

Additional file 5

Coordination of water molecules in cluster II

water molecule	ligand 1	ligand 2	ligand 3	ligand 4
1	Val15 backbone	Tyr82 side chain	water molecule 2	
2	water molecule 1	water molecule 3		
3	Gln11 side chain	Tyr82 side chain	water molecule 2	water molecule 4
4	Asn74 Seitenkette	Pro69 backbone	water molecule 3	water molecule 5
5	Pro68 backbone	Asn74 backbone	Asn74 side chain	water molecule 4