

Table S4. Halogen-ionic bridges at protein-ligand interfaces

Halogen Ion Portion							Bound Ligand/Residue Portion					
No.	PDB	Halogen ion	Number in PDB file	Occupancy	B-factor	Branch degree <i>a</i>	Ligand/Residue <i>b</i>	Atom <i>c</i>	Charged state <i>d</i>	<i>D</i> (Å) <i>e</i>	<i>d</i> (Å) <i>f</i>	θ (°) <i>g</i>
1	1AID	Cl	1519	0.50	23.02	3	THK201	N1	c	3.075	/	/
							Ile50 (A)	N	u	3.070	2.137	154.5
							Ile50 (B)	N	u	3.038	2.082	159.3
2	2AID	Cl	1519	1.00	28.41	3	THK201	N1	c	2.993	/	/
							Ile50 (A)	N	u	3.264	2.208	168.7
							Ile50 (B)	N	u	3.296	2.286	156.6
3	1DAN	Cl	4737	1.00	27.23	3	DPN1	N	c	3.118	/	/
							Arg3 (C)	NE	c	3.309	/	/
							Gly219 (H)	N	u	3.245	2.421	139.3
4	1E6C	Cl	2702	1.00	20.20	3	MRD903	O2	u	3.067	2.265	140.5
							Arg11 (A)	N	u	3.271	2.284	169.0
							Arg139 (A)	NH1	c	3.395	/	/
5	1JIF	Cl	1914	1.00	24.60	3	BLM402	NK	u	3.319	2.355	157.1
							BLM402	NL	u	3.256	2.253	167.5
							His117 (A)	NE2	c	4.431	/	/
6	1K6E	Br	2329	0.75	27.77	2	PGO2001	O1	u	3.157	2.295	149.1
							Asn38 (A)	ND2	u	3.398	2.435	161.2
7	1K6E	Cl	2331	0.25	46.26	2	PGO2001	O1	u	3.154	2.295	148.9
							Asn38 (A)	ND2	u	3.391	2.427	161.6
8	1KQ3	Cl	2795	1.00	11.51	3	TRS2922	O2	u	3.176	2.323	147.6
							Thr173 (A)	OG1	u	2.867	2.103	131.6
							His252 (A)	CE1	c	3.591	/	/
9	1N5M	I	8355	0.60	45.82	3	GMN951	O1	u	3.312	2.379	163.9
							GMN951	O2	u	3.034	2.133	155.8
							Phe295 (A)	N	u	3.399	2.455	157.1
10	1OYJ	Cl	7139	1.00	54.81	2	GSW803	N3	u	3.143	2.403	128.7
							Lys114 (C)	NZ	c	3.186	/	/
11	1OYJ	Cl	7144	1.00	74.98	3	GSW803	N1	c	3.234	/	/
							Arg113 (C)	NH2	c	3.114	/	/
							Lys55 (D)	NZ	c	3.066	/	/
12	1R89	Cl	3636	1.00	49.64	3	CTP501	O3'	u	3.054	2.097	174.8
							Gly46 (A)	N	u	3.160	2.346	137.9
							Arg50 (A)	NH1	c	3.189	/	/
13	1SD0	Cl	2825	1.00	14.26	2	ARG403	NH1	c	3.445	/	/
							Thr273 (A)	N	u	3.333	2.411	153.0
							Thr273 (A)	OG1	u	2.794	1.911	145.7
14	1TY8	Cl	1981	1.00	19.52	3	ADP285	N6	u	3.312	2.319	164.0
							His53 (A)	ND1	c	4.074	/	/
							Gln55 (A)	N	u	3.382	2.440	156.7
15	1U2Q	Cl	1201	1.00	41.91	3	GOL165	O1	u	2.824	1.979	145.6
							Ile15 (A)	N	u	2.739	1.756	166.8
							Cys16 (A)	N	u	2.754	2.025	127.8
16	1V1M	Cl	5665	1.00	37.99	2	TDP1401	N4'	u	3.341	2.460	144.3
							Tyr113 (A)	OH	u	3.307	2.313	173.0
17	1VME	Cl	6590	1.00	26.64	5	MSE263	N	u	3.398	2.682	128.6
							Tyr264 (B)	N	u	3.211	2.214	174.1
							Phe266 (B)	N	u	3.380	2.638	131.2
							Val267 (B)	N	u	3.484	2.503	166.8
							Ser262 (B)	OG	u	3.762	2.769	171.9
18							APK481	O3'	u	2.675	1.750	160.5

