

On the significance of weak hydrogen bonds in crystal packing: a large databank comparison of polymorphic structures

Leonardo Lo Presti^{a,b,c}

^a Università degli Studi di Milano, Department of Chemistry, Via Golgi 19 I-20133 Milano (Italy)

^b Centre for Materials Crystallography, Århus University, Langelandsgade 140, DK-8000 Århus C. (Denmark)

^c Istituto di Scienze e Tecnologie Molecolari, Italian CNR, Via Golgi 19 I-20133 Milano (Italy)

To whom correspondence should be addressed: leonardo.lopresti@unimi.it

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ELECTRONIC SUPPLEMENTARY INFORMATION

Table S1. List of CSD refcodes constituting the POLY-*all* dataset, in alphabetical order. Chemically related polymorphs are listed close to each other.

ABAKEV01	DADDER03	FUQWAQ01	KADPOU	NAJBEF	PROGST13
ABAKEV02	DAKFUQ	FUWFAG	KADPOU01	NAJBEF01	PUBMUU01
ABEYOY	DAKFUQ01	FUWFAG01	KADTEO	NANQUO	PUBMUU05
ABEYOY01	DATWUS	GAGSIR	KADTEO01	NANQUO02	PUBMUU07
ABIZAP	DATWUS01	GAGSIR01	KADTEO02	NAPQAZ	PUGVUK
ABIZAP01	DAXTIH	GEBSOV	KAGCIE02	NAPQAZ01	PUGVUK01
ACEDAN	DAXTIH01	GEBSOX	KAGCIE03	NAPTAN01	PUGWUK
ACEDAN01	DCLANT01	GEMGAG01	KANYUU02	NAPTAN02	PUGWUK01
ACRDIN04	DCLANT10	GEMGAG02	KANYUU03	NAXFUO	PURSEB
ACRDIN05	DCLBQN01	GOFVAZ	KAWJAU	NAXFUO01	PURSEB01
ACRDIN07	DCLBQN02	GOFVAZ01	KAWJAU01	NAYNUX	PURSEB02
AHAPEG	DCLNAP01	GOLLUO	KAZDUL01	NAYNUX01	PUVVUX
AHAPEG01	DCLNAP02	GOLLUO01	KAZDUL03	NEHREZ	PUVVUX01
AJETAL	DEBMUS	HAJYUN01	KETYAJ	NEHREZ01	PYMSUL10
AJETAL01	DEBNAZ	HAJYUN02	KETYAJ01	NEPTAZ	PYMSUL11
ANUKAW	DEMQUIW	HAKTAP	KIFHUC	NEPTAZ01	QAMNAT
ANUKAW01	DEMQUIW01	HAKTAP01	KIFHUC01	NIPSOV	QAMNAT01
APEPES	DEWCAK	HEHWOJ	KIGTOL	NIPSOV01	QANHAP
APEPES01	DEWCAK01	HEHWOJ01	KIGTOL01	NOQFII	QANHAP01
AZADAG	DIWKOK	HEWL0L01	KIJQEA01	NOQFII01	QEJZAH
AZADAG01	DIWKOK01	HEWL0L02	KIJQEA02	NORFUX	QEJZAH02
AZADAG02	DIWMOM02	HMHOCN07	KIZMAI	NORFUX01	QILYUH
BAHNUU	DIWMOM03	HMHOCN08	KIZMAI01	NUJLIN	QILYUH01
BAHNUU01	DIXBIW	HNIABZ11	KUDXAK	NUJLIN01	QIXFUY
BANHOO01	DIXBIW01	HNIABZ21	KUDXAK01	NUKMAH	QIXFUY01
BANHOO02	DMETSO04	HOFFEN	LEQPIH	NUKMAH02	QOGNEF01
BCOCAN01	DMETSO05	HOFFEN02	LEQPIH01	NUNCAB	QOGNEF02
BCOCAN03	DMFUSC03	HOKMAW	LIKBOU	NUNCAB02	QUZREJ01
BDTOLE13	DMFUSC04	HOKMAW01	LIKBOU01	NXENAM	QUZREJ03
BDTOLE14	DOLJET	IBOBUY	LIVQOY	NXENAM01	RAFFIO
BEBMAX	DOLJET01	IBOBUY01	LIVQOY05	OGOMON	RAFFIO01
BEBMAX01	DOZYAS	IBULIA	LOZYII	OGOMON01	RAFGAJ
BENCLN02	DOZYAS01	IBULIA01	LOZYII01	OHIBOW	RAFGAJ01
BENCLN05	DUDCUC	IHEMIR	LUFCIY	OHIBOW02	RAXRAK
BIINDO	DUDCUC01	IHEMIR01	LUFCIY01	OLATUR	RAXRAK01
BIINDO02	DUDCUC02	IPXUB08	LUKXAQ	OLATUR01	RIGHUK07
BILCOO10	DUDNAS	IPXUB11	LUKXAQ01	OMEFAN	RIGHUK09
BILCOO11	DUDNAS01	IPXUB13	MAFPOA	OMEFAN01	RUVZOY
BIRKIW02	DURZUM	IQAREY	MAFPOA01	OVEPUC	RUVZOY01
BIRKIW03	DURZUM01	IQAREY01	MANPIM01	OVEPUC01	SAXJEG
BOLMIZ	EDAXEM	IVATAC	MANPIM02	PABHAB	SAXJEG01
BOLMIZ02	EDAXEM01	IVATAC01	MATDEQ	PABHAB01	SAYVEV
BPHENO03	EGOPIB	IWUKAM	MATDEQ01	PANQUO	SAYVEV01
BPHENO18	EGOPIB01	IWUKAM01	MBYINO	PANQUO01	SEBTAU
BUDYOP	EKIPUL	IWUKAM02	MBYINO02	PAVBEU	SEBTAU01
BUDYOP01	EKIPUL01	JATFUF03	MEGYON01	PAVBEU01	SEMYIT
BUFTED	EROGUP	JATFUF04	MEGYON02	PEGWII	SEMYIT01
BUFTED01	EROGUP01	JATXOU	MEHROH	PEGWII01	SESYAR
BUYZUQ	EYIWU	JATXOU01	MEHROH02	PEJBUC	SESYAR01
BUYZUQ02	EYIWU01	JAVCEO02	MELVEE	PEJBUC01	SIHNII
CAFCUK	FABRAB10	JAVCEO04	MELVEE01	PEJHOD	SIHNII01
CAFCUK01	FABRAB11	JOTNAH	MEQVAG	PEJHOD01	SIRJUZ
CAFSIO	FATYOP	JOTNAH01	MEQVAG01	PEJJOF	SIRJUZ01
CAFSIO01	FATYOP01	JOWNAM	MIQKOM	PEJJOF01	SIWDEH
CARBIJ	FEFPEM	JOWNAM01	MIQKOM01	PHISCY01	SIWDEH01
CARBIJ01	FEFPEM01	JOWPAO	MIZHOT01	PHISCY02	SOCRUZ
CEWGAM	FEVNAV01	JOWPAO01	MIZHOT02	PIMTAZ01	SOCRUZ01
CEWGAM01	FEVNAV02	JUDRAB	MMANCN	PIMTAZ02	SOLSIW
CINYEE	FEVWUY	JUDRAB01	MMANCN02	PINPAD	SOLSIW01
CINYEE01	FEVWUY01	JULBUN	MONTIS	PINPAD01	SUBTIS02
CIVTUW	FOBSOE02	JULBUN01	MONTIS01	POFLAX	SUBTIS03
CIVTUW01	FOBSOE03	JULZAR	MSULIN04	POFLAX01	SUGGEG01
CYVTPA	FOVYOE	JULZAR01	MSULIN05	PRMDIN01	SUGGEG02
CYVTPA01	FOVYOE11	KADNEI	NAGNER	PRMDIN02	SUKNIW01
DADDER	FUQWAQ	KADNEI01	NAGNER01	PROGST12	SUKNIW02

TACRIB04	TUZYIY01	VISSOF01	XEPXOF	YAXCEH01	ZELDOJ
TACRIB07	UHULEQ	VUYPUC	XEPXOF01	YELHUS	ZELDOJ01
TADLIU01	UHULEQ01	VUYPUC01	XEWZAB	YELHUS01	ZILNOX
TADLIU02	UHULEQ02	WAMFAS01	XEWZAB01	YICDIZ	ZILNOX01
TALNAV01	UJICEX	WAMFAS03	XIYXIN	YICDIZ01	ZOGQAN03
TALNAV02	UJICEX01	WECCUC	XIYXIN01	YICDUL	ZOGQAN05
TELKUQ	USOGOZ	WECCUC01	XOCXUI01	YICDUL01	ZZZBLP02
TELKUQ01	USOGOZ02	WOVGIZ	XOCXUI02	YIVRIF	ZZZBLP03
TENMIK	VALLIE	WOVGIZ01	XOKYAZ	YIVRIF01	ZZZMUC08
TENMIK01	VALLIE01	WUXDOJ	XOKYAZ01	YIVRIF02	ZZZMUC09
TIZWAA	VECRUR02	WUXDOJ02	YAKYAL	YOLDAF01	ZZZWGK01
TIZWAA01	VECRUR03	XAJFOG	YAKYAL01	YOLDAF04	ZZZWGK03
TNBENZ11	VEJDUL	XAJFOG01	YAMHID	YORYAH	
TNBENZ12	VEJDUL01	XEBBOY	YAMHID03	YORYAH01	
TOQPUM	VEMTOW	XEBBOY01	YAPFIH	YORYAH02	
TOQPUM02	VEMTOW01	XEHHEX	YAPFIH01	YOWYOY	
TUDROZ	VIFVUC	XEHHEX01	YASKOS	YOWYOY02	
TUDROZ01	VIFVUC01	XEJNUV	YASKOS01	YUMKOH	
TUZYIY	VISSOF	XEJNUV01	YAXCEH	YUMKOH01	

Table S2. List of CSD refcodes constituting the POLY-*pix* dataset, in alphabetical order. Chemically related polymorphs are listed close to each other.

