

Supplementary data

Supplementary Table 1. Trp/Tyr hydrogen bonds (H...X distance up to 3.0 Å) with Cl⁻ and water molecules.

Partial occupancies shown in parentheses.

Tryptophanes 109, 111, 213b, 313b, 413b and Tyr411b do not form hydrogen bond neither with Cl⁻ nor with water.

Trp/Tyr No. (occupancy)	(Trp)NH ⁺ ...Cl ⁻		(Trp)NH ⁺ ...OH ₂	
	H...Cl ⁻ Distance [Å] (Cl number and occupancy)	N-H...Cl ⁻ Angle [°]	H...O Distance [Å] (H ₂ O number and occupancy)	N-H...O Angle [°]
113	2.48 (23; 0.15)	147	3.12 (85; 0.20)	131
	2.57 (22; 0.34)	155		
115	2.65 (24; 0.16)	132	2.18 (85; 0.20)	130
	2.90 (23; 0.15)	125		
209	2.37 (26; 0.28)	156	2.94 (86; 0.85)	147
211a (0.77)	2.10 (27; 0.12)	147		
211b (Tyr)(0.23)	2.21 (25; 0.05)	143		
213a (0.51)	2.34 (29; 0.30)	180		
215	2.53 (28; 0.16)	151		
309a (0.62)	2.92 (31; 0.36)	140		
311			2.14 (89; 0.50)	156
313	2.87 (24; 0.16)	139	3.20 (85; 0.20)	131
315a (0.68)	2.14 (21; 0.32)	154		
	2.61 (22; 0.34)	142		
409	2.38 (21; 0.32)	168		
	2.72 (22; 0.34)	129		
411a (0.81)	2.27 (29; 0.30)	162		
413a (0.47)	2.29 (25; 0.05)	157		
413b (0.54)	2.83 (25; 0.05)	112		
415	2.68 (26; 0.28)	159		
	2.90 (25; 0.05)	130		

Supplementary Table 2. Hydrogen bonds observed for chlorine acceptors.

Atom (occ.)	Cl ⁻ ...H	Cl ⁻ ...N(O)	Cl ⁻ ...H...N(O)	Cl ⁻ ...X(Cl ⁻ ,OH ₂)
<i>Cluster I</i>				
Cl⁻ 21 (0.32)				
Trp 315a	2.14	2.94	154	
Trp 409	2.38	3.22	168	
H ₂ O 85				3.40
Cl 22				2.10
Cl 23				2.73
Cl⁻ 22 (0.34)				
Trp 113	2.57	3.37	155	
Trp 315a	2.61	3.33	142	
Trp 409	2.70	3.31	129	
Trp 115	3.54	3.98	116	
H ₂ O 85				2.10
Cl 23				1.05
Cl 24				3.31
Cl⁻ 23 (0.15)				
Trp 113	2.48	3.23	147	
Trp 115	2.90	3.47	125	
Trp 315a	3.17	3.75	127	
Trp 313	3.65	4.09	116	
Trp 409	3.72	4.34	131	
H ₂ O 85				1.09
Cl 22				1.03
Cl 24				2.26
Cl⁻ 24 (0.16)				
Trp 115	2.65	3.29	132	
Trp 313	2.87	3.56	139	
Trp 113	3.54	3.95	113	
H ₂ O 85				1.20
Cl 22				3.31
Cl 23				2.26
<i>Cluster II</i>				
Cl⁻ 25 (0.05)				
Tyr 211	2.21	2.91	143	
Trp 413a	2.29	3.10	157	
Trp 413b	2.83	3.25	112	
Trp 415	2.90	3.51	130	
Trp 211	3.06	3.58	121	
Cl 26				3.15
Cl 27				2.61
Cl⁻ 26 (0.28)				
Trp 209	2.37	3.17	156	
Trp 415	2.68	3.49	159	
H ₂ O 86				2.33
Cl 25				3.15
Cl 27				3.23
Cl⁻ 27 (0.12)				
Trp 211	2.10	2.86	147	
Tyr 211	3.39	4.09	146	
H ₂ O 86				2.92
Cl 25				2.61
Cl 26				3.23
<i>a.Dispersed</i>				
Cl⁻ 28 (0.16)				
Trp 215	2.53	3.31	151	
Tyr 411	3.56	4.09	128	
H ₂ O 88				3.22
Cl⁻ 29 (0.30)				
Trp 411	2.27	3.10	162	
Trp 213a	2.34	3.19	180	

Cl⁻ 30 (0.18)				
Trp 213b	3.24	4,03	155	
Cl⁻ 31 (0.36)				
Trp 309a	2.92	3.61	140	
Cl⁻ 32 (0.13)				
H ₂ O 88				3.98