Water-mediated ionic interactions in protein structures

R Sabarinathan, K Aishwarya, R Sarani, M Kirti Vaishnavi and K Sekar

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Supplementary material

Supplementary table 1. List of complete water-mediated ionic interactions formed by different combinations of charged atoms and their corresponding occurrences

S. No.	Type	Number of water-mediated ionic interactions (within subunit)	Nature of water molecule	
			Buried	Surface
1	$N^{\delta1}$-W-$O^{\delta1}$ $N^{\delta1}$-W-$O^{\delta2}$	3	1	2
2	$N^{\varepsilon2}$-W-$O^{\delta1}$ $N^{\varepsilon2}$-W-$O^{\delta2}$	5	3	2
3	$N^{\delta1}$-W-$O^{\varepsilon1}$ $N^{\delta1}$-W-$O^{\varepsilon2}$	2	0	2
4	$N^{\varepsilon2}$-W-$O^{\varepsilon1}$ $N^{\varepsilon2}$-W-$O^{\varepsilon2}$	4	4	0
5	N^{ζ}-W-$O^{\delta1}$ N^{ζ}-W-$O^{\delta2}$	10	3	7
6	N^{ζ}-W-$O^{\varepsilon1}$ N^{ζ}-W-$O^{\varepsilon2}$	12	0	12
7	NH1-W-$O^{\delta1}$ NH2-W-$O^{\delta2}$	2	0	2
8	NH1-W-$O^{\delta2}$ NH2-W-$O^{\delta1}$	2	0	2
9	NH1-W-$O^{\delta1}$ NH2-W-$O^{\delta1}$	16	8	8
10	NH1-W-$O^{\delta2}$ NH2-W-$O^{\delta2}$	19	5	14
11	NH2-W-$O^{\delta1}$ N^{ε}-W-$O^{\delta1}$	24	12	12
12	NH2-W-$O^{\delta2}$ N^{ε}-W-$O^{\delta2}$	20	5	15
13	NH1-W-$O^{\delta1}$ NH1-W-$O^{\delta2}$	9	4	5
14	NH2-W-$O^{\delta1}$ NH2-W-$O^{\delta2}$	6	4	2
15	N^{ε}-W-$O^{\delta1}$ N^{ε}-W-$O^{\delta2}$	6	0	6
16	NH1-W-$O^{\varepsilon1}$ NH2-W-$O^{\varepsilon1}$	17	5	12
17	NH1-W-$O^{\varepsilon2}$ NH2-W-$O^{\varepsilon2}$	17	7	10
18	NH2-W-$O^{\varepsilon1}$ N^{ε}-W-$O^{\varepsilon1}$	15	3	12
19	NH2-W-$O^{\varepsilon2}$ N^{ε}-W-$O^{\varepsilon2}$	17	6	11
20	NH1-W-$O^{\varepsilon1}$ NH1-W-$O^{\varepsilon2}$	3	0	3

21	NH2-W- $O^{\varepsilon 1}$ NH2-W- $O^{\varepsilon 2}$	7	2	5
22	N^{ε} -W- $O^{\varepsilon 1}$ N^{ε} -W- $O^{\varepsilon 2}$	3	1	2
Total number of complete water-mediated ionic interactions		219	73	146

Supplementary table 2. List of incomplete water-mediated ionic interaction formed by different combinations of charged atoms and their corresponding numbers