ABAKEV01	MANPIM01	SIHNII
ABAKEV02	MANPIM02	TADLIU01
ABIZAP01	MEGYON01	TADLIU02
ABIZAP	MEGYON02	XEWZAB01
ACRDIN04	MIZHOT01	XEWZAB
ACRDIN05	MIZHOT02	YAKYAL01
ACRDIN07	MONTIS01	YAKYAL
AHAPEG01	MONTIS	ZZZBLP02
AHAPEG	MSULIN04	ZZZBLP03
ANUKAW01	MSULIN05	ZZZWGK01
ANUKAW	NANQUO02	ZZZWGK03
BCOCAN01	NANQUO	
BCOCAN03	NAPQAZ01	
BEBMAX01	NAPQAZ	
BEBMAX	NAPTAN01	
CINYEE	NAPTAN02	
CINYEE01	NIPSOV01	
DCLBQN01	NIPSOV	
DCLBQN02	NUJLIN01	
DEBMUS	NUJLIN	
DEBNAZ	NUKMAH02	
DIWKOK	NUKMAH	
DIWKOK01	OHIBOW02	
DUDNAS01	OHIBOW	
DUDNAS	PANQUO01	
FABRAB10	PANQUO	
FABRAB11	PEGWII01	
GAGSIR01	PEGWII	
GAGSIR	PEJBUC01	
HAJYUN01	PEJBUC	
HAJYUN02	PEJHOD01	
HEHWOJ01	PEJHOD	
HEHWOJ	PEJJOF01	
HOKMAW01	PEJJOF02	
HOKMAW	PHISCY01	
IBOBUY01	PHISCY02	
IBOBUY	QAMNAT01	
JATFUF03	QAMNAT	
JATFUF04	QOGNEF01	
KAWJAU01	QOGNEF02	
KAWJAU	RIGHUK07	
LIKBOW01	RIGHUK09	
LIKBOW	SAYVEV01	
LOZYII01	SAYVEV	
LOZYII	SESYAR01	
MAFPOA01	SESYAR	
MAFPOA	SIHNII01	

Table S3. Number of close contacts in POLY-*all*, as a function of the chemical nature of the donor and acceptor group, depending on the distance cutoff P (see text).

	N_c^a				$R_{av}/\text{\AA}^b$		
<i>Donor: Aromatic H</i>							
<i>Acceptor</i>	$P=$	0.90	0.95	1.00	0.90	0.95	1.00
Aliphatic Nitrogen		0	0	10	// ^c	// ^c	2.67(1)
N aromatic		14	72	157	2.38(2)	2.512(9)	2.594(8)
–CN or –N=N		14	48	91	2.40(1)	2.50(1)	2.58(1)
–O– ether		12	28	78	2.377(8)	2.44(1)	2.56(1)
C=O (Oxygen)		108	254	423	2.324(6)	2.413(6)	2.490(6)
N=O (Oxygen)		31	89	149	2.33(1)	2.437(9)	2.506(9)
S=O (Oxygen)		10	26	47	2.34(2)	2.425(2)	2.51(2)
–S–		0	8	44	// ^c	2.73(1)	2.819(9)
C=S (Sulphur)		0	1	2	// ^c	// ^c	2.81(8)
O=S (Sulphur)		0	1	1	// ^c	// ^c	// ^c
–F		0	5	22	// ^c	2.39(1)	2.48(1)
–Cl		0	6	43	// ^c	2.69(1)	2.780(9)
<i>Donor: Acetilenic H</i>							
<i>Acceptor</i>	$P=$	0.90	0.95	1.00	0.90	0.95	1.00
CN or –N=N		2	2	3	2.3(1)	2.3(1)	2.4(1)
<i>Donor: Aliphatic CH,CH₂,CH₃</i>							
<i>Acceptor</i>	$P=$	0.90	0.95	1.00	0.90	0.95	1.00
Aliphatic Nitrogen		1	6	16	// ^c	2.540(2)	2.62(2)
N aromatic		2	17	47	2.43(1)	2.53(1)	2.622(1)
–CN or –N=N		0	11	34	// ^c	2.52(1)	2.633(2)
–O– ether		10	55	132	2.33(3)	2.46(1)	2.551(8)
C=O (Oxygen)		67	170	328	2.351(5)	2.428(6)	2.520(6)
N=O (Oxygen)		22	68	122	2.35(1)	2.441(9)	2.52(1)
S=O (Oxygen)		14	29	46	2.32(2)	2.41(2)	2.49(2)
–S–		0	7	20	// ^c	2.73(1)	2.81(2)
C=S (Sulphur)		0	2	13	// ^c	2.65(2)	2.82(2)
O=S (Sulphur)		0	0	1	// ^c	// ^c	// ^c
–F		0	1	12	// ^c	// ^c	2.47(1)
–Cl		0	3	13	// ^c	2.69(2)	2.78(2)

^a Number of contacts satisfying the close contact requirements detailed in Section 2.2.

^b Average H...A distance in Å, with the estimated standard deviation in parentheses.

^c No averages are performed if the number of contacts is lower than 2.

Table S4. AA–CLP cohesive energies ($\text{kJ}\cdot\text{mol}^{-1}$), with the corresponding decomposition into Coulomb (E_c), polarization (E_p), dispersion (E_d), repulsion (E_r) and dipole (E_{dip}) terms, for the POLY–*all* dataset. Entries in the Table are organized as follows (from left to right): CSD refcode, space group label, E_c , E_p , E_d , E_r , E_{dip} and E_{coh} .

ABAKEV01	'P 21 21 21'	-10.9	-16	-90.6	27.5	0	-89.9
ABAKEV02	'P 21/c'	-11.7	-16	-91	30.5	0	-88.3
ABEYOY	'P 21 21 21'	-38	-63.2	-166.8	73.7	0	-194.3
ABEYOY01	'P 21'	-19.7	-63.1	-168	77.1	-22.1	-195.8
ABIZAP	'P -1'	-23.8	-28.1	-130.5	46.6	0	-135.8
ABIZAP01	'P 21/n'	-34.7	-29.7	-133.5	54	0	-143.9
ACEDAN	'P 21/c'	-7.6	-21.6	-142.2	50.7	0	-120.6
ACEDAN01	'P 21/c'	-5	-22.4	-149.2	60.1	0	-116.6
ACRDIN04	'P 21/n'	-5.9	-13.5	-120.3	33.9	0	-105.8
ACRDIN05	'C c'	-12.5	-12.9	-110.3	31.2	-2.8	-107.2
ACRDIN07	'P 21/c'	-8.8	-12.8	-109.4	28.3	0	-102.7
AHAPEG	'C 2/c'	-27.7	-37.2	-190.5	73.3	0	-182.2
AHAPEG01	'C 2/c'	-20	-35.7	-176.3	59.5	0	-172.5
AJETAL	'C 2/c'	-7.6	-36.2	-151.5	57.9	0	-137.4
AJETAL01	'P 21/c'	-12.7	-35.9	-146.3	56.6	0	-138.3
ANUKAW	'P -1'	-28.2	-41.3	-198.1	90	0	-177.7
ANUKAW01	'C 2'	-26.2	-44.7	-202.3	102.1	0	-171.1
APEPES	'P 21/n'	-17.4	-36.6	-180.2	70.8	0	-163.4
APEPES01	'P -1'	-17.1	-39.7	-204.1	92.6	0	-168.3
AZADAG	'P 21/c'	-26.8	-23.4	-132.7	53.7	0	-129.1
AZADAG01	'P -1'	-15.8	-22.3	-124.7	42.9	0	-119.8
AZADAG02	'P b c a'	-16.3	-20.8	-116.3	62.3	0	-91.1
BAHNUU	'P 21/n'	-4.5	-4.9	-139.8	29	0	-120.3
BAHNUU01	'P 21/c'	4.9	-5.4	-140.5	27.1	0	-114
BANHO001	'C c'	-20.2	-29.9	-154.8	54.7	-8.8	-159
BANHO002	'C c'	-20.9	-28	-147	59.9	-9.3	-145.4
BOCAN01	'C c'	-29.7	-25.5	-120	40.8	-3.3	-137.7
BOCAN03	'P 21/c'	-37.9	-27.9	-133.9	67	0	-132.8
BDOLE13	'P 21/n'	5.6	-21.9	-116.7	27.1	0	-106
BDOLE14	'P -1'	-3.7	-20.2	-104.9	24.3	0	-104.5
BEEMAX	'C m c 21'	-13.5	-46.3	-185.2	63.3	-8.5	-190.2
BEEMAX01	'P b c n'	-21.8	-45.7	-186.5	74.9	0	-179
BENCLN02	'P c c n'	-18	-25.4	-116.6	78.4	0	-81.6
BENCLN05	'P 21/c'	-22.9	-22.7	-98.7	49.6	0	-94.8
BIINDO	'P 21/n'	-27.9	-27.1	-148.9	60.4	0	-143.5
BIINDO02	'F d d 2'	-26.8	-28.4	-159.5	73.1	0	-141.6
BILCOO10	'P 21/n'	-4.6	-29.8	-119.4	40.2	0	-113.6
BILCOO11	'P 21/c'	-3.1	-33	-138.6	50.4	0	-124.4
BIRKIWO2	'C c'	-12.7	-20.2	-149.9	35.8	0	-147
BIRKIWO3	'P -1'	-13.6	-21.8	-168.5	47.4	0	-156.4
BOLMIZ	'P 21/c'	-15.8	-16.5	-158	41.1	0	-149.2
BOLMIZ02	'P b c n'	-14.6	-16.8	-167.2	44	0	-154.6
BPHEO03	'C 2/c'	-16.6	-13.8	-97.8	33.5	0	-94.6
BPHEO18	'P 21 21 21'	-16.3	-14.2	-107.5	38.5	0	-99.4
BUDYOP	'C c'	-17	-19.2	-139.8	50.5	-2.9	-128.3
BUDYOP01	'P 21/c'	-21	-17.2	-115.8	35.8	0	-118.1
BUFTED	'P 21'	-38.9	-47.4	-135.4	66.5	-0.7	-155.8
BUFTED01	'P 21'	-39.2	-49.1	-140.6	78	0	-150.8
BUYZUQ	'P 21 21 21'	-32	-39.4	-98	50.5	0	-118.9
BUYZUQ02	'P 21'	-29.3	-42.2	-110.1	51.4	-2.5	-132.6
CAFCUK	'P -1'	-28.3	-58.8	-119.6	61.6	0	-145.1
CAFCUK01	'P 21/c'	-34.7	-58.2	-114.8	63.6	0	-144.1
CAFSIO	'P 21'	8.2	-34.6	-160.5	66.3	-26.1	-146.7
CAFSIO01	'P 21/c'	-26.1	-34.9	-164.8	64.3	0	-161.5
CARBJ	'P 21/n'	-6.2	-23.4	-203.3	52.3	0	-180.6
CARBJ01	'P c c n'	-11.8	-23.3	-200.5	52.3	0	-183.4
CEWGAM	'P 21/c'	-6.4	-38.5	-143.4	39.2	0	-149.2
CEWGAM01	'P -1'	-8.4	-39.5	-152.7	47	0	-153.5
CINYE	'P 21'	-11.1	-30.5	-181.7	60.6	-2	-164.7
CINYE01	'P 21 21 21'	-13.1	-29.7	-174.6	72.9	0	-144.6
CIVTUW	'P 21 21 21'	-52	-48.2	-158.3	99.7	0	-158.9
CIVTUW01	'P 1 1 21/n'	-44.4	-45.6	-150.2	78	0	-162.1
CVTPA	'B 1 1 2/b'	-19.1	-32.7	-151.7	48.7	0	-154.8
CVTPA01	'P b c a'	-18.2	-36	-165.8	53.5	0	-166.5
DADDER	'P 21/n'	-20.7	-20.2	-119.7	38.7	0	-121.9
DADDER03	'P -1'	-18.4	-19.8	-121.4	36.9	0	-122.7
DAKFUQ	'P 21/n'	-28.4	-21.4	-127.3	32.4	0	-144.7
DAKFUQ01	'C 2/c'	-24.4	-21.5	-125.5	36.6	0	-134.8
DATWUS	'P 21/c'	3.2	-31	-151.8	49.4	0	-130.2
DATWUS01	'P 21/c'	3.5	-30.5	-148.7	46.7	0	-129
DAXTIH	'P 21/c'	-23.1	-30.7	-173.3	74.7	0	-152.4
DAXTIH01	'P -1'	-21	-31	-181.8	107.4	0	-126.5
DCLANT01	'P -1'	-0.5	-8.6	-145.4	35.1	0	-119.5
DCLANT10	'P 21/a'	-1.3	-8.7	-146.7	36.1	0	-120.6
DCLBQ01	'P 21/c'	-40.1	-19.9	-88.7	53.7	0	-95.1
DCLBQ02	'P -1'	-40.6	-20.5	-92.8	57.9	0	-95.9
DCLNAP01	'P b 21 a'	1.5	-15.3	-117	41.3	-2.5	-92.1
DCLNAP02	'P -1'	-12.1	-15.4	-118.6	44.6	0	-101.4
DEBMUS	'P 21 21 21'	-9.9	-27.3	-163.2	51.5	0	-149
DEBNAZ	'P n a 21'	-8.7	-26.2	-155.8	47.1	0	-143.7
DEMQUIW	'P 21/c'	-0.8	-7.5	-56.5	19.5	0	-45.3
DEMQUIW01	'P 21/c'	-0.7	-7.2	-52.7	16.3	0	-44.3
DEWCAK	'P -1'	-9.6	-66.7	-230.7	73.3	0	-233.6
DEWCAK01	'P b c a'	-18.7	-71.7	-256.7	107.2	0	-239.9

