**Constraints list**

***HADDOCK AIR restraints for 1st molecule***

Residues 33, 57 and 88

**HADDOCK AIR restraints for 2st molecule**

1. **PRE of S33C-MTSL probe**
   1. ***0.05<0.2***: 56, 59
   2. ***0.2<0.6***: 2, 7, 33, 52, 53, 54, 55, 58, 65
2. **PRE of S57C-MTSL probe**
   1. ***<0.05***: 35
   2. **0.05<0.2**: 2, 36, 54, 56, 84, 85
   3. **0.2<0.6**: 7, 11, 15, 17, 33, 34, 37, 52, 53, 55, 59, 65, 83, 87, 88
3. **PRE of S88C-MTSL probe**
4. **<0.05**: 52, 53, 54, 55, 56
5. **0.2 < 0.6**: 7, 12, 33, 63, 65, 67, 68, 69
6. **Crosslinking-MASS spectrometry: S57C-MTS-diazirine**
7. 35, 36, 46, 51, 52, 55, 64, 82, 83