Table S4 Weak Interactions in the crystals in this study

No.	E(SM)%		Interaction			Ang(^{0})	sym. cod.
1	23.5	π ··· π	Plane 3-3	3.47	3.67	18.7	-x+1,-y,-z+1
	14.2	CH/ π	C4-H16...P2	2.65	3.43	128.8	-x+1,y-1/2,-z+1/2
	8.6	HB	C10-H20...O24		3.39	113.9	x,y-1,z
	6.3	HB	O24-H25...O24		3.39	103.6	-x+1,-y-1,-z+1
	1.7	HB	C11-H21...Cl17		3.70	123.0	x-1,-y+1/2,z-1/2
2	15.9	CH/ π	C7-H19...P1	2.85	3.76	141.7	x+1/2,-y+1/2,-z+1
	15.9	HB	C4-H6...Cl18		3.59	118.1	-x+1/2,-y+1,z-1/2
	8.5	HB	C12-H22...O24		3.56	152.0	-x,y+1/2,-z+3/2
	7.0	CH/ π	C15-H29...P2	2.51	3.53	158.2	-x+1,y-1/2,-z+3/2
3	22.4	π ··· π	Plane1-1	3.77	3.93	16.7	x,y-1,z
	7.2	CH/ π	C6-H18...P3	3.11	4.02	147.8	x-1/2,-y+3/2,-z-1
	5.1	Cl/Cl	C10-Cl20...Cl22-C12	3.79	149.2	83.3	-x-1,y+1/2,-z-3/2
	1.8	HB	C4-H16...Cl22		3.68	115.3	-x-3/2,-y+2,z-1/2
4	14.9	CH/ π	C8-H26....P2	2.91	3.56	118.3	-x-1/2,-y,z-1/2
	8.3	CH/ π	C6-H18...P2	2.81	3.63	138.2	-x-1,y-1/2,-z-1/2
	7.2	HB	C3-H15...O24		3.30	125.2	x,y,z-1
	6.5	HB	C12-H22....N1		3.74	138.1	x-1/2,-y-1/2,-z-1
5	21.5	π ··· π	Plane 1-1	3.30	4.48	42.6	x,y-1,z
	21.5	π ··· π	Plane 2-2	3.35	4.48	41.6	x,y-1,z
	5.6	HB	C8-H26...O24		3.40	151.5	x+1/2,-y+1,z
	4.6	HB	C7-H19...O24		3.38	106.8	x+1/2,-y+2,z
6	21.5	π ··· π	Plane3-3	3.68	3.89	18.7	-x+1,-y,-z+1
	11.9	HB	C10-H20...O15		3.69	156.6	-x+1,-y-1,-z+1
	9.1	HB	C8-H25...O15		3.29	116.5	x,y-1,z
	8.3	CH/ π	C7-H19...P1	2.70	3.47	128.1	-x+1/2,y-1/2,-z+3/2
	6.4	CH/ π	C13-H23...P2	2.83	3.65	132.3	-x+3/2,y-1/2,-z+3/2
	1.6	HB	C6-H18...Cl22		3.56	126.3	x+1,y,z
7	20.5	π ··· π	Plane 1-1	3.38	4.82	45.4	x,y-1,z
	20.5	π ··· π	Plane 2-2	3.54	4.82	42.7	x,y-1,z
	5.0	CH/ π	C11-H21...P3	3.25	4.11	137.2	-x+1,y+1/2,-z+1
	1.5	Cl/Cl	C12-Cl22...Cl16-C4	3.61	106.8	99.5	x+1,y-2,z
8	21.4	π ··· π	Plane 1-1	3.36	4.75	45.0	x,y-1,z
	21.4	π ··· π	Plane 2-2	3.56	4.75	41.5	x,y-1,z
	5.2	HB	C13-H23...N1		3.59	135.5	-x+1,y+1/2,-z+2
	2.9		C10-H20...Cl16		3.74	114.6	-x,y+3/2,-z+1
9	21.4	CH/ π	C5-H17...P1	3.52	3.89	105.1	x,y-1,z
	21.4	π ··· π	Plane 1-1	3.31	4.74	45.8	x,y-1,z
	21.4	π ··· π	Plane2-2	3.50	4.74	44.2	x,y-1,z
	5.1	CH/ π	C11-H21...P3	3.29	4.05	137.2	-x-1,y+1/2,-z+1
	0.4	HB	C11-H21...N1		3.56	133.7	-x-1,y+1/2,-z-1
10	16.9	π ··· π	Plane 2-2	3.42	3.82	26.7	-x+2,-y+1,-z+2