	1VS0	Cl	4876	1.00	38.61	4	Ala463 (A)	N	u	3.346	2.366	166.5
							Lys635 (A)	NZ	c	3.686	/	/
							Arg629 (A)	NH1	c	3.934	/	/
19							APK481	O3'	u	2.674	1.735	164.9
	1VS0	Cl	4881	1.00	54.13	4	Ala463 (B)	N	u	3.181	2.196	168.2
							Lys635 (B)	NZ	c	4.038	/	/
							Arg629 (B)	NH2	c	4.429	/	/
20	1X7W	Cl	5643	1.00	32.62	2	TDP801	N4'	u	3.106	2.285	136.5
							Tyr113 (A)	OH	u	3.211	2.228	167.4
21	1X7X	Cl	5574	1.00	41.15	2	TDP801	N4'	u	3.009	2.183	136.9
							Tyr113 (A)	OH	u	3.241	2.252	169.7
22	1X7Y	Cl	5671	1.00	36.00	2	TDP901	N4'	u	3.210	2.389	136.8
							Tyr113 (A)	OH	u	3.312	2.333	165.9
23	1X80	Cl	5563	1.00	37.83	2	TDP801	N4'	u	3.066	2.305	130.3
							Tyr113 (A)	OH	u	3.178	2.196	166.8
24	1XC6	I	7850	0.70	28.66	2	BMA3004	O2	u	3.785	3.102	129.5
							Glu378 (A)	N	u	3.882	2.945	156.5
25	1XC6	I	7894	0.50	67.67	2	NAG4001	N2	u	3.178	2.177	166.7
							Arg154 (A)	NE	c	3.506	/	/
26							CME1014	N	u	2.893	2.031	135.6
	1XV5	Cl	3307	1.00	34.42	4	Val1016 (A)	N	u	3.212	2.535	124.8
							Thr1017 (A)	N	u	3.187	2.251	155.4
							Thr1017 (A)	OG1	u	3.613	2.844	134.1
27	1YB5	Cl	4923	1.00	31.03	3	NAP801	O3B	u	3.626	2.842	139.5
							Gly159 (A)	N	u	3.251	2.608	122.1
							Gly162 (A)	N	u	2.844	1.951	147.2
28	1YB5	Cl	4995	1.00	32.76	3	NAP801	O3B	u	3.596	2.795	141.5
							Gly159 (B)	N	u	3.221	2.538	125.3
							Gly162 (B)	N	u	2.848	1.942	149.4
29	1YQZ	Cl	7005	1.00	21.38	3	COA442	N4P	u	3.441	2.567	138.4
							Tyr361 (A)	OH	u	3.198	2.203	173.4
							Cys43 (B)	N	u	3.513	2.726	135.8
30							LI8501	N25	u	3.796	2.759	163.2
	1Z5M	Cl	2262	1.00	26.08	4	LI8501	N29	u	3.537	2.517	159.0
							Lys111 (A)	NZ	c	3.222	/	/
							Thr222 (A)	OG1	u	3.137	2.157	166.3
31							GOL2012	O3	u	3.171	2.438	133.0
	2AF6	I	15384	0.30	49.19	4	FAD2600	O2'	u	3.718	2.867	148.2
							Ser71 (D)	N	u	3.312	2.444	144.9
							Arg190 (D)	NH2	c	3.974	/	/
32	2B4G	Br	9754	0.40	32.69	2	GOL3401	O3	u	3.430	2.651	138.6
							Leu23 (C)	N	u	3.528	2.567	161.2
33							BU11501	O5	u	3.814	2.973	146.9
	2B9Y	Cl	3460	1.00	50.31	3	Arg88 (A)	NE	c	3.401	/	/
							Tyr297 (A)	OH	u	3.285	2.287	175.1
34							B121	N3	u	3.352	2.481	143.0
	2BB6	Cl	13021	1.00	23.93	4	Gln269 (A)	N	u	3.346	2.391	159.5
							Asn270 (A)	N	u	3.228	2.278	158.3
							Gln394 (A)	NE2	u	3.273	2.274	177.5
35							B121	N3	u	3.319	2.404	148.7
	2BB6	Cl	13113	1.00	24.48	4	Gln269 (B)	N	u	3.324	2.360	161.6
							Asn270 (B)	N	u	3.232	2.288	157.0
							Gln394 (B)	NE2	u	3.232	2.235	174.8
36							B121	N3	u	3.428	2.534	146.1

