2v61

Conclusions: The pairs found by the new routine that are not found by the old routine, and not found by CaPTURE, are very much off center.

The new method reports 17 cations, 16 aromatics. The old method reports 20 cations, 22 aromatics.

The Old routine shows 4 unpaired aromatics and 0 unpaired cations. The new method shows no unpaired residues.

The pairs K271:Y393 and K296:Y60(B) reported by old but not new (and not CaPTURE) have some ring atoms >6. Therefore I guess each residue must be within a compensating atom of another partner but I did not investigate this.

TEST METHOD: To apply the old method, reduce the cutoff to 1000 atoms (catPiLimitNewAlgorithm in modeldat.js)

 Gray = unpaired. CaPTURE **Bold: found by old but not new.**

|  |  |  |
| --- | --- | --- |
| Old | New |  |
| [TYR]44:A.CA #289[TYR]53:A.CA #369**[TYR]60:A.CA #418**[TYR]311:A.CA #2469[TYR]337:A.CA #2663[TYR]383:A.CA #3029[TRP]388:A.CA #3076[TYR]393:A.CA #3123[TYR]410:A.CA #3254[PHE]423:A.CA #3369[TRP]463:A.CA #3672[TYR]44:B.CA #4261[TYR]53:B.CA #4341[TYR]60:B.CA #4390[TYR]311:B.CA #6441[TYR]337:B.CA #6635[TYR]383:B.CA #7001[TRP]388:B.CA #7048**[TYR]393:B.CA #7095**[TYR]410:B.CA #7226[PHE]423:B.CA #7341[TRP]463:B.CA #7644 | [TYR]44:A.CA #289[TYR]53:A.CA #369[TYR]337:A.CA #2663[TYR]383:A.CA #3029[TRP]388:A.CA #3076[TYR]410:A.CA #3254[PHE]423:A.CA #3369[TRP]463:A.CA #3672[TYR]44:B.CA #4261[TYR]53:B.CA #4341[TYR]337:B.CA #6635[TYR]383:B.CA #7001[TRP]388:B.CA #7048[TYR]410:B.CA #7226[PHE]423:B.CA #7341[TRP]463:B.CA #7644 | Off center R38K296Off center K52, Note 1Off center K357.R268Off center R38Off center K52, Note 1Off center K357.K271R268 |
| [ARG]38:A.CA #245**[LYS]52:A.CA #360**[ARG]282:A.CA #2219[ARG]288:A.CA #2270**[LYS]296:A.CA #2328**[LYS]332:A.CA #2626[ARG]350:A.CA #2761[LYS]357:A.CA #2820[LYS]386:A.CA #3059[ARG]445:A.CA #3530[ARG]38:B.CA #4217[LYS]52:B.CA #4332**[LYS]271:B.CA #6100**[ARG]282:B.CA #6191[ARG]288:B.CA #6242[LYS]332:B.CA #6598[ARG]350:B.CA #6733[LYS]357:B.CA #6792[LYS]386:B.CA #7031[ARG]445:B.CA #7502 | [ARG]38:A.CA #245[ARG]282:A.CA #2219[ARG]288:A.CA #2270[LYS]332:A.CA #2626[ARG]350:A.CA #2761[LYS]357:A.CA #2820[LYS]386:A.CA #3059[ARG]445:A.CA #3530[ARG]38:B.CA #4217[LYS]52:B.CA #4332[ARG]282:B.CA #6191[ARG]288:B.CA #6242[LYS]332:B.CA #6598[ARG]350:B.CA #6733[LYS]357:B.CA #6792[LYS]386:B.CA #7031[ARG]445:B.CA #7502 | Off center Y44Note 2Y60Off center Y410.Off center Y383.Off center Y44Note 1Y393Off center Y410.Off center Y383. |

1. K52:B fails 6A for Y53B. Succeeds 6A with Y337 but is WAY off center, thus FG picks K52:B but not CaPTURE. CaPTURE is OK with K332:Y53. FG picks Y337 because it barely makes 6A to K332 (off center).

2. K52:A fails 6A for both nearby rings, Y337:A and Y53:A, but the 6A subset of the atoms from both rings evidently provide all looked for by the old algorithm.