 | -6.4477  | -48.3331 | [[0,0,0,0,0,0,0] | 68 71 12 7 | [0,0,0,0,0,0,0] |
| 40 | 1407034.00 | -4.5481  | -48.2409 | [[0,0,0,0,0,0,0] | 87 21 169  | [0,0,0,0,0,0,0] |
| 41 | 1407034.00 | -5.7336  | -48.2256 | [[0,0,0,0,0,0,0] | 21 31 97 4 | [0,0,0,0,0,0,0] |
| 42 | 1407034.00 | -6.1698  | -47.5906 | [[0,0,0,0,0,0,0] | 47 115 18  | [0,0,0,0,0,0,0] |
| 43 | 1407034.00 | -3.6924  | -47.0855 | [[0,0,0,0,0,0,0] | 173 3 100  | [0,0,0,0,0,0,0] |
| 44 | 1407034.00 | -4.4214  | -46.7796 | [[0,0,0,0,0,0,0] | 88 180 181 | [0,0,0,0,0,0,0] |
| 45 | 1407034.00 | -4.3033  | -46.5818 | [[0,0,0,0,0,0,0] | 186 187 18 | [0,0,0,0]       |

|    | clus |
|----|------|
| 1  | 4    |
| 2  | 3    |
| 3  | 3    |
| 4  | 0    |
| 5  | 0    |
| 6  | 0    |
| 7  | 5    |
| 8  | 0    |
| 9  | 2    |
| 10 | 0    |
| 11 | 0    |
| 12 | 0    |
| 13 | 0    |
| 14 | 0    |
| 15 | 0    |
| 16 | 0    |
| 17 | 1    |
| 18 | 0    |
| 19 | 0    |
| 20 | 5    |
| 21 | 0    |
| 22 | 0    |
| 23 | 0    |
| 24 | 2    |
| 25 | 1    |
| 26 | 1    |
| 27 | 0    |
| 28 | 5    |
| 29 | 0    |
| 30 | 0    |
| 31 | 0    |
| 32 | 0    |
| 33 | 1    |
| 34 | 0    |
| 35 | 0    |
| 36 | 0    |
| 37 | 0    |
| 38 | 5    |
| 39 | 0    |
| 40 | 0    |
| 41 | 0    |
| 42 | 0    |
| 43 | 0    |
| 44 | 0    |
| 45 | 0    |

|    | mol  | receptor | rseq | mseq | S        | rmsd_ref... |
|----|------|----------|------|------|----------|-------------|
| 46 | 1VTQ | DnmA     | 1    | 1    | -46.5529 | 0.9895      |
| 47 | 1VTQ | DnmA     | 1    | 1    | -46.4143 | 0.8798      |
| 48 | 1VTQ | DnmA     | 1    | 1    | -45.6044 | 2.0984      |
| 49 | 1VTQ | DnmA     | 1    | 1    | -45.2909 | 1.3425      |
| 50 | 1VTQ | DnmA     | 1    | 1    | -45.2697 | 0.8971      |
| 51 | 1VTQ | DnmA     | 1    | 1    | -45.1307 | 1.5884      |
| 52 | 1VTQ | DnmA     | 1    | 1    | -44.9729 | 0.8088      |
| 53 | 1VTQ | DnmA     | 1    | 1    | -44.9341 | 1.6969      |
| 54 | 1VTQ | DnmA     | 1    | 1    | -44.8276 | 0.8681      |
| 55 | 1VTQ | DnmA     | 1    | 1    | -44.6953 | 5.4332      |
| 56 | 1VTQ | DnmA     | 1    | 1    | -44.5358 | 2.4182      |
| 57 | 1VTQ | DnmA     | 1    | 1    | -44.3602 | 2.5514      |
| 58 | 1VTQ | DnmA     | 1    | 1    | -44.1268 | 3.8594      |
| 59 | 1VTQ | DnmA     | 1    | 1    | -44.0539 | 1.2922      |
| 60 | 1VTQ | DnmA     | 1    | 1    | -43.8291 | 3.6215      |
| 61 | 1VTQ | DnmA     | 1    | 1    | -43.5571 | 1.6061      |
| 62 | 1VTQ | DnmA     | 1    | 1    | -42.9197 | 1.6732      |
| 63 | 1VTQ | DnmA     | 1    | 1    | -42.6796 | 2.6172      |
| 64 | 1VTQ | DnmA     | 1    | 1    | -42.5065 | 0.5469      |
| 65 | 1VTQ | DnmA     | 1    | 1    | -41.9945 | 1.1213      |
| 66 | 1VTQ | DnmA     | 1    | 1    | -41.9399 | 3.1490      |
| 67 | 1VTQ | DnmA     | 1    | 1    | -41.6986 | 0.5615      |
| 68 | 1VTQ | DnmA     | 1    | 1    | -41.3057 | 2.8742      |
| 69 | 1VTQ | DnmA     | 1    | 1    | -40.9262 | 11.3473     |
| 70 | 1VTQ | DnmA     | 1    | 1    | -40.4849 | 4.2592      |
| 71 | 1VTQ | DnmA     | 1    | 1    | -39.7497 | 0.7068      |
| 72 | 1VTQ | DnmA     | 1    | 1    | -39.6331 | 2.3019      |
| 73 | 1VTQ | DnmA     | 1    | 1    | -39.3315 | 0.8594      |
| 74 | 1VTQ | DnmA     | 1    | 1    | -39.3235 | 1.9620      |
| 75 | 1VTQ | DnmA     | 1    | 1    | -39.3041 | 2.2239      |
| 76 | 1VTQ | DnmA     | 1    | 1    | -38.5578 | 2.2004      |
| 77 | 1VTQ | DnmA     | 1    | 1    | -38.0105 | 6.1549      |
| 78 | 1VTQ | DnmA     | 1    | 1    | -37.7820 | 2.9029      |
| 79 | 1VTQ | DnmA     | 1    | 1    | -37.6732 | 3.0624      |
| 80 | 1VTQ | DnmA     | 1    | 1    | -37.3294 | 3.9571      |
| 81 | 1VTQ | DnmA     | 1    | 1    | -37.3263 | 2.0469      |
| 82 | 1VTQ | DnmA     | 1    | 1    | -35.2369 | 1.8203      |
| 83 | 1VTQ | DnmA     | 1    | 1    | -34.9550 | 1.7006      |
| 84 | 1VTQ | DnmA     | 1    | 1    | -34.9289 | 2.1718      |
| 85 | 1VTQ | DnmA     | 1    | 1    | -34.8272 | 8.7828      |
| 86 | 1VTQ | DnmA     | 1    | 1    | -33.6755 | 1.8190      |
| 87 | 1VTQ | DnmA     | 1    | 1    | -33.1202 | 1.8625      |
| 88 | 1VTQ | DnmA     | 1    | 1    | -31.8262 | 1.1536      |
| 89 | 1VTQ | DnmA     | 1    | 1    | -31.0959 | 1.7535      |
| 90 | 1VTQ | DnmA     | 1    | 1    | -30.7633 | 4.5787      |