	2BB6	Cl	13205	1.00	23.74	4	Gln269 (C)	N	u	3.260	2.291	162.8
							Asn270 (C)	N	u	3.185	2.247	155.6
							Gln394 (C)	NE2	u	3.235	2.239	173.6
37							B121	N3	u	3.279	2.390	145.0
	2BB6	Cl	13297	1.00	24.67	4	Gln269 (D)	N	u	3.302	2.339	161.4
							Asn270 (D)	N	u	3.193	2.252	156.3
							Gln394 (D)	NE2	u	3.247	2.251	173.5
38							B121	N33	u	3.241	2.308	151.5
	2BBC	Cl	3256	1.00	37.10	4	Gln269 (A)	N	u	3.118	2.133	167.7
							Asn270 (A)	N	u	3.094	2.230	143.7
							Gln394 (A)	NE2	u	3.276	2.281	173.1
39							STU1302	N4	u	3.290	2.353	152.2
	2BUJ	Cl	4551	1.00	65.28	2	Arg59 (A)	NH1	c	3.535	/	/
40							U5P404	O3'	u	3.776	2.843	164.4
							Arg99 (V)	NH1	c	3.825	/	/
	2C37	Cl	46454	1.00	45.90	5	Gly137 (V)	N	u	3.489	2.798	126.7
							Arg139 (V)	N	u	3.588	2.603	168.1
							Arg139 (V)	NE	c	3.575	/	/
41							EDO1141	O1	u	2.704	2.089	120.4
	2CDP	Cl	4156	1.00	27.96	2	Gly72 (B)	N	u	2.863	1.983	145.4
42							GOL501	O2	u	3.187	2.595	120.2
	2CUN	Cl	6462	1.00	64.09	3	Arg114 (A)	NH2	c	3.270	/	/
							Arg154 (A)	NE	c	2.945	/	/
43							ACL703	NE	c	3.079	/	/
	2FIR	Cl	4728	1.00	41.78	3	ACL703	NH2	c	3.429	/	/
							Gly219 (H)	N	u	3.221	2.578	122.0
44							MSE1	N	u	3.600	2.668	155.1
	2FPO	Cl	8458	1.00	35.31	2	Ala110 (C)	N	u	3.291	2.621	124.4
45							MSE406	N	u	3.642	2.762	146.9
	2FPO	Cl	8461	1.00	35.38	3	Asn109 (F)	ND2	u	3.756	3.044	129.1
							Ala110 (F)	N	u	3.120	2.348	133.3
46							EDO251	O2	u	3.085	2.203	152.2
	2HI0	Cl	3783	1.00	23.64	3	Gly48 (B)	N	u	3.131	2.180	158.2
							Gly50 (B)	N	u	3.130	2.251	145.9
47							MSE106	N	u	3.185	2.351	140.3
	2I6G	Cl	2988	1.00	36.80	2	Ala135 (A)	N	u	3.148	2.206	156.4
48							MSE106	N	u	3.181	2.283	148.9
	2I6G	Cl	3017	1.00	50.38	2	Ala135 (B)	N	u	3.345	2.427	152.3
49							IZA300	NO	u	3.194	2.205	162.9
	2J90	Cl	4267	1.00	24.35	3	Lys42 (A)	NZ	c	3.328	/	/
							Asp161 (A)	N	u	3.232	2.355	146.0
50							IZA300	NO	u	3.198	2.211	162.2
	2J90	Cl	4295	1.00	38.83	3	Lys42 (B)	NZ	c	3.311	/	/
							Asp161 (B)	N	u	3.208	2.353	143.1
51							GOL1244	O2	u	3.281	2.416	149.7
	2JH7	Cl	1783	1.00	20.07	3	Ser17 (A)	OG	u	3.063	2.131	154.5
							Asp90 (A)	N	u	3.173	2.184	169.6
52							GOL1244	O2	u	3.216	2.306	158.1
	2JHD	Cl	1782	1.00	27.83	3	Ser17 (A)	OG	u	3.153	2.239	151.3
							Asp90 (A)	N	u	3.186	2.191	173.2
53							GOL300	O3	u	3.212	2.302	157.9
	2NMO	Cl	1190	1.00	10.08	4	Arg151 (A)	NH1	c	4.438	c	c
							Lys226 (A)	N	u	3.186	2.260	153.5
							Lys227 (A)	N	u	3.503	2.620	147.2