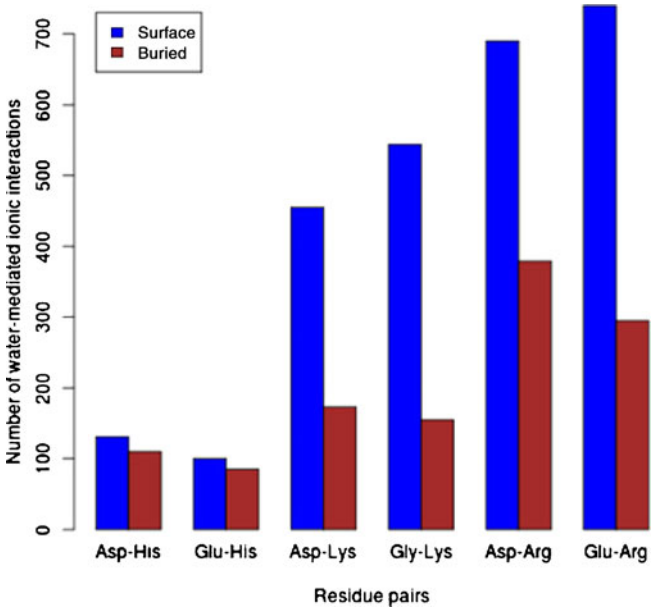
		Number of water-mediated ionic interactions			Nature of water molecule	
S. No.	Type	Within subunit	Between subunits	Total	Buried	Surface
1	$N^{\delta 1}$-W- $O^{\delta 1}$	57	0	57	22	35
2	$N^{\delta 1}$-W- $O^{\delta 2}$	41	0	41	18	23
3	$N^{\varepsilon 2}$-W- $O^{\delta 1}$	61	2	63	34	29
4	$N^{\varepsilon 2}$-W- $O^{\delta 2}$	70	1	71	29	42
5	$N^{\delta 1}$-W- $O^{\varepsilon 1}$	30	0	30	15	15
6	$N^{\delta 1}$-W- $O^{\varepsilon 2}$	38	0	38	22	16
7	$N^{\varepsilon 2}$-W- $O^{\varepsilon 1}$	50	0	50	20	30
8	$N^{\varepsilon 2}$-W- $O^{\varepsilon 2}$	59	1	60	25	35
9	N^{ζ} -W- $O^{\delta 1}$	338	1	339	85	254
10	N^{ζ} -W- $O^{\delta 2}$	313	4	317	82	235
11	N^{ζ} -W- $O^{\varepsilon 1}$	356	6	362	89	273
12	N^{ζ} -W- $O^{\varepsilon 2}$	316	2	318	67	251
13	NH1-W- $O^{\delta 1}$	167	1	168	60	108
14	NH2-W- $O^{\delta 1}$	153	2	155	51	104
15	N^{ε} -W- $O^{\delta 1}$	119	0	119	44	75
16	NH1-W- $O^{\delta 2}$	170	2	172	54	118
17	NH2-W- $O^{\delta 2}$	197	0	197	57	140
18	N^{ε} -W- $O^{\delta 2}$	76	3	79	38	41
19	NH1-W- $O^{\varepsilon 1}$	158	1	159	62	97
20	NH2-W- $O^{\varepsilon 1}$	142	1	143	38	105
21	N^{ε} -W- $O^{\varepsilon 1}$	90	1	91	35	56
22	NH1-W- $O^{\varepsilon 2}$	163	2	165	43	122
23	NH2-W- $O^{\varepsilon 2}$	162	1	163	39	124
24	N^{ε} -W- $O^{\varepsilon 2}$	78	3	81	28	53
Total number of incomplete water-mediated ionic interactions				3438	1057	2381

Supplementary table 3. Water-mediated ionic interaction networks observed within the subunits of different protein chains

No	Type	Number of water-mediated ionic interaction networks
1	$N^{\varepsilon 2}$ (a)-W- $O^{\delta 2}$ (c) $N^{\varepsilon 2}$ (b)-W- $O^{\delta 2}$ (c)	3
2	$N^{\varepsilon 2}$ (c)-W- $O^{\delta 1}$ (a) $N^{\varepsilon 2}$ (c)-W- $O^{\varepsilon 2}$ (b)	5
3	$N^{\delta 1}$ (c)-W- $O^{\delta 1}$ (a) $N^{\varepsilon 2}$ (c)-W- $O^{\varepsilon 1}$ (b)	3
4	N^{ζ} (a)-W- $O^{\delta 1}$ (c) $N^{\varepsilon 2}$ (b)-W- $O^{\delta 2}$ (c)	6
5	N^{ζ} (a)-W- $O^{\varepsilon 1}$ (c) $N^{\varepsilon 2}$ (b)-W- $O^{\varepsilon 2}$ (c)	4
6	N^{ζ} (a)-W- $O^{\varepsilon 1}$ (c) N^{ζ} (b)-W- $O^{\varepsilon 2}$ (c)	9
7	N^{ζ} (a)-W- $O^{\delta 2}$ (c) N^{ζ} (b)-W- $O^{\delta 2}$ (c)	4
8	N^{ζ} (c)-W- $O^{\delta 2}$ (a) N^{ζ} (c)-W- $O^{\delta 2}$ (b)	3
9	N^{ζ} (c)-W- $O^{\delta 1}$ (a) N^{ζ} (c)-W- $O^{\varepsilon 1}$ (b)	9
10	N^{ζ} (c)-W- $O^{\delta 1}$ (a) N^{ζ} (c)-W- $O^{\varepsilon 2}$ (b)	5
11	N^{ζ} (c)-W- $O^{\delta 2}$ (a) N^{ζ} (c)-W- $O^{\varepsilon 1}$ (b)	13
12	N^{ζ} (c)-W- $O^{\delta 2}$ (a) N^{ζ} (c)-W- $O^{\varepsilon 2}$ (b)	7
13	N^{ζ} (c)-W- $O^{\delta 1}$ (a) N^{ζ} (c)-W- $O^{\delta 2}$ (b)	12
14	N^{ζ} (c)-W- $O^{\varepsilon 1}$ (a) N^{ζ} (c)-W- $O^{\varepsilon 2}$ (b)	14
15	NH1(a)-W- $O^{\delta 1}$ (c) NH2(b)-W- $O^{\delta 2}$ (c)	6
16	NH1(a)-W- $O^{\varepsilon 1}$ (c) NH2(b)-W- $O^{\varepsilon 2}$ (c)	5
17	NH1(c) -W- $O^{\delta 2}$ (a) NH2(c) -W- $O^{\delta 2}$ (b)	4
18	NH1(c)-W- $O^{\delta 2}$ (a) NH2(c)-W- $O^{\varepsilon 1}$ (b)	5
19	NH1(c)-W- $O^{\delta 2}$ (a) NH2(c)-W- $O^{\varepsilon 2}$ (b)	3
20	NH2(c)-W- $O^{\varepsilon 1}$ (a) NH2(c)-W- $O^{\varepsilon 2}$ (b)	3
21	NH2(c)-W- $O^{\delta 2}$ (a) NH2(c)-W- $O^{\delta 2}$ (b)	3
22	NH2(c)-W- $O^{\delta 1}$ (a) NH2(c)-W- $O^{\varepsilon 1}$ (b)	4
23	NH2(c)-W- $O^{\delta 2}$ (a) NH2(c)-W- $O^{\varepsilon 1}$ (b)	3
24	NH2(c)-W- $O^{\delta 2}$ (a) NH2(c)-W- $O^{\varepsilon 1}$ (b)	3
25	NH2(c)-W- $O^{\delta 1}$ (a) NH2(c)-W- $O^{\delta 2}$ (b)	3
26	NH2(a)-W- $O^{\varepsilon 2}$ (c)	3

