Table 1. List of structures having short *X*···O contacts from a survey of the July 2004 release of the Protein Data Bank (PDB)

Bound group	Halogen	PDB code	Res., Å	*d*, Å	Θ_1	Θ_2	Ψ
Structures containing halogenated nucleotides							
P–O	Br	1RLG	2.7	3.12/3.13	174/161	104/114	
		1P54	1.9	3.03	169	117	
		376D	2.1	3.09	162	127	
	I	454D	1.2	3.13/3.06	176/163	110/118	
		1UE2	1.4	3.14	168	115	
C=O	Br	1J6S	1.4	2.99/2.95	158 /158	110/112	
O2'–H	Br	1J6S	1.4	3.12	166	134	
Complexes with proteins involving halogenated ligands							
C=O (peptide)	Cl	1L7X	2.3	3.25	121	137	P
		1PMQ	2.2	2.96	160	90	P
		1PMN	2.2	2.82	159	96	P
		1LKD	1.7	3.02	164	131	P
		1KZN	2.3	3.19	144	107	P
		1QYE	2.1	2.91	142	101	P
		1LEV	2.2	3.10	161	137	P
		1M78	1.7	3.25/3.24	130/133	146/147	L/L
		1RHR	3.0	3.11	144	106	P
		1J3J	2.3	3.05/3.22	175/169	104/114	P/P
		1JW7	2.3	3.01	167	122	L
		1RRV	2.0	3.08	125	96	P
		1C1E	1.9	2.98/2.85	148/153	74/81	P/P
		1G3M	1.7	3.13	147	123	L
		1C14	2.0	3.25	173	115	L
		1G0N	2.0	3.09	164	85	P
		1S1W	2.7	3.23	156	97	P
		1VJF	2.5	3.13	157	125	L
		1IEI	2.5	3.15	157	99	P
	Br	1N1G	2.5	3.28	128	126	L
		1GXZ	2.1	3.15	169	122	L
		1KI4	2.3	2.92/3.16	136/138	142/122	L/P
		1KGJ	2.3	3.29/3.35	138/150	84/102	P/P
		1E7B	2.4	3.21	151	122	L
		1E7C	2.4	3.17	149	127	L
		1RV1	2.3	3.05/3.14	163/160	123/122	P/P
		6STD	1.8	3.36/3.25/3.21	165/165/163	83/86/87	P/P/P
		1SEZ	2.9	3.30	177	88	P
		1J91	2.2	3.30	164	106	P
		1P5E	2.2	3.00/2.90/3.23/2.87/3.04	169/165/144/177/172	154/132/110/121/151	L/P/P/P/L
	I	1GJD	1.8	3.41	164	157	L
		1NQ0	2.4	3.32	173	124	P
		1NQ2	2.4	3.07	171	125	P
		1QK0	2.1	3.40	149	135	L
		1OPM	2.1	3.39	152	98	P

Bound group	Halogen	PDB code	Res., Å	*d*, Å	Θ_1	Θ_2	Ψ
		1SDW	1.9	3.45	149	96	P
		1THA	2.0	3.44/3.24/3.21	173/161/145	113/114/84	P/P/P
		1ETA	1.7	3.12/3.12	149/161	106/102	P/P
		1ETB	1.7	3.26/3.23	160/161	93/92	P/P
		1ICT	3.0	3.30/3.46/3.23	166/132/161	102/91/80	P/P/P
		1IE4	2.5	3.06	158	101	P
		1HKL	2.7	3.23/3.28/3.46	147/170/151	127/131/102	L/L/P
		1HK2	2.8	3.29/3.33/3.21	152/162/144	130/130/114	L/L/P
		1HK3	2.8	3.40/3.47/3.14	154/169/143	134/127/120	L/L/P
		1HK4	2.4	3.20	132	114	L
		1HK5	2.7	3.46	133	111	L
		1KGI	1.8	3.08/3.08	130/154	95/103	P/P
		1KED	2.2	2.84	167	90	P
		2ROX	2.0	2.79/3.25	163/167	95/90	P/P
		1F86	1.1	3.03/3.20	168/167	90/91	P/P
		1LIJ	1.9	3.34	162	113	P
COO^- (Asp/Glu)	Cl	1H1R	2.0	2.83	140	111	
		1CKP	2.0	3.04	130	97	
		1J51	2.2	3.04	135	129	
	Br	1FVT	2.2	3.21	127	87	
		1M5C	1.6	3.25	168	104	
	I	1ML7	1.2	3.29	174	108	
$CONH_2$ (Asn)	Cl	1PZO	1.9	3.06	148	101	
SO_4^{2-}	I	2GSQ	2.2	3.04	124	119	
OH(Ser/Thr/Tyr)	Cl	2GSS	1.9	3.09/3.07	169/164	114/114	
		1PY2	2.8	3.06	139	161	
		1GXF	2.7	3.12/3.14	149/146	108/112	
		1VJ3	2.1	2.72	145	110	
		1D8R	2.1	2.72	176	145	
	Br	1PWL	1.1	3.02	157	132	
		1M5D	1.7	3.27	136	96	
		1O27	2.3	3.24/3.20/3.13	120/121/121	114/110/113	
		1THC	2.3	3.05			
		1US0	0.7	2.97	153	132	
	I	1SO2	2.4	3.33/3.33	149/151	103/102	
		1ICT	3.0	3.30	166	102	

Ψ corresponds to the N–C=O···X torsion angle for halogen bonds involving the carbonyl group of the peptide backbone (see Fig. 3*d*). P, Perpendicular interactions involving the π system of the C=O bond; L, interactions involving the lone pair electrons of the oxygen of the C=O bond; Res, resolution. For a definition of *d*, Θ_1, and Θ_2, see Fig. 1.