|    | E_conf     | E_place | E_refine | PLIF_raw           | FP:PLIF    | PLIF_ligidx       |
|----|------------|---------|----------|--------------------|------------|-------------------|
| 46 | 1407034.00 | -9.8383 | -46.5529 | [[0,0,0,0,0,0,0,0] | 47 190 50  | [0,0,0,0,0,0,0,0] |
| 47 | 1407034.00 | -7.0854 | -46.4143 | [[0,0,0,0,0,0,0,0] | 58 30 59 4 | [0,0,0,0,0,0,0,0] |
| 48 | 1407034.00 | -7.5189 | -45.6044 | [[0,0,0,0,0,0,0,0] | 30 31 18 9 | [0,0,0,0,0,0,0,0] |
| 49 | 1407034.00 | -9.0425 | -45.2909 | [[0,0,0,0,0,0,0,0] | 46 80 51 8 | [0,0,0,0,0,0,0,0] |
| 50 | 1407034.00 | -3.6690 | -45.2697 | [[0,0,0,0,0,0,0,0] | 11 58 30 5 | [0,0,0,0,0,0,0,0] |
| 51 | 1407034.00 | -6.9720 | -45.1307 | [[0,0,0,0,0,0,0,0] | 3 101 103  | [0,0,0,0,0,0,0,0] |
| 52 | 1407034.00 | -6.6094 | -44.9729 | [[0,0,0,0,0,0,0,0] | 48 81 134  | [0,0,0,0,0,0,0,0] |
| 53 | 1407034.00 | -4.6113 | -44.9341 | [[0,0,0,0,0,0,0,0] | 11 58 30 5 | [0,0,0,0,0,0,0,0] |
| 54 | 1407034.00 | -4.8884 | -44.8276 | [[0,0,0,0,0,0,0,0] | 30 46 47 1 | [0,0,0,0,0,0,0,0] |
| 55 | 1407034.00 | -3.6963 | -44.6953 | [[0,0,0,0,0,0,0,0] | 48 49 50 5 | [0,0,0,0,0,0]     |
| 56 | 1407034.00 | -4.4659 | -44.5358 | [[0,0,0,0,0,0,0,0] | 201 202 20 | [0,0,0,0,0,0,0,0] |
| 57 | 1407034.00 | -7.5245 | -44.3602 | [[0,0,0,0,0,0,0,0] | 46 47 115  | [0,0,0,0,0,0,0]   |
| 58 | 1407034.00 | -7.3797 | -44.1268 | [[0,0,0,0,0,0,0,0] | 47 51 82 1 | [0,0,0,0,0,0,0,0] |
| 59 | 1407034.00 | -7.0285 | -44.0539 | [[0,0,0,0,0,0,0,0] | 46 47 115  | [0,0,0,0,0,0,0,0] |
| 60 | 1407034.00 | -5.6664 | -43.8291 | [[0,0,0,0,0,0,0,0] | 46 47 115  | [0,0,0,0,0,0,0]   |
| 61 | 1407034.00 | -5.4064 | -43.5571 | [[0,0,0,0,0,0,0,0] | 68 42 20 1 | [0,0,0,0,0,0,0,0] |
| 62 | 1407034.00 | -6.1031 | -42.9197 | [[0,0,0,0,0,0,0,0] | 213 214 30 | [0,0,0,0,0,0,0,0] |
| 63 | 1407034.00 | -4.3162 | -42.6796 | [[0,0,0,0,0,0,0,0] | 51 52 103  | [0,0,0,0,0,0,0,0] |
| 64 | 1407034.00 | -4.8584 | -42.5065 | [[0,0,0,0,0,0,0,0] | 42 88 43 9 | [0,0,0,0,0,0,0]   |
| 65 | 1407034.00 | -7.9752 | -41.9945 | [[0,0,0,0,0,0,0,0] | 213 11 47  | [0,0,0,0,0,0,0,0] |
| 66 | 1407034.00 | -3.8385 | -41.9399 | [[0,0,0,0,0,0,0,0] | 219 220 22 | [0,0,0,0,0,0,0,0] |
| 67 | 1407034.00 | -5.1663 | -41.6986 | [[0,0,0,0,0,0,0,0] | 82 134 53  | [0,0,0,0,0,0,0]   |