DIWKOK	'P 21'	-18.4	-31.7	-135.2	65.2	-6	-126
DIWKOK01	'P 21 21 21'	-26.2	-32	-136.7	67.6	0	-127.2
DIWMOM02	'P 2/c'	-7.8	-16.3	-145.9	38.7	0	-131.3
DIWMOM03	'P 21/c'	-7.9	-16.4	-147.4	39.5	0	-132.2
DIXBIW	'P -1'	-33.7	-34.2	-176.1	83.8	0	-160.1
DIXBIW01	'P 21/n'	-40.5	-32.5	-158.7	80.3	0	-151.3
DMETSO04	'P 21/c'	-13.2	-27.2	-49.1	36.1	0	-53.4
DMETSO05	'P -1'	-13.2	-28.9	-53.3	40.5	0	-54.9
DMFUSC03	'P 21/c'	-26.2	-24	-155.6	61.5	0	-144.3
DMFUSC04	'P 21 21 21'	-25.6	-24.5	-161.1	81.4	0	-129.8
DOUJET	'P -1'	-29.1	-48.8	-184.9	60.7	0	-202.1
DOUJET01	'P 1 1 21/a'	-27.1	-50.8	-196.1	63.4	0	-210.6
DOZYAS	'P 21/n'	-21.4	-41.5	-174	58.9	0	-178.1
DOZYAS01	'P -1'	-22.2	-44.5	-200	75.7	0	-191
DUDCUC	'C 2/c'	-11.1	-22.3	-135.2	46.6	0	-122
DUDCUC01	'P -1'	-8.4	-22.6	-140.5	47.4	0	-124.2
DUDCUC02	'P 21 21 21'	-13.3	-21.9	-135.1	46.4	0	-123.9
DUDNAS	'P 21/n'	-30.1	-29.9	-147.3	67.7	0	-139.7
DUDNAS01	'P b c a'	-29.6	-26.6	-126.2	50.8	0	-131.6
DURZUM	'P 21/n'	-20.3	-20.5	-135.5	43	0	-133.3
DURZUM01	'P 21/c'	-21.2	-20.2	-133.3	44.4	0	-130.3
EDAXEM	'P -1'	-29	-52.5	-179.7	83.4	0	-177.8
EDAXEM01	'P 21/n'	-35.4	-51.4	-174.1	67	0	-193.9
EGOPIB	'P -1'	-35.4	-49.6	-170.8	39.2	0	-216.6
EGOPIB01	'P 21/c'	-17.2	-46.7	-157.7	34.6	0	-187
EKIPUL	'P 21 21 2'	-12.4	-44.9	-245.2	78.1	0	-224.5
EKIPUL01	'P 21 21 21'	-9	-45.9	-258.4	89.9	0	-223.5
EROGUP	'P 21/c'	-7.9	-33.1	-245.8	87.5	0	-199.2
EROGUP01	'P 21/c'	-15.7	-31.8	-227.3	66.6	0	-208.2
EYIWU	'P -1'	-7.4	-42.9	-197.1	80.4	0	-167.1
EYIWU01	'P 21/c'	-9.2	-41	-182.3	75.9	0	-156.6
FABRAB10	'C 2/c'	-15.9	-25.9	-121.6	50.9	0	-112.4
FABRAB11	'P 21/n'	-12.1	-27.2	-130.7	44.6	0	-125.5
FATYOP	'P 21/c'	-24.2	-29	-141.7	54.9	0	-140
FATYOP01	'P 21/c'	-25.5	-29	-140.1	52	0	-142.6
FEPEM	'P 21/c'	-18.1	-26.3	-128.3	55.8	0	-116.9
FEPEM01	'P -1'	-12	-23.7	-108.6	36.7	0	-107.6
FEVNAV01	'P 21/c'	-18.9	-16.6	-97	33.1	0	-99.4
FEVNAV02	'P 31'	-18.2	-16.5	-100.6	41.2	-0.5	-94.6
FEVWUY	'P 21/a'	-31.9	-43.2	-164.9	73.3	0	-166.8
FEVWUY01	'P -1'	-30.1	-40.7	-144.9	70.5	0	-145.1
FOBSEO02	'C 2/c'	-12.4	-23.9	-183.7	52.7	0	-167.3
FOBSEO03	'P 21 21 21'	-12.4	-25.1	-193.7	49.1	0	-182.1
FOVYOE	'P 21/n'	-19	-29.1	-141	55.3	0	-133.7
FOVYOE11	'P 21'	-17.6	-29.9	-146.2	56.4	0	-137.2
FUQWAQ	'P -1'	-27.2	-74	-219.5	114.9	0	-205.8
FUQWAQ01	'P -1'	-42.8	-73.4	-215	142.4	0	-188.8
FUWFAG	'P -1'	-12.9	-24.5	-199.5	68.3	0	-168.5
FUWFAG01	'P 21/c'	-12.9	-24.7	-200.4	68.9	0	-169
GAGSIR	'P -1'	-27.2	-30.6	-116.3	60.2	0	-113.9
GAGSIR01	'P 21/n'	-27.5	-31.5	-116.7	56.5	0	-119.1
GEBSOV	'P 21 21 21'	-29.9	-36	-126	52.6	0	-139.3
GEBSOX	'C 2/c'	-15.7	-36.3	-134.8	53.3	0	-133.6
GEMGAG01	'P 21/c'	-29	-43.9	-186	82.2	0	-176.7
GEMGAG02	'P 21/n'	-33.7	-40	-166	78.3	0	-161.4
GOFVAZ	'C 2/c'	-10.1	-25.4	-138.1	45.2	0	-128.4
GOFVAZ01	'P 21/n'	-7.7	-26.5	-147.8	50.2	0	-131.8
GOLLUO	'P 21/n'	-29	-22.8	-85	46.8	0	-90.1
GOLLUO01	'P b c a'	-34.6	-22.9	-87.3	56.1	0	-88.6
HAIYUN01	'P -1'	-22	-56	-184.3	72.9	0	-189.4
HAIYUN02	'P 21/c'	-30	-53.1	-176.1	78.1	0	-181
HAKTAP	'P 21/n'	-26	-52.9	-143.7	54.6	0	-168
HAKTAP01	'P 21/c'	-24.6	-54.3	-150.5	76.8	0	-152.5
HEHWJO	'P 21/c'	-64.7	-38.2	-132.6	63.3	0	-172.1
HEHWJO01	'P 21/n'	-34.4	-40.5	-144.3	57.1	0	-162.1
HEWLLOL01	'P 21/c'	-19.2	-26.8	-185.3	83.1	0	-148.2
HEWLLOL02	'P 21/c'	-21	-25.1	-164.8	47.7	0	-163.2
HMHOCN07	'P 21/c'	-5.2	-48.1	-94.1	38.6	0	-108.8
HMHOCN08	'P 21/c'	-8.1	-48.8	-99.1	49	0	-107
HNIABZ11	'P 21/a'	-60.7	-65.3	-186.6	116.2	0	-196.3
HNIABZ21	'P 21'	-67.7	-63.2	-176.9	104.1	-0.1	-203.7
HOFFEN	'P 21/c'	-20.2	-18.9	-135.1	39.5	0	-134.7
HOFFEN02	'P 21/c'	-20.3	-20.2	-143.4	47.7	0	-136.2
HOKMAW	'C 2/c'	-25	-26.4	-131.3	66.1	0	-116.6
HOKMAW01	'P c a 21'	-16.9	-25.9	-124.3	60.3	0	-106.8
IBOBUY	'P 21 21 21'	-41.7	-59.3	-190.1	118.7	0	-172.4
IBOBUY01	'P 21/c'	-38.4	-56.8	-182	85.2	0	-192.1
IBULIA	'P 21/c'	-5	-21.6	-116.4	34.9	0	-108.2
IBULIA01	'P 21/c'	-8.9	-21.2	-113.7	35.6	0	-108.2
IHEMIR	'P 21/n'	-39.7	-14.5	-85.4	44	0	-95.6
IHEMIR01	'P 21/n'	-42.3	-14.4	-85.3	44.5	0	-97.5
IPIXUB08	'P 21/c'	-5.8	-15.6	-152.1	46.6	0	-126.9
IPIXUB11	'P 21'	-2.8	-19.4	-172.6	78.8	0	-116.1
IPIXUB13	'P 1'	-3.5	-21.4	-189.3	90	-0.1	-124.3