54	2NN8	Cl	1234	1.00	12.55	3	GOL600	O3	u	3.249	2.319	162.9
							Lys226 (A)	N	u	3.157	2.219	155.5
							Lys227 (A)	N	u	3.563	2.713	143.0
55	2OGS	Cl	3867	0.65	33.17	2	OCS408	N	u	3.859	2.814	165.4
							Ala407 (A)	N	u	3.777	2.890	148.4
56	2PJM	Cl	7088	1.00	22.56	3	PGO335	O2	u	3.859	3.045	143.5
							Gly100 (B)	N	u	3.224	2.494	129.4
							Cys102 (B)	N	u	3.169	2.196	163.7
57	2Q7X	Cl	4853	1.00	38.81	4	MSE225	N	u	3.308	2.331	165.3
							Asn223 (A)	ND2	u	4.100	3.180	153.5
							Ile224 (A)	N	u	3.194	2.502	126.1
							His308 (A)	CE1	c	4.093	/	/
58	2QKI	Br	17891	0.60	54.82	3	GOL824	O2	u	3.488	2.850	124.7
							Lys337 (D)	NZ	c	3.197	/	/
							Arg508 (D)	NH2	c	3.501	/	/
59	2QSZ	Cl	1566	1.00	42.87	2	MSE63	N	u	3.135	2.318	169.0
							Glu64 (A)	N	u	3.573	2.674	149.8
60	2V3N	Cl	3278	1.00	32.65	4	B121001	N33	u	3.492	2.525	158.2
							Gln269 (A)	N	u	3.105	2.112	172.1
							Asn270 (A)	N	u	3.165	2.267	148.7
							Gln394 (A)	NE2	u	3.218	2.224	172.2
61	2V3P	Cl	3271	1.00	43.35	4	B121415	N33	u	3.500	2.547	155.4
							Gln269 (A)	N	u	2.997	2.016	166.4
							Asn270 (A)	N	u	3.041	2.224	137.8
							Gln394 (A)	NE2	u	3.225	2.235	170.3
62	2VJK	Cl	6732	1.00	27.03	2	COA1169	N4P	u	3.491	2.488	155.8
							Gln262 (A)	N	u	3.042	2.130	150.8
63	2VJL	Cl	6765	1.00	28.81	2	COA1169	N4P	u	3.488	2.524	157.3
							Gln262 (A)	N	u	3.179	2.276	149.6
64	2VJX	Cl	13850	1.00	21.72	4	EDO1881	O2	u	3.526	2.740	139.6
							His627 (A)	CE1	c	3.676	/	/
							Gln685 (A)	N	u	3.200	2.227	164.0
							His774 (A)	CE1	c	3.763	/	/
65	2VJX	Cl	13942	1.00	25.50	4	EDO1881	O2	u	3.529	2.856	127.9
							His627 (B)	CE1	c	3.795	/	/
							Gln685 (B)	N	u	3.220	2.235	168.2
							His774 (B)	CE1	c	3.653	/	/
66	2VL4	Cl	13937	1.00	23.28	4	EDO1891	O2	u	3.748	3.055	130.4
							His627 (B)	CE1	c	3.768	/	/
							Gln685 (B)	N	u	3.245	2.268	165.3
							His774 (B)	CE1	c	3.716	/	/
67	2VX3	Cl	11123	1.00	45.41	3	D15600	NAT	u	3.258	2.318	152.5
							Lys188 (A)	NZ	c	3.098	/	/
							Asp307 (A)	N	u	3.432	2.754	125.4
68	2VX3	Cl	11197	1.00	47.87	3	D15600	NAT	u	3.177	2.187	163.3
							Lys188 (B)	NZ	c	3.307	/	/
							Asp307 (B)	N	u	3.468	2.795	125.1
69	2VX3	Cl	11282	1.00	61.57	3	D15600	NAT	u	3.318	2.540	132.7
							Lys188 (C)	NZ	c	3.113	/	/
							Asp307 (C)	N	u	3.414	2.760	123.4
70	2VX3	Cl	11347	1.00	56.35	2	D15600	NAT	u	3.111	2.355	130.1
							Lys188 (D)	NZ	c	2.961	/	/
71	2WBK	Cl	13644	1.00	37.85	2	EDO1878	O1	u	3.502	2.878	123.6
							Ile578 (B)	N	u	3.176	2.202	164.2

