Supplementary Table S1. List of double conformations in all BT models. Only the occupancy of the A conformation is indicated, the B conformation is complementary. The minus sign ('-') indicates that no additional conformation was modeled.

		model				
residue		**BT1**	**BT2**	**BT3**	**BT4**	**BT5**
Val	31	0.64	0.60	0.62	0.62	0.58
Tyr	39	0.55	0.55	0.43	0.50	0.38
Asn	48	0.64	0.61	0.62	0.57	0.59
Gln	50	0.57	0.59	0.73	0.66	0.56
Val	53	0.56	0.59	0.55	0.58	0.64
Leu	67	0.49	0.55	0.60	0.55	0.59
Ser	84	0.63	0.62	0.65	0.56	0.61
Ser	86	0.73	0.73	0.81	0.83	0.78
Lys	87	0.57	0.62	-	-	-
Ser	88	0.72	0.70	0.62	0.62	0.64
Pro	92	-	0.66	0.58	0.69	0.64
Met	104	0.59	0.60	0.57	0.56	0.54
Ser	113	0.69	0.71	0.65	0.70	0.71
Arg	117	0.51	0.61	0.60	0.55	0.70
Ser	120	0.76	0.71	0.68	0.70	0.69
Ser	122	0.77	0.72	0.67	0.73	0.73
Pro	124	0.56	0.60	0.71	0.56	0.59
Thr	125	0.56	0.60	0.71	0.56	0.59
Ser	127	0.56	0.60	0.71	0.56	0.59
Thr	134	0.64	0.62	0.56	0.53	0.52
Gln	135	0.64	0.62	0.56	0.53	0.52
Lys	145	0.67	0.61	0.62	0.52	0.69
Ser	147	0.58	0.54	0.62	0.60	0.65
Gly	148	0.58	0.54	0.62	0.60	0.65
Thr	149	0.58	0.54	0.62	0.60	0.65
Pro	152	0.69	0.72	0.78	0.74	0.69
Asp	153	0.69	0.72	0.78	0.74	0.69
Lys	156	0.55	0.56	0.55	0.50	0.54
Asp	165	0.56	0.55	0.70	0.58	0.62
Ser	170	0.76	0.71	0.75	0.66	0.71
Lys	1188	0.59	0.56	0.56	0.66	0.58
Gln	192	0.61	0.56	0.51	0.57	0.55
Ser	217	0.68	0.65	0.63	0.63	0.63
Lys	224	0.80	0.64	0.59	0.57	0.75
Ser	236	0.42	0.50	0.41	0.42	0.41
Gln	240	0.56	0.67	0.76	0.76	0.71
Ser	244	0.65	0.65	0.56	0.60	0.60

Supplementary Table S2. Pairwise σ level of the occupancies of ligand and solvent molecules in all BT models. The column title BT1-BT2 indicates that the distances between BT1 and BT2 are compared.

	BT1-BT2	BT1-BT3	BT1-BT4	BT1-BT5	BT2-BT3	BT2-BT4	BT2-BT5	BT3-BT4	BT3-BT5	BT4-BT5
BEN-A	1.2	0.9	2.0	0.4	0.1	1.0	0.6	0.6	0.6	1.4
BEN-B	1.2	0.9	2.0	0.4	0.1	1.0	0.6	0.6	0.6	1.4
SO4-1	0.8	6.8	0.7	4.1	6.5	1.5	3.7	7.5	2.2	4.8
SO4-2	3.8	9.6	14.5	10.8	6.8	12.5	8.2	5.8	1.8	3.8
GOL	8.5	11.3	16.3	10.6	2.8	7.8	2.1	4.9	0.7	5.7