IQAREY	'P 21 21 21'	-20.6	-23	-95.6	45	0	-94.2
IQAREY01	'P 21'	-15.6	-22.8	-94.3	40.4	0	-92.2
IVATAC	'P b c a'	-0.8	-43.2	-137.7	48	0	-133.7
IVATAC01	'P b c a'	-3	-45.1	-149.8	55	0	-143
IWUKAM	'P n a 21'	-4.8	-77.1	-189.6	57.3	-0.1	-214.3
IWUKAM01	'P n a 21'	-10.6	-82.3	-213.9	87.3	0	-219.5
IWUKAM02	'P 21/n'	-29.9	-85.7	-229.4	109.4	0	-235.7
JATFUF03	'R 3 c'	-14.9	-52.2	-98	38	0	-127
JATFUF04	'P n m a'	-13	-52.4	-98.4	38.5	0	-125.3
JATXOU	'P -1'	-23.8	-23.3	-135.4	68.2	0	-114.3
JATXOU01	'P c a 21'	-28.2	-22.6	-130.4	58.9	0	-122.2
JAVCEO02	'A b a 2'	-20	-27.7	-156.6	75.5	-5.5	-134.3
JAVCEO04	'P b c a'	-20	-28.9	-158.6	61.7	0	-145.7
JOTNAH	'P -1'	-23.4	-31.6	-107.8	37	0	-125.8
JOTNAH01	'P 21/c'	-23.5	-31.2	-106.7	42.1	0	-119.3
JOWNAM	'P -1'	-23.2	-35.3	-129.8	50.8	0	-137.5
JOWNAM01	'P -1'	-20.7	-36.6	-152	62.2	0	-147.2
JOWPAO	'P -1'	-22.1	-22	-172.7	51	0	-165.8
JOWPAO01	'P b c 21'	-16.2	-22.1	-170.6	55	-0.6	-154.5
JUDRAB	'P 32 2 1'	-11.4	-46.9	-119.5	47.3	0	-130.5
JUDRAB01	'P 32 2 1'	-12.8	-49.7	-138.7	83.8	0	-117.4
JULBUN	'P 21/c'	-31.1	-24.6	-88.5	36.3	0	-107.8
JULBUN01	'P 21/n'	-37.2	-24.8	-91.6	43.3	0	-110.4
JULZAR	'P 21/a'	-38.8	-15.4	-83.3	40	0	-97.5
JULZAR01	'P c a 21'	-36.1	-14.2	-75.2	31.8	0	-93.7
KADNEI	'P 21/n'	-29.1	-38.9	-210.3	78.2	0	-200.1
KADNEI01	'P n a 21'	-28.5	-39.2	-213.3	86.7	-3.3	-197.6
KADPOU	'P 41'	-9.6	-57.5	-157	50.5	0	-173.6
KADPOU01	'P -1'	-10.1	-59.5	-166.9	56.4	0	-180.2
KADTEO	'P 21/c'	-17	-37.4	-123.3	69.5	0	-108.1
KADTEO01	'P 21 21 21'	-33.7	-40.3	-141.4	88.7	0	-126.7
KADTEO02	'P 21/c'	-16.9	-37.7	-124.8	71.2	0	-108.2
KAGCIE02	'P 21'	-29	-76	-183.6	91.3	0	-197.3
KAGCIE03	'P 21 21 21'	-30.9	-73.7	-175.7	85.8	0	-194.5
KANYUU02	'A b a 2'	-17.6	-27.5	-255.2	75.2	0	-225
KANYUU03	'P b c a'	-6	-29.6	-279.4	86.1	0	-228.8
KAWJAU	'P 21'	-18.1	-34.5	-157.3	57.4	-2	-154.5
KAWJAU01	'P 42/n'	-23.5	-32.3	-140.5	52.1	0	-144.2
KAZDUL01	'P 21/n'	-37.1	-41.3	-163.4	66.2	0	-175.6
KAZDUL03	'P b c a'	-32	-44	-170.8	66.2	0	-180.6
KETYAJ	'P 21/n'	-2.5	-17.1	-115.9	37.6	0	-97.9
KETYAJ01	'P -1'	-1.7	-16.4	-105	31.1	0	-92.1
KIFHUC	'P 1 1 21/a'	-29.6	-41.3	-142.3	65.3	0	-147.9
KIFHUC01	'P 21/n'	-24.4	-38.4	-134.5	54.5	0	-142.8
KIGTOL	'P 21/c'	-6.1	-41.9	-275.3	67.5	0	-255.8
KIGTOL01	'P 21/n'	-20.5	-41.4	-270.5	69.8	0	-262.7
KIJEFA01	'C 2/c'	-8.2	-40	-288.6	72.1	0	-264.7
KIJEFA02	'P 21/c'	-16.4	-38.6	-276.3	75.5	0	-256
KIZMAI	'P 21 21 2'	-13.4	-17.4	-123.4	42.3	0	-111.9
KIZMAI01	'P 21'	-14.8	-17	-119.6	52.2	0	-99.1
KUDXAK	'P 21/c'	-31.6	-47.1	-149.8	77.9	0	-150.7
KUDXAK01	'P 21/c'	-37.1	-49.5	-157.1	102	0	-141.7
LEQPIH	'P 21'	-14.2	-27.7	-126.9	35.5	-0.1	-133.4
LEQPIH01	'P -1'	-18.2	-26.7	-125.5	40	0	-130.4
LIKROW	'P b c a'	-18.1	-33	-125.2	43.8	0	-132.5
LIKROW01	'P n a 21'	-8.6	-32.8	-122.5	45	-11	-129.9
LIVQOY	'C 2/c'	-20.7	-31.1	-162.8	51.4	0	-163.3
LIVQOY05	'P b c a'	-27.1	-31.6	-169.4	56	0	-172
LOZYII	'P 21/n'	-23.9	-59	-138.1	55.3	0	-165.7
LOZYII01	'P 21/n'	-16.6	-57.2	-128.9	51.2	0	-151.5
LUFCIY	'P 21/c'	-7.4	-18	-163	38.5	0	-149.9
LUFCIY01	'P 21 21 21'	-11.6	-18.7	-165.5	43.4	0	-152.4
LUKXAK	'P 21'	-17	-58.5	-166.4	69.8	0	-172.1
LUKXAK01	'P 21'	-18.4	-57.3	-162.9	70.3	-0.1	-168.4
MAFPOA	'P 21/n'	-24.8	-23.7	-135.7	57.2	0	-127.1
MAFPOA01	'P b c a'	-21.8	-24.4	-145.6	60.4	0	-131.4
MANPIM01	'P 21/c'	-22.5	-24.6	-123.4	44.6	0	-126
MANPIM02	'P -1'	-25.9	-24.8	-121.7	51.4	0	-121.1
MATDEQ	'P 21/c'	-23.3	-55.8	-152.4	68.1	0	-163.4
MATDEQ01	'P -1'	-25.5	-55.4	-144.4	66	0	-159.3
MBYINO	'P 21/c'	-21.8	-28.5	-160.5	64.9	0	-145.8
MBYINO02	'P 21/c'	-25.5	-27.4	-157.5	62.7	0	-147.7
MEGYON01	'P n a 21'	-17.3	-24.2	-169.2	65.8	0	-145.1
MEGYON02	'P 21/c'	-21.2	-23.4	-164.6	59.4	0	-149.9
MEHROH	'P 21/c'	-29.1	-24.4	-128	56.6	0	-124.9
MEHROH02	'P 21'	-25.8	-23.8	-123.1	46.3	-7.3	-133.6
MELVEE	'P 21'	-20.4	-28.9	-176.8	74.2	0	-151.9
MELVEE01	'P 21'	-24.1	-30.3	-190.9	70.5	-0.4	-175.1
MEQVAG	'P 21 21 21'	-53	-31.2	-120.2	61.8	0	-142.7
MEQVAG01	'C c'	-56.6	-31.1	-119.6	67.9	-1.8	-141.2
MIQKOM	'P 21/c'	-27.7	-50	-163.2	71.4	0	-169.4
MIQKOM01	'P 21/c'	-17.2	-49.3	-165.1	70	0	-161.5
MIZHOT01	'P 21/c'	-10.4	-35.9	-164.6	56.9	0	-154
MIZHOT02	'P 21'	-9.2	-35.8	-163.3	53.9	-1.7	-156.2
MMANCN	'P 1'	-13.3	-21.2	-95.3	28.1	-2	-103.7
MMANCN02	'C 2/c'	-16.3	-21.2	-98.1	33.7	0	-101.8
MONTIS	'P 21 21 21'	-31.6	-31.9	-168	61.2	0	-170.3
MONTIS01	'P 21'	-28.9	-31	-163.2	58.1	-0.1	-165
MSULIN04	'P 21/c'	-30.4	-36.1	-111.1	73	0	-104.6
MSULIN05	'P 21 21 21'	-27.8	-36.6	-108.4	58.9	0	-113.9
NAGNER	'P 1'	-14.8	-24.4	-168.2	66.3	0	-141