| 68 | 1407034.00 | -3.9102 | -41.3057 | [[0,0,0,0,0,0,0,0] | 30 31 170  | [0,0,0,0,0,0,0,0] |
| 69 | 1407034.00 | -3.9929 | -40.9262 | [[0,0,0,0,0,0,0,0] | 47 51 82 1 | [0,0,0,0,0,0,0,0] |
| 70 | 1407034.00 | -4.6299 | -40.4849 | [[0,0,0,0,0,0,0,0] | 48 81 134  | [0,0,0,0,0,0,0,0] |
| 71 | 1407034.00 | -4.3537 | -39.7497 | [[0,0,0,0,0,0,0,0] | 131 232 18 | [0,0,0,0,0,0,0,0] |
| 72 | 1407034.00 | -4.5293 | -39.6331 | [[0,0,0,0,0,0,0,0] | 81 51 82 1 | [0,0,0,0,0,0,0]   |
| 73 | 1407034.00 | -5.3340 | -39.3315 | [[0,0,0,0,0,0,0,0] | 48 81 233  | [0,0,0,0,0,0,0,0] |
| 74 | 1407034.00 | -4.5646 | -39.3235 | [[0,0,0,0,0,0,0,0] | 30 47 83 8 | [0,0,0,0,0,0]     |
| 75 | 1407034.00 | -4.1540 | -39.3041 | [[0,0,0,0,0,0,0,0] | 53 108 109 | [0,0,0,0,0,0]     |
| 76 | 1407034.00 | -4.1788 | -38.5578 | [[0,0,0,0,0,0,0,0] | 175 237 14 | [0,0,0,0,0,0,0,0] |
| 77 | 1407034.00 | -7.7032 | -38.0105 | [[0,0,0,0,0,0,0,0] | 47 48 82 8 | [0,0,0,0,0]       |
| 78 | 1407034.00 | -4.7074 | -37.7820 | [[0,0,0,0,0,0,0,0] | 46 47 115  | [0,0,0,0,0,0,0,0] |
| 79 | 1407034.00 | -3.7321 | -37.6732 | [[0,0,0,0,0,0,0,0] | 47 48 81 2 | [0,0,0,0,0,0,0,0] |
| 80 | 1407034.00 | -6.7163 | -37.3294 | [[0,0,0,0,0,0,0,0] | 48 241 242 | [0,0,0,0,0,0,0,0] |
| 81 | 1407034.00 | -3.6391 | -37.3263 | [[0,0,0,0,0,0,0,0] | 47 115 146 | [0,0,0,0,0,0,0,0] |
| 82 | 1407034.00 | -4.0171 | -35.2369 | [[0,0,0,0,0,0,0,0] | 221 243 24 | [0,0,0,0,0,0,0,0] |
| 83 | 1407034.00 | -4.8314 | -34.9550 | [[0,0,0,0,0,0,0,0] | 48 81 233  | [0,0,0,0,0,0,0,0] |
| 84 | 1407034.00 | -9.0406 | -34.9289 | [[0,0,0,0,0,0,0,0] | 51 82 198  | [0,0,0,0,0,0,0,0] |
| 85 | 1407034.00 | -6.2155 | -34.8272 | [[0,0,0,0,0,0,0,0] | 46 47 48 4 | [0,0,0,0,0,0,0]   |
| 86 | 1407034.00 | -5.3564 | -33.6755 | [[0,0,0,0,0,0,0,0] | 136 141 10 | [0,0,0,0,0]       |
| 87 | 1407034.00 | -5.4221 | -33.1202 | [[0,0,0,0,0,0,0,0] | 51 82 198  | [0,0,0,0,0,0]     |
| 88 | 1407034.00 | -4.8239 | -31.8262 | [[0,0,0,0,0,0,0,0] | 48 81 212  | [0,0,0,0,0,0,0,0] |
| 89 | 1407034.00 | -3.9012 | -31.0959 | [[0,0,0,0,0,0,0,0] | 48 51 82   | [0,0,0,0]         |
| 90 | 1407034.00 | -3.7663 | -30.7633 | [[0,0,0,0,0,0,0,0] | 101 103 21 | [0,0,0,0,0,0,0,0] |

