Table S3. HADDOCK active residues for Bcl-x  $\!_{L}$  and cytochrome c.

| Bcl-x <sub>L</sub>       | cytochrome c             |
|--------------------------|--------------------------|
| Q88, E129, D133, T190,   | Q16, V20, G24, H26, G29, |
| F191 <sup>a</sup> , G196 | G41, A50, K79, M80, V83  |

a The residue was considered active although it does not result solvent accessible from NACCESS calculations based on the solution structure 1LXL.