

Additional file 3

Coordination of water molecules in cluster I

water molecule	ligand 1	ligand 2	ligand 3	ligand 4
1	Glu188 side chain	Asp223 side chain	Ala225 backbone	water molecule 2
2		water molecule 1	water molecule 3	water molecule 4
3	Leu278 backbone	Leu277 backbone	Ala275 backbone	water molecule 2
4	water molecule 3	water molecule 5	water molecule 7	water molecule 8
5	Thr229 side chain	Ala274 backbone	water molecule 4	water molecule 6
6	Pro260 backbone	water molecule 5	water molecule 7	
7	water molecule 4	water molecule 5	water molecule 6	water molecule 8
8	Asp223 backbone	Asp223 side chain	water molecule 6	water molecule 7