	NH2(b)-W- $O^{\varepsilon 2}$ (c)	
27	NH1(c)-W- $O^{\delta 1}$ (a) NH1(c)-W- $O^{\varepsilon 1}$ (b)	3
28	NH1(c)-W- $O^{\delta 2}$ (a) NH1(c)-W- $O^{\varepsilon 1}$ (b)	4
29	NH1(c)-W- $O^{\delta 1}$ (a) NH1(c)-W- $O^{\delta 2}$ (b)	5
30	NH1(c)-W- $O^{\varepsilon 1}$ (a) NH2(c)-W- $O^{\varepsilon 2}$ (b)	3
31	N^{ε} (c)-W- $O^{\delta 1}$ (a) N^{ε} (c)-W- $O^{\varepsilon 1}$ (b)	3
32	N^{ε} (c)-W- $O^{\delta 1}$ (a) N^{ε} (c)-W- $O^{\varepsilon 2}$ (b)	3
33	N^{ε} (c)-W- $O^{\delta 1}$ (a) N^{ε} (c)-W- $O^{\delta 2}$ (b)	3
34	N^{ζ} (a)-W- $O^{\delta 1}$ (c) NH2(b)-W- $O^{\delta 1}$ (c)	8
35	N^{ζ} (a)-W- $O^{\delta 2}$ (c) NH2(b)-W- $O^{\delta 2}$ (c)	3
36	N^{ζ} (a)-W- $O^{\varepsilon 2}$ (c) NH2(b)-W- $O^{\varepsilon 2}$ (c)	4
37	N^{ζ} (a)-W- $O^{\varepsilon 1}$ (c) NH2(b)-W- $O^{\varepsilon 1}$ (c)	3
38	N^{ζ} (a)-W- $O^{\delta 1}$ (c) NH2(b)-W- $O^{\delta 2}$ (c)	7
39	N^{ζ} (a)-W- $O^{\varepsilon 1}$ (c) NH2(b)-W- $O^{\varepsilon 2}$ (c)	6
40	N^{ζ} (a)-W- $O^{\delta 1}$ (c) N^{ε} (b)-W- $O^{\delta 1}$ (c)	3
41	NH2(a)-W- $O^{\varepsilon 2}$ (c) N^{ε} (b)-W- $O^{\varepsilon 2}$ (c)	3
42	NH2(a)-W- $O^{\varepsilon 1}$ (c) N^{ε} (b)-W- $O^{\varepsilon 2}$ (c)	5
43	NH1(a)-W- $O^{\delta 1}$ (c) N^{ε} (b)-W- $O^{\delta 2}$ (c)	3
44	NH1(a)-W- $O^{\varepsilon 1}$ (c) N^{ε} (b)-W- $O^{\varepsilon 2}$ (c)	3
45	NH1(c)-W- $O^{\delta 1}$ (a) N^{ε} (c)-W- $O^{\delta 1}$ (b)	3
46	NH1(c)-W- $O^{\varepsilon 2}$ (a) N^{ε} (c)-W- $O^{\varepsilon 2}$ (b)	3
47	N^{ζ} (a)-W- $O^{\delta 1}$ (c) NH1(b)-W- $O^{\delta 2}$ (c)	4
48	N^{ζ} (a)-W- $O^{\varepsilon 1}$ (c) NH1(b)-W- $O^{\varepsilon 2}$ (c)	3
49	NH2(a)-W- $O^{\delta 1}$ (c) $N^{\varepsilon 2}$ (b)-W- $O^{\delta 2}$ (c)	5

The characters (a, b and c) within the parentheses refer to different residues involved in the formation of hydrated ion pair networks.



Supplementary figure 1. Distribution of water-mediated ionic interactions formed by surface (S) and buried (B) water molecules.