NAGNER01	'P 21 21 21'	-28.6	-23.1	-155.3	57.2	0	-149.9
NAJBEE	'P 21/n'	-35.8	-27.7	-137.4	58.4	0	-142.6
NAJBEEF01	'P 21/c'	-44.1	-28.5	-140.6	53.4	0	-159.8
NANQUO	'P 21/n'	-45.1	-31.6	-99.5	46.3	0	-129.9
NANQUO02	'P -1'	-47.4	-35.3	-119.2	72	0	-129.9
NAPQAZ	'P -1'	-15.6	-30.6	-132	41.9	0	-136.4
NAPQAZ01	'P 21/n'	-15.4	-31	-133.6	44.8	0	-135.2
NAPTAN01	'P 21 21 21'	-23.9	-22.8	-116.6	43.8	0	-119.5
NAPTAN02	'P 21/c'	-21.3	-22.7	-115.2	42.7	0	-116.6
NAXFUO	'P 21/n'	-36.8	-40.6	-87.8	57.4	0	-107.8
NAXFUO01	'P 21/c'	-37.5	-41.1	-89.2	62	0	-105.9
NAYNUX	'P -1'	-46.4	-65.5	-155	120.6	0	-146.4
NAYNUX01	'P 31'	-49.4	-67.9	-162.4	121.4	-1.9	-160.1
NEHREZ	'P 21/c'	-14.7	-30.7	-148.9	51.6	0	-142.7
NEHREZ01	'P 21/c'	-14.4	-30.6	-147.6	51.1	0	-141.5
NEPTAZ	'P n a 21'	-10.4	-17.8	-114.5	30.6	-0.1	-112.2
NEPTAZ01	'P b c a'	-6.9	-19.8	-134.2	41.5	0	-119.4
NIPSOV	'P 21 21 21'	-16.9	-20.4	-163.7	51.5	0	-149.6
NIPSOV01	'P 21/c'	-12.2	-20.6	-167.7	45.1	0	-155.5
NOQFII	'P -1'	-5.2	-23.7	-179.7	46.3	0	-162.3
NOQFII01	'P 21/n'	-13.8	-23.6	-177.8	46	0	-169.2
NORFUX	'C 2/c'	-18.3	-25.7	-90.5	42.5	0	-92
NORFUX01	'P 21/n'	-16.2	-25.9	-92.5	47.5	0	-87
NUJLIN	'P m n 21'	-17.1	-29.2	-160.6	46.4	-10.5	-171.1
NUJLIN01	'P 21/n'	82.4	-33.9	-174.5	51.1	0	-74.8
NUKMAH	'P b c a'	-8.4	-24.4	-131.6	38.3	0	-126
NUKMAH02	'i 2/a'	-9.3	-26	-151.3	57.1	0	-129.4
NUNCAB	'P 21/n'	-32.8	-25.6	-149.4	68.4	0	-139.3
NUNCAB02	'i 41 c d'	-30.7	-23.8	-134.7	51.8	-0.3	-137.7
NXENAM	'P c a 21'	-33.9	-39.9	-113.8	79.9	-7.7	-115.4
NXENAM01	'P 21/c'	-34.7	-41	-115.3	78.3	0	-112.7
OGOMON	'P 21/n'	-19.4	-17.4	-141.6	48.7	0	-129.8
OGOMON01	'P 21/c'	-19.3	-17.6	-142.7	48.7	0	-130.9
OHIBOW	'P c a 21'	-27.5	-28.8	-208.3	77	0	-187.7
OHIBOW02	'P -1'	-27.9	-29.9	-226.9	75.3	0	-209.4
OLATUR	'P 21 21 21'	-31.1	-29.5	-132.2	65.9	0	-126.9
OLATUR01	'P 21'	-30.6	-32.6	-156.5	75.9	-9.6	-153.3
OMEFAN	'P -1'	-54.4	-45.3	-227.8	93.6	0	-234
OMEFAN01	'P -1'	-61.5	-46.4	-233	98.2	0	-242.7
OVEPUC	'P 21/n'	-16.9	-32.2	-194.3	69.1	0	-174.3
OVEPUC01	'P -1'	-25.8	-33.4	-205.3	78.4	0	-186
PABHAB	'P 21/c'	-83.7	-66.8	-183.1	110.4	0	-223.2
PABHAB01	'P 21/a'	-75.1	-68.5	-186.1	109.6	0	-220.1
PANQUO	'P b c a'	-35.5	-27.1	-113.2	55.7	0	-120.1
PANQUO01	'P b c a'	-25.6	-28	-118.9	52	0	-120.5
PAVBEU	'P 21/n'	-2.7	-19	-125.4	29.5	0	-117.6
PAVBEU01	'P 21/n'	-2.6	-19.1	-122.7	25.3	0	-119.2
PEGWII	'P 21/n'	-21.2	-15.8	-153.4	48.6	0	-141.9
PEGWII01	'P -1'	-23.3	-16.3	-156.3	46.6	0	-149.3
PEJBUC	'P 21/n'	-28.1	-32.8	-159	70.7	0	-149.1
PEJBUC01	'P 21'	-26.6	-34	-160.3	83	-2.8	-140.7
PEJHOD	'P 21/c'	-27.2	-23.8	-182.2	74.6	0	-158.6
PEJHOD01	'P 21/c'	-34.2	-24.5	-189	86.5	0	-161.1
PEJOF	'P -1'	-25.4	-23.7	-184.1	87.6	0	-145.5
PEJOF01	'P 21/c'	-28.6	-23.4	-180.2	81.1	0	-151.1
PHISCY01	'F d d 2'	-27.6	-44.4	-190.9	70.1	0	-192.7
PHISCY02	'C 2/c'	-6.5	-43.9	-190.5	71.8	0	-169.1
PIMTAZ01	'P 21/n'	-17	-20.9	-114.3	36.6	0	-115.6
PIMTAZ02	'P 21/c'	-17.8	-21.7	-121.2	41.4	0	-119.2
PINPAD	'P 21/n'	-15.4	-48.8	-84.9	74.6	0	-74.5
PINPAD01	'P 21/c'	-12.8	-51	-89.3	65.3	0	-87.8
POFLAX	'P 21 21 21'	-13.1	-38.7	-133	46.4	0	-138.4
POFLAX01	'P -1'	-10.2	-40.5	-140.3	51	0	-140
PRMDIN01	'P n a 21'	-10.1	-11.7	-60.6	24.8	-0.6	-58.3
PRMDIN02	'P n a 21'	-9.4	-10.7	-52.7	17.9	-0.6	-55.5
PROGST12	'P 21 21 21'	-22	-52	-143.1	70.8	0	-146.2
PROGST13	'P 21 21 21'	-19	-52.8	-144	77.1	0	-138.8
PUBMUU01	'P b 21 a'	-62.3	-72.4	-170	116.7	-0.1	-188.2
PUBMUU05	'P 21/n'	-72.7	-76.8	-189.8	157.8	0	-181.5
PUBMUU07	'P 21/n'	-73.6	-73.6	-182	154.5	0	-174.7
PUGVUK	'P b c a'	-14.7	-43	-249.1	72.8	0	-234
PUGVUK01	'P 21/n'	7.7	-45.1	-264.3	67.8	0	-234
PUGWUK	'P 21/c'	-7.8	-41.6	-116.3	40.2	0	-125.6
PUGWUK01	'P 21/n'	-8.2	-40.6	-112.7	46	0	-115.5
PURSEB	'P -1'	-42.2	-55.7	-229.8	94.7	0	-233
PURSEB01	'P 21/n'	-30.1	-58.4	-242.1	107.9	0	-222.7
PURSEB02	'P n a 21'	-45.6	-56.8	-236.6	95.2	-0.4	-244.2
PUVVUX	'P 21/a'	-38.8	-31	-72.8	37.7	0	-104.9
PUVVUX01	'P c a 21'	-40	-32.5	-79.1	46.4	0	-105.2
PYMSUL10	'P -1'	-10.7	-24.6	-114	30.8	0	-118.5
PYMSUL11	'P -4 21 c'	-11.6	-26.4	-127.9	46.8	0	-119.1
QAMNAT	'P 21/c'	-11.1	-16.4	-132.8	41.6	0	-118.7
QAMNAT01	'P 21/c'	-11.3	-16.3	-126.3	39.7	0	-114.2
QANHAP	'P c'	-18.7	-26.4	-211.4	59.4	-3.8	-201
QANHAP01	'P c a 21'	-21.2	-26.4	-214.6	59.9	-0.8	-203.2
QEJZAH	'C 2/c'	-36.7	-25.8	-98.4	55.1	0	-105.7
QEJZAH02	'P 21/c'	-25.8	-26.4	-106.4	57.5	0	-101.2
QILYUH	'P 21/c'	-3.8	-19.3	-125.4	34.7	0	-113.7
QILYUH01	'C 2/c'	-2.6	-20.9	-137.3	43	0	-117.7
QIXFUY	'P 21/c'	-14	-41.4	-122.8	51.4	0	-126.9
QIXFUY01	'P 21/n'	-12.1	-41.9	-123.8	46.9	0	-130.8

