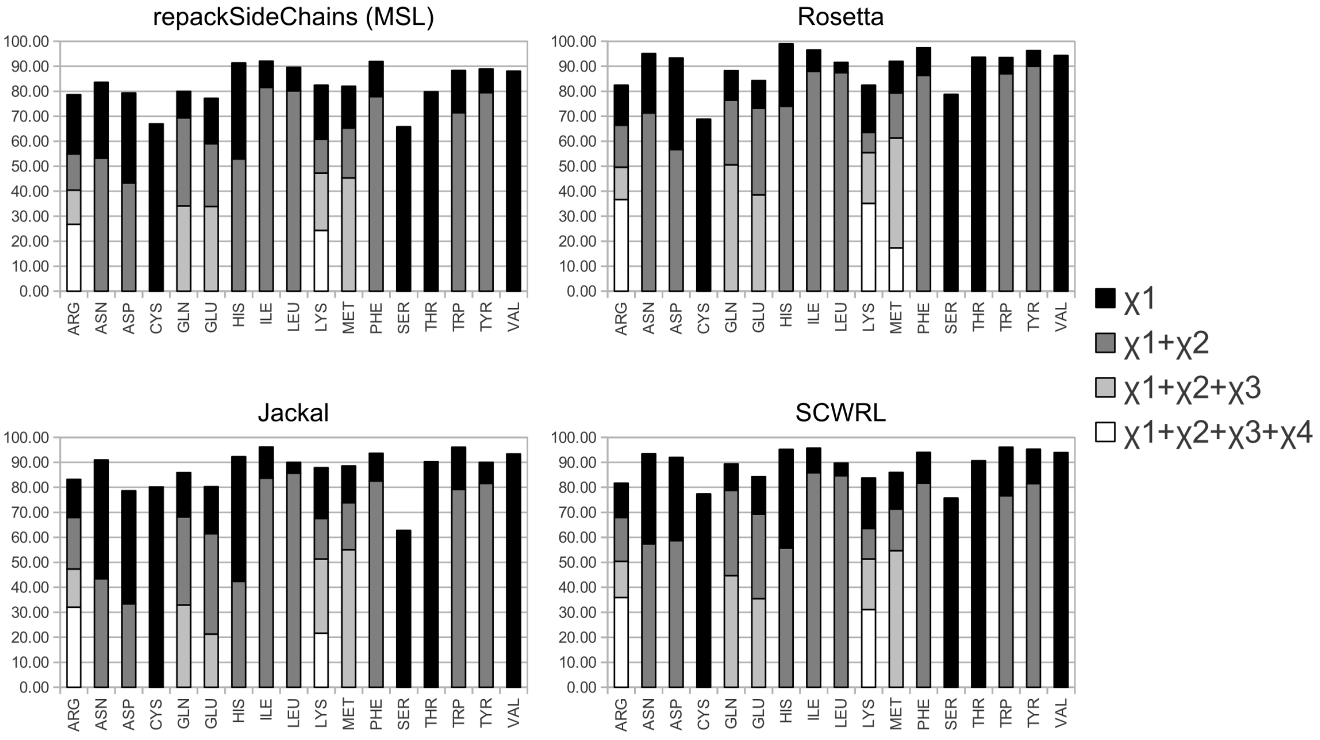
Supporting Information for: DW. Kulp, S Subramaniam, JE. Donald, BT. Hannigan, BK. Mueller, G Grigoryan, and A Senes “Structural informatics, modeling and design with an open-source Molecular Software Library (MSL)” *Journal of Computational Chemistry* (2012)

Supplementary Figure



Supplementary Fig. 1 Comparison of the performance of MSL's *repackSideChains* with other side chain prediction programs, detailed version. Detailed side chain recovery performance on a set of 34 proteins (same data of Fig. 8), subdivided by amino acid type and χ angle (χ1, χ1+χ2, χ1+χ2+χ3 and χ1+χ2+χ3+χ4, when applicable)

Supplementary methods

Side chain prediction program comparison

The side chain prediction comparison was performed on the following set of pdb files: 1B2P, 1DTJ, 1DUA, 1E6F, 1EO6, 1ES6, 1FA8, 1FQN, 1GQN, 1H03, 1IJY, 1J1I, 1J33, 1JYK, 1K50, 1KYH, 1NRI, 1OI7, 1OQW, 1QYU, 1R3D, 1RWZ, 1RZ2, 1TMI, 1U7I, 1UXZ, 1V6T, 1VC1, 1WR2, 1XDZ, 1XQO, 1Y5H, 1YT4, 2BJV. All programs were run on a dual Quad-Core Intel Xeon Processor E5440 computers equipped with 16 GB of RAM running Ubuntu Linux 8.10 served edition. The programs were run with the following options:

RepackSideChains (MSL version 0.2.22.9):

```
--rotlibfile EBL_11-2011_CHARMM22.txt --rotlevel SL85.00 --charmmtopfile top_all22_prot.inp
--charmmparfile par_all22_prot.inp --hbondparfile par_hbond_1.txt --rungreedy true
--greedycycles 3 --excludeenergyterm CHARMM_ELEC --onthefly true
```

Rosetta (version 3.3):

```
fixbb.static.linuxgccrelease -database rosetta3.3_bundles/rosetta_database -dun10 true
```

```
-multi_cool_annealer 10 -linmem_ig 10 -no_his_his_pairE true -minimize_sidechains true
-ignore_unrecognized_res true -no_optH false -nstruct 1 -resfile resfile.txt
```

Scwrl (version 4): no specific option.

Jackal:

```
scap -prm 1 -rtm 1 -seed 1 -min 4 -out 0 -self 0
```

The recovery analysis was performed with the MSL program *getChiRecovery*, which is available from the MSL repository.