72	2WO6	CI	5709	1.00	47.32	2	D15600 Lys188 (B)	N NZ	u c	3.217 2.831	2.340 /	143.4 /
73	2ZHP	CI	1901	1.00	19.58	3	BY6301 BY6301 His117 (A)	NK NL NE2	u u c	3.317 3.273 3.469	2.387 2.274 /	151.2 165.7 /
74	2ZHP	CI	1994	1.00	25.75	3	BY6301 BY6301 His117 (B)	NK NL NE2	u u c	3.213 3.157 3.837	2.291 2.159 /	149.7 165.7 /
75	3BGU	CI	1708	1.00	20.64	3	EDO105 Ala33 (A) His73 (A)	O1 N CE1	u u c	2.948 2.928 4.462	2.099 1.949 /	146.6 165.8 /
76	3BYQ	CI	4458	1.00	25.00	4	EDO197 Lys81 (A) Arg106 (A) Val116 (A)	O1 NZ NH1 N	u c c u	3.044 3.355 3.479 3.389	2.377 /	126.2 /
77	3BYQ	CI	4502	1.00	24.20	4	EDO202 Lys81 (B) Arg106 (B) Val116 (B)	O1 NZ NH1 N	u c c u	3.016 3.243 3.337 3.364	2.289 /	131.9 /
78	3C8V	CI	14334	1.00	74.40	2	EDO487 Arg32 (B)	O1 NH1	u c	3.623 3.666	2.734 /	154.2 /
79	3C8V	CI	14376	1.00	59.51	3	EDO485 Arg32 (D) Tyr39 (D)	O2 NH1 OH	u c u	4.393 3.946 3.742	3.447 /	169.4 /
80	3C34	CI	4201	1.00	36.84	3	GOL403 Arg31 (A) Leu55 (A)	O1 NH1 N	u c u	3.472 3.275 2.888	2.841 /	124.1 /
81	3CLO	CI	6161	1.00	54.59	2	MSE81 Val57 (C)	N N	u u	3.497 4.034	2.565 3.133	155.0 150.5
82	3CLV	CI	1429	1.00	67.49	3	GDP211 GDP211 Lys186	N2 N3 NZ	u u c	2.924 3.600 4.310	1.919 2.838 /	167.7 131.8 /
83	3CNG	CI	5814	0.80	40.03	2	GOL501 Val150 (A)	O3 N	u u	2.911 3.192	2.016 2.275	154.1 151.8
84	3G3K	CI	9691	0.56	38.46	3	IPA266 Arg149 (A) Lys237 (B)	O2 NH2 NZ	u c c	3.063 3.278 4.429	2.305 /	135.4 /
85	3I6Y	CI	4548	1.00	12.33	3	MSE149 Leu55 (A) Ser148 (A)	N N OG	u u u	3.140 3.131 3.057	2.256 2.132 2.165	146.7 178.5 147.5
86	3I6Y	CI	4565	1.00	13.03	3	MSE149 Leu55 (B) Ser148 (B)	N N OG	u u u	3.135 3.165 2.960	2.173 2.165 2.050	160.7 177.8 150.1
87	3I7U	CI	4496	1.00	22.05	2	EDO163 Phe5 (D)	O2 N	u u	2.971 3.224	2.247 2.252	131.4 163.6
88	3IXQ	CI	7280	1.00	22.06	3	PGO233 Gly100 (B) Cys102 (B)	O1 N N	u u u	3.888 3.234 3.175	3.091 2.506 2.204	141.5 129.5 163.5
89	1Y8Z	CI	6741	1.00	36.06	4	CME1014 Val1016 (B) Thr1017 (B) Thr1017 (B)	N N N OG1	u u u u	3.138 3.114 3.383 3.809	2.295 2.374 2.447 2.884	134.4 130.1 155.7 154.3
90	2JLV	CI	7543	1.00	21.03	4	ANP1619 Arg418 (A)	O2' N	u u	3.322 3.385	2.679 2.457	124.9 154.2

								Arg418 (A)	NE	c	3.462	/	/
								Arg463 (A)	NE	c	3.810	/	/
91								ANP1619	O2'	u	3.471	2.850	123.2
	2JLV	Cl	7582	1.00	23.79	4		Arg418 (B)	N	u	3.326	2.400	153.7
								Arg418 (B)	NE	c	3.471	/	/
								Arg463 (B)	NE	c	3.852	/	/

a Branch degree: the number of atoms/groups that are bound to the central halogen ion.

b Ligand/Residue: the name and numbering of ligand/residue are same to that in PDB file; the letter in parenthesis is the chain name that the residue belongs to.

c Atom: atomic symbol is same to that in PDB file.

d Charged state: 'u' denotes uncharged and 'c' charged.

e D: the distance between the halogen ion and its bound heavy atom.

f d: the distance between the halogen ion and its bound hydrogen atom. This value, as well as the value of θ mentioned below, are not provided for those halogen-ionic bonds with charged atoms/groups, since these interactions are possibly not hydrogen bond and/or in which the hydrogen's position is difficult to be determined accurately due to the proton transfer.

g θ : the angle $\angle(X^{\cdot\cdot}H-Y)$, where $X^{\cdot\cdot}$ represents the halogen ion, H denotes the bound hydrogen atom, and Y is the hydrogen-bonded heavy atom.