QOGNEF01	'P n a 21'	-25.1	-35.8	-162.3	61.2	-3	-164.9
QOGNEF02	'P 21/c'	-5.5	-41.6	-157.2	65.8	0	-138.4
QUZREJ01	'P -1'	-27.1	-36.7	-182.2	82.1	0	-163.9
QUZREJ03	'P -1'	-30.7	-36.4	-180.9	80.4	0	-167.6
RAFFIO	'P 21 21 21'	-8.3	-15.6	-91.4	24.7	0	-90.6
RAFFIO01	'P 21/n'	-10	-15.6	-92.8	26.8	0	-91.6
RAFGAJ	'P 21 21 21'	-10.2	-20.6	-157.3	43.9	0	-144.1
RAFGAJ01	'P -1'	-10.8	-20.8	-155.6	39.4	0	-147.8
RAXRAK	'P 21 21 21'	-38.9	-41.2	-111.4	58.4	0	-133
RAXRAK01	'P 21/c'	-28.6	-43.2	-122.2	55.9	0	-138
RIGHUK07	'P 21/c'	-28.3	-31.4	-126.1	52.8	0	-133
RIGHUK09	'P 21/c'	-22.9	-30.5	-120.6	47.4	0	-126.6
RUVZOY	'P -1'	-5.4	-12.3	-136.8	36.1	0	-118.3
RUVZOY01	'P 21/n'	-2.2	-12.3	-134.1	32.5	0	-116.1
SAXJEG	'P -1'	-3.7	-18.9	-172.6	41.1	0	-154.2
SAXJEG01	'P 21/n'	7.8	-19.5	-177.7	42.7	0	-146.6
SAYVEV	'C 2/c'	-59.8	-43.4	-199.7	104.2	0	-198.7
SAYVEV01	'P 21/c'	-59.7	-41.8	-197.4	92	0	-206.9
SEBTAU	'P 21/c'	-36.5	-41.2	-162.2	58.3	0	-181.5
SEBTAU01	'P -1'	-39.4	-39.7	-153.1	59.3	0	-172.9
SEMYIT	'P n a 21'	-29.5	-41.2	-129.1	75.7	-11	-135.1
SEMYIT01	'P 21/c'	-36.5	-40	-124.2	59.8	0	-140.9
SESYAR	'P 21/c'	-27	-28.8	-146.1	64.3	0	-137.5
SESYAR01	'P -1'	-21.4	-29	-146.2	61.6	0	-135
SIHNII	'P -1'	-45.6	-51.6	-245.1	117.9	0	-224.4
SIHNII01	'P 21/c'	-54.7	-52.2	-247.8	108.8	0	-245.9
SIRJUZ	'P n a 21'	-18.4	-32.7	-214.9	75.1	0	-190.9
SIRJUZ01	'P 21/c'	-16.7	-33.1	-217.4	74.7	0	-192.5
SIWDEH	'P -1'	-30.4	-24.6	-208.1	70.3	0	-192.7
SIWDEH01	'P 21 n b'	-11.5	-24.8	-209.6	53.3	0	-192.5
SOCRUZ	'C c'	1.2	-30.4	-156.8	57.2	-18	-146.8
SOCRUZ01	'P 21/c'	-30.5	-27.9	-136.3	49.2	0	-145.5
SOLSIW	'P 21 21 21'	-32.9	-48.2	-142.1	57.6	0	-165.4
SOLSIW01	'P 21 21 21'	-32.8	-48.4	-143.2	58.6	0	-165.8
SUBTIS02	'P -1'	-24.7	-39.1	-178.9	63.9	0	-178.8
SUBTIS03	'P b c a'	-30.9	-37.3	-171.8	67	0	-172.9
SUGGEG01	'P 21/n'	-22.9	-33.8	-123.4	53.6	0	-126.5
SUGGEG02	'P -1'	-24.8	-34.9	-130.4	62.6	0	-127.6
SUKNIW01	'C c'	-14.1	-21.2	-120	33.9	-5.2	-126.6
SUKNIW02	'P -1'	-14.3	-22.8	-133	43.5	0	-126.6
TACRIB04	'P 21'	-44.4	-84.7	-153.1	94.8	-0.1	-187.6
TACRIB07	'P 21 21 21'	-52.2	-78.6	-136.9	92.6	0	-175.2
TADLIU01	'P -1'	-19	-47	-169.9	80.7	0	-155.2
TADLIU02	'P 21/n'	-24.6	-45.3	-168.7	68.4	0	-170.1
TALNAV01	'P 21 21 21'	-32.8	-43.5	-114.2	67.3	0	-123.2
TALNAV02	'P 21 21 21'	-34.3	-43.4	-114.5	56.8	0	-135.3
TELKUQ	'P b c a'	-27.2	-63.8	-172.7	78.5	0	-185.3
TELKUQ01	'P -1'	-12.3	-62	-163.2	62.6	0	-175
TENMIK	'P -1'	-24.1	-25.4	-156	55.9	0	-149.6
TENMIK01	'P 21/c'	-21.4	-26	-164.8	55.5	0	-156.7
TIZWAA	'P -1'	-34.4	-36.1	-254	88.3	0	-236.2
TIZWAA01	'P -1'	-3.9	-34	-243.5	73	0	-208.4
TNBENZ11	'P b c a'	-35.9	-34.3	-106.9	70.6	0	-106.6
TNBENZ12	'P c a 21'	-40	-33.3	-105.8	74	0	-105
TOQPUM	'C 2/c'	-19.5	-22.9	-162.3	54.5	0	-150.3
TOQPUM02	'P b c n'	-15.5	-23.8	-171.1	49.7	0	-160.7
TUDROZ	'P b c a'	-2.6	-16	-136.8	37.9	0	-117.5
TUDROZ01	'P 21/n'	-6	-15.4	-131.9	36.2	0	-117.1
TUZYIY	'P 21/c'	-36.6	-52.9	-148.2	80.4	0	-157.3
TUZYIY01	'P 21/c'	-40.7	-54.1	-158.4	75.4	0	-177.9
UHULEQ	'P 21 21 21'	-29.6	-57.2	-141.4	77.7	0	-150.6
UHULEQ01	'P 21 21 21'	-29.2	-57.5	-141.3	77.8	0	-150.2
UHULEQ02	'P 21 21 21'	-35.7	-56.5	-142	95	0	-139.3
UIICEX	'P 21/c'	-21.7	-45.6	-137.2	65.4	0	-139.1
UIICEX01	'P -1'	-23.7	-51.3	-165.2	84.9	0	-155.3
USOGOZ	'P -1'	-30.1	-34.2	-152.2	70.8	0	-145.7
USOGOZ02	'P 21/c'	-31.8	-33.2	-146.7	69.7	0	-142
VALLIE	'P 21'	-6.8	-50	-234.8	78.7	-5	-217.9
VALLIE01	'P 21'	-10	-50.5	-237.7	77.2	0	-221
VECRUR02	'P 21/n'	-28.5	-23.8	-125.3	56.7	0	-121
VECRUR03	'C 2'	-25.1	-23.3	-120.4	50.7	-8.1	-126.1
VEJDUL	'P 21/n'	-19.7	-20.6	-146.2	47.6	0	-139
VEJDUL01	'P 21'	-19.5	-20.7	-149.9	56	0	-134.2
VEMTOW	'P c'	-27.7	-46.6	-153.9	82.8	-0.3	-145.7
VEMTOW01	'P 21/c'	-22.3	-44.1	-142.4	72.2	0	-136.6
VIFVUC	'P b c a'	-28.1	-16.5	-128.9	53	0	-120.5
VIFVUC01	'P 21'	-25.5	-17	-136.3	52.6	-2.7	-125
VISSOF	'P 21/c'	-12.4	-34.5	-156.6	53.6	0	-150

VISSOF01	'P 21 21 21'	-21.4	-32.9	-150.7	54.6	0	-150.5
VUYPUC	'P 21/c'	-22.5	-18.3	-135.5	39.9	0	-136.5
VUYPUC01	'P b c a'	-25.1	-19.4	-150.8	53.2	0	-142.1
WAMFAS01	'P 21/n'	-28.2	-43	-203.4	91.8	0	-182.8
WAMFAS03	'P 21/c'	-24.1	-45.4	-224.3	79.4	0	-214.4
WECCUC	'P 21 21 21'	-62	-127.7	-205	99	0	-295.7
WECCUC01	'P 21 21 21'	-40.8	-122.3	-189.4	85.4	0	-267.1
WOVGIZ	'P -1'	-8.7	-12.1	-178	55.5	0	-143.3
WOVGIZ01	'P 21/n'	-7.9	-11.6	-175.6	56.4	0	-138.7
WUXDOJ	'P 21/c'	-27.4	-22	-122.5	44.9	0	-127.1
WUXDOJ02	'P 21 21 21'	-30.9	-21.7	-121.8	46	0	-128.4
XAJFOG	'P -1'	-6	-43	-254.8	89.6	0	-214.2
XAJFOG01	'P -1'	-6.4	-42.7	-254.3	90.4	0	-213
XEBBOY	'P 21 21 21'	-66.9	-57.7	-270.4	117.7	0	-277.3
XEBBOY01	'P 21/c'	-69	-60.3	-284.1	131.4	0	-282
XEHHEX	'P 21/n'	-2.1	-20.2	-138.7	32	0	-129
XEHHEX01	'P 21/a'	0	-19.8	-137.7	31.8	0	-125.8
XEJNUV	'P 1'	-23.8	-17.2	-100.4	30.4	0	-111
XEJNUV01	'P 21 21 21'	-25.6	-18.7	-114.4	36.6	0	-122.1
XEPXOF	'P c a 21'	-13.1	-21	-138.5	42.7	-0.2	-130.1
XEPXOF01	'P 21/c'	-10	-20.8	-141.5	40.2	0	-132
XEWZAB	'P 21/c'	-30.1	-37.1	-193.8	54	0	-207.1
XEWZAB01	'P 21/n'	-17.5	-38.8	-203.2	55.1	0	-204.5
XIYXIN	'P -1'	-21.2	-51.5	-126.2	77.2	0	-121.7
XIYXIN01	'P 21/n'	-30.5	-48.4	-114.1	69.2	0	-123.9
XOCXUI01	'P 21/c'	-29.2	-30.7	-138.7	54.3	0	-144.3
XOCXUI02	'P 21/c'	-24.5	-28.4	-138.3	52.6	0	-138.6
XOKYAZ	'P n a 21'	-1.6	-37.5	-165.3	61.8	0	-142.5
XOKYAZ01	'P -1'	-5.3	-35.1	-153.3	57.6	0	-136.1
YAKYAL	'P -1'	-11.1	-33.7	-133	54.9	0	-122.8
YAKYAL01	'P 21/n'	-14.1	-32.3	-125.9	51.6	0	-120.7
YAMHID	'P 21/c'	-17.1	-17.9	-78.3	23.1	0	-90.2
YAMHID03	'P 21/c'	-18.7	-18.5	-84.3	29.6	0	-91.9
YAPFIH	'P -1'	4.1	-16.8	-216.8	50.9	0	-178.7
YAPFIH01	'P 21/n'	-9.2	-16.4	-199.8	45.4	0	-180
YASKOS	'P 21/c'	-1.7	-13.1	-186.3	56	0	-145
YASKOS01	'P -1'	-1.7	-13.3	-203.6	68	0	-150.6
YAXCEH	'P 21/c'	-14.2	-14.5	-116.4	31.9	0	-113.1
YAXCEH01	'l b a 2'	-11.9	-15.1	-123.6	37.7	-0.1	-113
YELHUS	'P 21/c'	-25.9	-36.9	-213.2	62.7	0	-213.3
YELHUS01	'P 21/c'	-18.1	-36.4	-210.1	62.9	0	-201.8
YICIDZ	'P 21/n'	-6.4	-10.1	-54.3	15.5	0	-55.3
YICIDZ01	'P n a 21'	-5.2	-11.8	-69.2	28.2	0	-58
YICDUL	'P 21/n'	-6.1	-10.7	-53.1	17.4	0	-52.5
YICDUL01	'P b c a'	-5.3	-13.6	-78.3	37.1	0	-60
YIVRIF	'P 21/c'	-15.4	-36.5	-170.4	59.5	0	-162.8
YIVRIF01	'P 21/c'	-12.2	-35.4	-163.6	51.8	0	-159.4
YIVRIF02	'P 21'	-7.4	-35.8	-161.2	50.8	-11.3	-164.8
YOLDAF01	'P 21/c'	-5.7	-3.8	-70.4	26.2	0	-53.8
YOLDAF04	'P 1 1 21/n'	-12.3	-4.5	-90.5	46.8	0	-60.4
YORYAH	'C c'	-25	-25.7	-176.8	52.5	-0.1	-175.1
YORYAH01	'P -1'	-24.9	-25.7	-180.3	55.1	0	-175.8
YORYAH02	'P 21/n'	-27.3	-25.4	-175.1	52.4	0	-175.4
YOWYOY	'P 21/n'	-31.7	-41.9	-160.5	76.5	0	-157.6
YOWYOY02	'P 21/n'	-23.4	-45.2	-177.3	90.7	0	-155.1
YUMKOH	'P 21/n'	-33.1	-36.5	-151.6	73.2	0	-148.1
YUMKOH01	'P b c a'	-38.1	-39.1	-168.9	75.5	0	-170.6
ZELDOJ	'P 21/n'	-8.5	-11.3	-63.4	30.3	0	-52.8
ZELDOJ01	'C 2/c'	-8.6	-11.6	-66.9	32.9	0	-54.2
ZILNOX	'P 21/c'	-23.4	-53.4	-88.8	52.3	0	-113.2
ZILNOX01	'P -1'	-26	-53.1	-89.3	55.1	0	-113.3
ZOGQAN03	'P 21/c'	-35.9	-38.7	-177.5	79.1	0	-173.1
ZOGQAN05	'P 21/c'	-38	-39.4	-180.3	87.2	0	-170.5
ZZZBLP03	'P 21/c'	0.6	-10.6	-157.3	45.3	0	-121.9
ZZZBLP02	'P n a 21'	0.5	-10.4	-154.3	43.8	0	-120.4
ZZZMUC08	'P 21/a'	-40.2	-41.7	-123.4	83.8	0	-121.6
ZZZMUC09	'P c a 21'	-40	-41.4	-121.5	80.7	0	-122.2
ZZZWGK01	'P 21 21 21'	-17	-22	-59.6	27.7	0	-70.9
ZZZWGK03	'P b c a'	-16.8	-21.1	-56.3	25.4	0	-68.9