|    | clus |
|----|------|
| 46 | 0    |
| 47 | 0    |
| 48 | 0    |
| 49 | 0    |
| 50 | 0    |
| 51 | 1    |
| 52 | 1    |
| 53 | 0    |
| 54 | 0    |
| 55 | 2    |
| 56 | 0    |
| 57 | 0    |
| 58 | 0    |
| 59 | 0    |
| 60 | 0    |
| 61 | 0    |
| 62 | 0    |
| 63 | 0    |
| 64 | 0    |
| 65 | 0    |
| 66 | 0    |
| 67 | 1    |
| 68 | 0    |
| 69 | 0    |
| 70 | 1    |
| 71 | 0    |
| 72 | 0    |
| 73 | 2    |
| 74 | 0    |
| 75 | 0    |
| 76 | 0    |
| 77 | 0    |
| 78 | 0    |
| 79 | 2    |
| 80 | 0    |
| 81 | 0    |
| 82 | 0    |
| 83 | 2    |
| 84 | 0    |
| 85 | 0    |
| 86 | 0    |
| 87 | 2    |
| 88 | 2    |
| 89 | 0    |
| 90 | 0    |

|           | <b>mol</b> | <b>receptor</b> | <b>rseq</b> | <b>mseq</b> | <b>S</b> | <b>rmsd_ref...</b> |
|-----------|------------|-----------------|-------------|-------------|----------|--------------------|
| <b>91</b> | 1VTQ       | DnmA            | 1           | 1           | -30.0450 | 1.5046             |
| <b>92</b> | 1VTQ       | DnmA            | 1           | 1           | -26.3779 | 26.2549            |
| <b>93</b> | 1VTQ       | DnmA            | 1           | 1           | -25.1760 | 12.6288            |
| <b>94</b> | 1VTQ       | DnmA            | 1           | 1           | -21.9407 | 45.3100            |
| <b>95</b> | 1VTQ       | DnmA            | 1           | 1           | -15.7578 | 19.2011            |
| <b>96</b> | 1VTQ       | DnmA            | 1           | 1           | -12.6603 | 37.7707            |

|    | E_conf     | E_place  | E_refine | PLIF_raw          | FP:PLIF    | PLIF_ligidx     |
|----|------------|----------|----------|-------------------|------------|-----------------|
| 91 | 1407034.00 | -4.9074  | -30.0450 | [[0,0,0,0,0,0,0,0 | 47 48 81 5 | [0,0,0,0,0]     |
| 92 | 1407034.00 | -4.9188  | -26.3779 | [[0,0,0,0,0,0,0,0 | 101 175 23 | [0,0,0,0,0,0,0] |
| 93 | 1407034.00 | -4.2971  | -25.1760 | [[0,0,0,0,0,0,0,0 | 46 47 91   | [0,0,0]         |
| 94 | 1407034.00 | -4.3383  | -21.9407 | [[0,0,0,0,0,0,0,0 | 74 254 71  | [0,0,0,0]       |
| 95 | 1407034.00 | -4.1776  | -15.7578 | [[0,0,0,0,0,0,0,0 | 255 256 25 | [0,0,0,0,0,0]   |
| 96 | 1407034.00 | -10.2642 | -12.6603 | [[0,0,0,0,0,0,0,0 | 249 217    | [0,0]           |



|    | clus |
|----|------|
| 91 | 0    |
| 92 | 0    |
| 93 | 0    |
| 94 | 0    |
| 95 | 0    |
| 96 | 0    |