	8.5	CH/π	C4-H16...P1	2.84	3.62	138.6	-x+1,y+1/2,-z+3/2
	8.2	CH/π	C6-H18...P2	2.78	3.48	130.2	x+1,y,z
	5.0	HB	C13-H23...Cl21		3.62	117.5	x,y-1,z
11	21.5	CH/π	C8-H25...P3	3.61	3.76	89.8	x+1/2,-y+1/2,-z+2
	5.5	HB	C14-H24...Br21		3.96	141.8	-x+1,y-1/2,-z+5/2
	5.5	HB	C7-H19...Cl16		3.86	146.7	-x+1,y-1/2,-z+5/2
	5.2	HB	C7-H19...Br21		3.91	113.6	-x+1/2,-y+1,z-1/2
12	27.0	π ··· π	Plane 3-3	3.42	3.59	17.7	-x,-y+1,-z+1
	11.3	π ··· π	Plane 2-2	3.56	3.70	16.1	-x,-y,-z+1
	8.9	CH/π	C25-H31...P1	2.96	3.84	156.4	-x-1,y-1/2,-z+1/2
13	23.0	π ··· π	Plane1-1	3.71	4.55	35.5	-x+1,-y+2,-z+1
	23.0	π ··· π	Plane3-3	3.37	3.77	26.8	-x+1,-y+2,-z+1
	23.0	HB	C26-H31...Cl21		3.68	137.7	-x+1,-y+2,-z+1
	6.0	Cl/Cl	C11-Cl21...Cl23-C13	3.68	86.8	104.6	x,-y+3/2,z-1/2
	2.0	HB	C4-H16...Cl21		3.68	141.2	x-1,-y+2,-z+1
14	23.7	π ··· π	Plane 3-3	3.39	3.55	17.1	-x+1,-y,-z+1
	22.3	π ··· π	Plane 3-3	3.53	3.84	23.4	-x+2,-y,-z+1
	14.6	HB	O23-H26...O2		2.77	148.9	-x+1,-y+1,-z+1
	6.3	HB	C4-H16...Cl19		3.65	116.2	x,y+1,z
	6.3	HB	C4-H16...O24		3.48	106.0	x,y+1,z
15	15.3	CH/π	C12-H12...P1		3.47	126.9	-x+1,-y+1,-z+1
	15.3	CH/π	C13-H13...P3		3.65	121.7	-x+1,-y+1,-z+1
	15.3	π ··· π	Plane3-3	4.24	4.66	24.66	-x+1,-y+1,-z+1
	12.6	CH/π	C10-H10...P3		3.63	138.8	x,-y+1/2,z+1/2
	12.6	HB	C6-H6...N2		3.48	126.8	x,-y+1/2,z+1/2
	0.2	HB	C14-H14B...Cl1		3.73	174.5	x+1,y,z-1

_geom_table_footnote_B
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Plane 3: the central part C-C=N-C.
P1, P2, P3 are respectively the centers of the corresponding planes.
For the definitions of the planes 1 & 2, see Table 3.
CH/π (Dmezawa, 1998): two phenyl rings take "T" shape through C-H in a phenyl ring, directing towards the center of another phenyl ring or the center of a π -conjugative system, Parameters followed are the distance between the C and the center (P) of the ring and the angle C-H...P, respectively.
π ··· π (Sharma, 1993): two parallel phenyl rings or π -systems are stacked closely, which makes most of the atoms involved very closely. The parameters followed are respectively the distances between the planes, the centers and the shearing angle.
For type, T: translation, S: screw, I: inversion, G: glide.
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