Table S5. PIXEL cohesive energies ($\text{kJ}\cdot\text{mol}^{-1}$), with the corresponding decomposition into Coulomb (E_c), polarization (E_p), dispersion (E_d), repulsion (E_r) and dipole (E_{dip}) terms, for the POLY-*pix* dataset. Entries in the Table are organized as follows (from left to right): CSD refcode, E_c , E_p , E_d , E_r , E_{dip} and E_{coh} .

ABAKEV01	-24.3	-9.1	-77.3	49.3	0.0	-61.5
ABAKEV02	-28.4	-10.5	-78.0	51.3	0.0	-65.6
ABIZAP01	-53.5	-19.5	-109.6	104.3	0.0	-78.3
ABIZAP	-51.6	-19.8	-107.8	93.8	0.0	-85.4
ACRDIN04	-26.3	-16.5	-108.6	78.0	0.0	-73.4
ACRDIN05	-29.1	-14.7	-100.8	72.8	-1.3	-73.2
ACRDIN07	-22.9	-13.1	-99.8	61.7	0.0	-74.2
AHAPEG01	-45.6	-21.7	-151.9	109.3	0.0	-109.9
AHAPEG	-73.6	-30.8	-161.2	145.9	0.0	-119.6
ANUKAW01	-55.7	-28.7	-160.3	134.6	-0.2	-110.3
ANUKAW	-58.4	-26.5	-158.6	129.2	0.0	-114.3
BCOCAN01	-37.9	-18.5	-100.1	65.3	-3.3	-94.5
BCOCAN03	-51.7	-24.5	-108.5	95.3	0.0	-89.4
BEBMAX01	-60.4	-25.1	-149.3	112.1	0.0	-122.7
BEBMAX	-38.7	-23.0	-153.3	103.4	-11.7	-123.3
CINYE01	-42.7	-21.1	-157.1	119.2	0.0	-101.7
CINYE	-41.1	-19.4	-164.8	120.1	-0.9	-106.0
DCLBQN01	-42.7	-15.0	-72.8	71.4	0.0	-59.0
DCLBQN02	-45.7	-16.4	-76.1	80.5	0.0	-57.8
DEBMUS	-45.5	-20.8	-160.3	104.4	0.0	-122.2
DEBNAZ	-40.5	-18.2	-153.9	96.0	0.0	-116.7
DIWKOK01	-35.4	-23.5	-112.1	97.2	0.0	-73.8
DIWKOK	-36.4	-24.8	-111.3	94.3	-2.6	-80.8
DUDNAS01	-47.7	-18.5	-104.5	82.2	0.0	-88.5
DUDNAS	-55.6	-24.1	-120.7	111.0	0.0	-89.4
FABRAB10	-30.6	-14.7	-109.7	73.1	0.0	-81.8
FABRAB11	-27.8	-13.3	-119.4	77.2	0.0	-83.2
GAGSIR01	-45.4	-15.5	-84.4	76.1	0.0	-69.1
GAGSIR	-48.3	-17.8	-91.8	89.7	0.0	-68.2
HAJYUN01	-44.8	-19.2	-143.1	102.7	0.0	-104.5
HAJYUN02	-64.5	-22.5	-137.7	122.3	0.0	-102.4
HEHWOJ01	-72.1	-22.8	-112.7	99.3	0.0	-108.3
HEHWOJ	-78.6	-26.5	-102.1	100.4	0.0	-106.8
HOKMAW01	-31.6	-10.7	-88.8	57.0	0.0	-74.1
HOKMAW	-35.5	-11.4	-93.1	67.7	0.0	-72.3
IBOBUY01	-71.4	-25.9	-150.2	127.1	0.0	-120.4
IBOBUY	-74.5	-30.7	-154.6	137.7	0.0	-122.1
JATFUF03	-36.5	-12.3	-81.0	51.3	0.0	-78.4
JATFUF04	-40.7	-12.2	-81.1	59.1	0.0	-75.0
KAWJAU01	-40.5	-16.2	-122.6	80.5	0.0	-98.8
KAWJAU	-44.9	-19.0	-137.1	101.6	-0.7	-100.1
LIKROW01	-31.9	-15.4	-105.1	77.1	-5.9	-81.2
LIKROW	-33.6	-15.2	-106.7	75.0	0.0	-80.4
LOZYII01	-59.3	-22.0	-114.8	70.7	0.0	-125.3
LOZYII	-59.2	-21.9	-122.5	85.9	0.0	-117.7
MAFPOA01	-48.4	-21.1	-124.4	103.0	0.0	-90.9
MAFPOA	-49.3	-19.6	-117.2	94.1	0.0	-92.0
MANPIM01	-41.4	-16.8	-104.3	70.7	0.0	-91.7
MANPIM02	-45.4	-17.4	-102.4	77.5	0.0	-87.6
MEGYON01	-51.6	-22.2	-148.9	119.7	-0.1	-102.9
MEGYON02	-51.5	-24.3	-146.0	117.7	0.0	-104.1
MIZHOT01	-40.5	-19.6	-142.0	96.7	0.0	-105.4
MIZHOT02	-38.4	-19.7	-140.7	94.7	-1.8	-105.9
MONTIS01	-53.6	-19.0	-140.6	95.2	0.0	-118.1
MONTIS	-56.0	-20.2	-144.7	100.1	0.0	-120.7
MSULIN04	-75.5	-32.0	-90.4	105.6	0.0	-92.3
MSULIN05	-63.9	-25.1	-91.2	87.6	0.0	-92.6

NANQUO02	-65.4	-22.8	-93.9	107.5	0.0	-74.6
NANQUO	-50.0	-15.1	-80.5	65.4	0.0	-80.3
NAPQAZ01	-39.6	-16.2	-120.0	82.3	0.0	-93.5
NAPQAZ	-38.7	-14.8	-118.9	78.8	0.0	-93.7
NAPTAN01	-36.3	-13.5	-94.2	68.0	0.0	-76.1
NAPTAN02	-41.5	-17.5	-93.3	63.4	0.0	-88.9
NIPSOV01	-41.9	-18.5	-150.1	100.4	0.0	-110.1
NIPSOV	-48.8	-20.2	-145.8	105.6	0.0	-109.3
NUJLIN01	-47.4	-22.6	-156.0	108.5	0.0	-117.6
NUJLIN	-42.7	-19.0	-143.4	97.5	-0.1	-107.7
NUKMAH02	-36.4	-20.3	-135.4	105.9	0.0	-86.3
NUKMAH	-28.4	-14.9	-121.3	70.1	0.0	-94.5
OHIBOW02	-59.5	-29.2	-198.4	135.1	0.0	-152.0
OHIBOW	-58.2	-26.8	-180.9	122.9	0.0	-143.1
PANQUO01	-42.6	-16.4	-96.3	77.4	0.0	-77.8
PANQUO	-45.1	-21.2	-92.1	75.5	0.0	-82.9
PEGWII01	-51.7	-23.6	-143.0	104.7	0.0	-113.6
PEGWII	-53.9	-25.1	-139.3	106.0	0.0	-112.3
PEJBUC01	-60.6	-24.5	-135.4	124.2	-1.1	-97.4
PEJBUC	-55.5	-27.4	-134.5	115.6	0.0	-101.8
PEJHOD01	-65.3	-30.1	-168.1	150.8	0.0	-112.7
PEJHOD	-59.3	-26.5	-163.3	137.2	0.0	-111.9
PEJJOFO1	-52.9	-26.5	-161.2	134.7	0.0	-106.0
PEJJOFO2	-56.4	-26.9	-175.1	143.7	0.0	-114.6
PHISCY01	-53.1	-31.0	-161.9	128.6	0.0	-117.3
PHISCY02	-58.4	-30.8	-162.7	131.0	0.0	-120.9
QAMNAT01	-33.0	-14.7	-110.8	70.1	0.0	-88.6
QAMNAT	-32.5	-15.7	-116.1	80.3	0.0	-84.0
QOGNEFO1	-57.8	-27.2	-135.8	121.8	-8.4	-107.5
QOGNEFO2	-65.5	-31.2	-130.8	124.0	0.0	-103.5
RIGHUK07	-43.7	-15.3	-101.4	66.3	0.0	-94.1
RIGHUK09	-38.3	-15.1	-97.5	58.2	0.0	-92.7
SAYVEV01	-75.8	-32.6	-159.2	147.9	0.0	-119.7
SAYVEV	-76.0	-32.5	-161.9	144.5	0.0	-125.9
SESYAR01	-49.4	-19.2	-120.5	100.2	0.0	-88.8
SESYAR	-56.1	-21.9	-120.8	101.5	0.0	-97.3
SIHNII01	-91.2	-43.0	-207.7	186.8	0.0	-155.0
SIHNII	-102.0	-45.9	-205.6	188.8	0.0	-164.7
TADLIU01	-53.0	-23.8	-145.7	120.6	0.0	-101.8
TADLIU02	-52.6	-23.8	-147.5	112.9	0.0	-110.9
XEWZAB01	-44.7	-30.3	-180.2	112.5	0.0	-142.7
XEWZAB	-54.8	-23.1	-169.4	113.7	0.0	-133.7
YAKYAL01	-34.9	-16.4	-107.6	81.6	0.0	-77.2
YAKYAL	-37.2	-17.5	-113.3	90.8	0.0	-77.3
ZZZBLP02	-35.5	-17.2	-147.5	107.4	0.0	-92.8
ZZZBLP03	-35.2	-17.7	-144.6	103.7	0.0	-93.8
ZZZWGK01	-19.9	-8.2	-51.1	40.9	0.0	-38.3
ZZZWGK03	-20.5	-7.8	-48.6	36.6	0.0	-40.3

Figure S1. ΔE_{el} vs ΔE_{dr} scatterplot (see main text, Section 3.4). Values are given in $\text{kJ}\cdot\text{mol}^{-1}$. Blue points refer to the POLY-*all* databank (254 structure pairs), whereas the red ones are relative to the POLY-*pix* one (52 structure pairs).

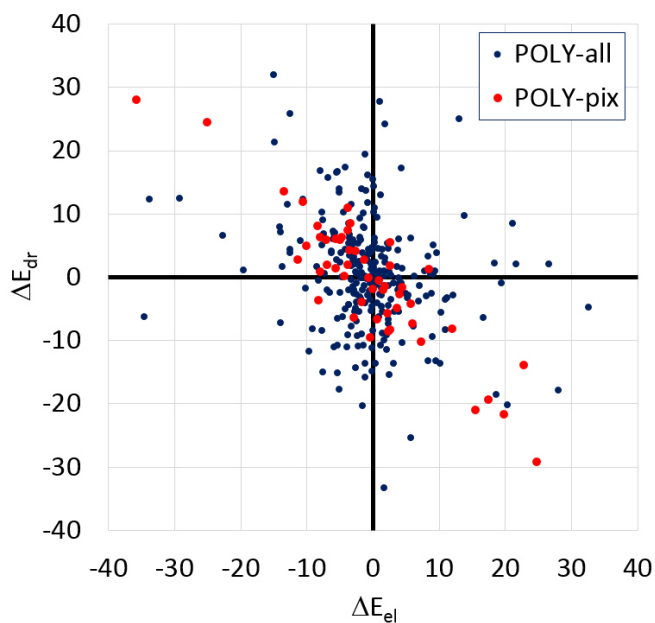


Figure S2. Weak correlation among the shortness parameter, B_s , of weak hydrogen bonds and the sum of AA-CLP purely electrostatic terms ($E_c + E_p$).

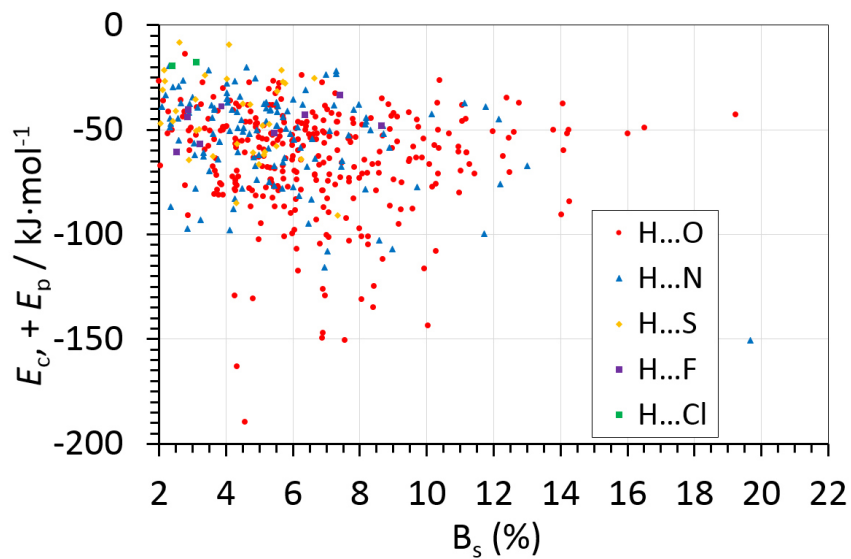


Table S6. Number distribution of compounds *vs.* differences between average contact distances, $\Delta\langle d_{\text{H}\cdots\text{X}}\rangle$, for $\text{H}\cdots\text{X}$ interactions among the polymorphs of each substance within the POLY-*all* databank. See Figure 4a in the main text and S2 below for the corresponding histogram.

$\Delta\langle d_{\text{H}\cdots\text{X}}\rangle / \text{\AA}$	$\text{H}\cdots\text{O}$	$\text{H}\cdots\text{N}$	$\text{H}\cdots\text{S}$	$\text{H}\cdots\text{Cl}$	$\text{H}\cdots\text{F}$
0.000–0.025	33	13	7	4	3
0.025–0.050	46	12	2	3	1
0.050–0.075	33	11	1	2	0
0.075–0.100	17	12	3	1	0
0.100–0.125	11	7	1	0	0
0.125–0.150	4	2	0	0	1
0.150–0.175	6	3	0	0	0
0.175–0.200	7	1	0	0	0
0.200–0.225	1	1	0	0	0
0.225–0.250	1	0	0	0	0
0.250–0.275	3	1	0	0	0
0.275–0.300	0	0	0	0	0
0.300–0.325	0	0	0	0	0
0.325–0.350	2	0	0	0	0
0.350–0.375	0	0	0	0	0
0.375–0.400	0	0	0	0	0
0.400–0.425	0	0	0	0	0
0.425–0.450	0	0	0	0	0
0.450–0.475	0	0	0	0	0
0.475–0.500	0	0	0	0	0
0.500–0.525	0	0	0	0	0
0.525–0.550	0	0	0	0	0
0.550–0.575	0	0	0	0	0
0.575–0.600	0	0	0	0	0
>0.600	0	0	0	0	0

Table S7. Number distribution of compounds vs. differences between average shortness index, ΔB_s , for H $\cdots$ X interactions among the polymorphs of each substance within the POLY-*all* databank. See Figure 4b in the main text and S2 below for the corresponding histogram.

$\Delta\langle B_s \rangle$	H $\cdots$ O	H $\cdots$ N	H $\cdots$ S	H $\cdots$ Cl	H $\cdots$ F
0–0.5	21	6	3	4	1
0.5–1	16	7	5	2	2
1–1.5	22	5	1	0	1
1.5–2	26	7	0	1	0
2–2.5	18	6	1	2	0
2.5–3	15	10	2	0	0
3–3.5	8	4	1	1	0
3.5–4	8	8	1	0	0
4–4.5	5	2	0	0	0
4.5–5	1	2	0	0	0
5–5.5	2	0	0	0	0
5.5–6	4	1	0	0	1
6–6.5	4	3	0	0	0
6.5–7	3	0	0	0	0
7–7.5	5	0	0	0	0
7.5–8	0	1	0	0	0
8–8.5	0	0	0	0	0
8.5–9	1	0	0	0	0
9–9.5	0	1	0	0	0
9.5–10	2	0	0	0	0
10–11	1	0	0	0	0
11–12	0	0	0	0	0
12–13	2	0	0	0	0
13–14	0	0	0	0	0
>14	0	0	0	0	0

Figure S3. Distribution of differences between average contact distances (a), Δd , and shortness index (b), ΔB_s , for $H\cdots X$ interactions among the polymorphs of each substance within the POLY-*all* databank.

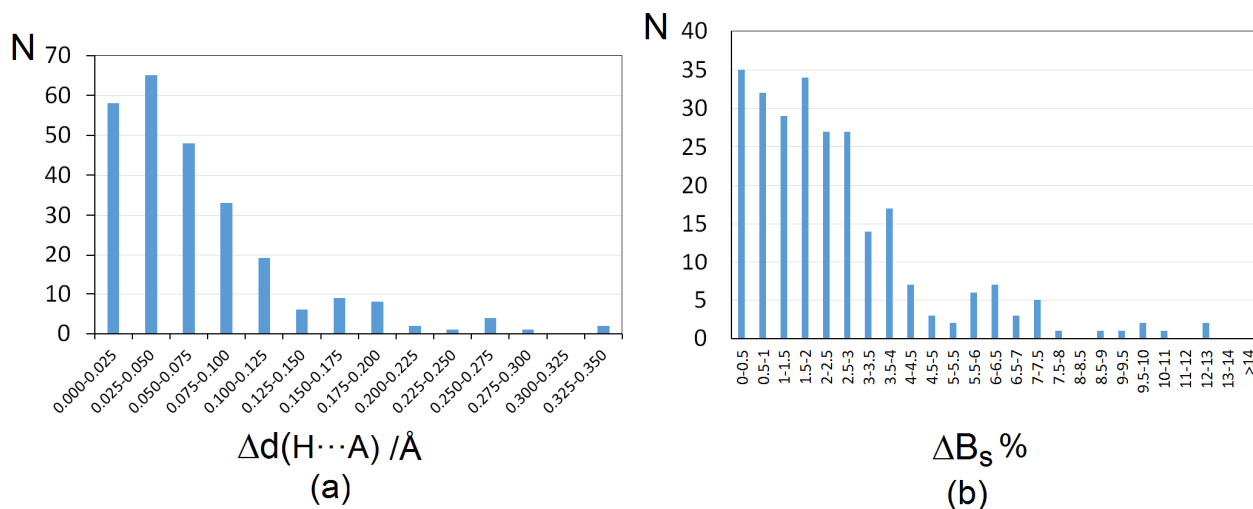


Figure S4. In-crystal PIXEL interaction energies, E_{mol} ($\text{kJ}\cdot\text{mol}^{-1}$) of molecular pairs bonded by weak HB that are conserved between polymorphs of the same substance vs. (a) $CH\cdots X$ ($X = N, O, S, Cl$) distances and (b) shortness parameter, B_s , of individual HB. The following thresholds were applied for considering a $H\cdots X$ contact as “conserved”: E_{mol} : 20 %; $H\cdots X$ distance: 20 %; $C-H\cdots X$ angle: 12 %. (c) and (d): As (a) and (b), with no thresholds on E_{mol} and 10 % / 6 % thresholds on $H\cdots X$ distance / $C-H\cdots X$ angle.

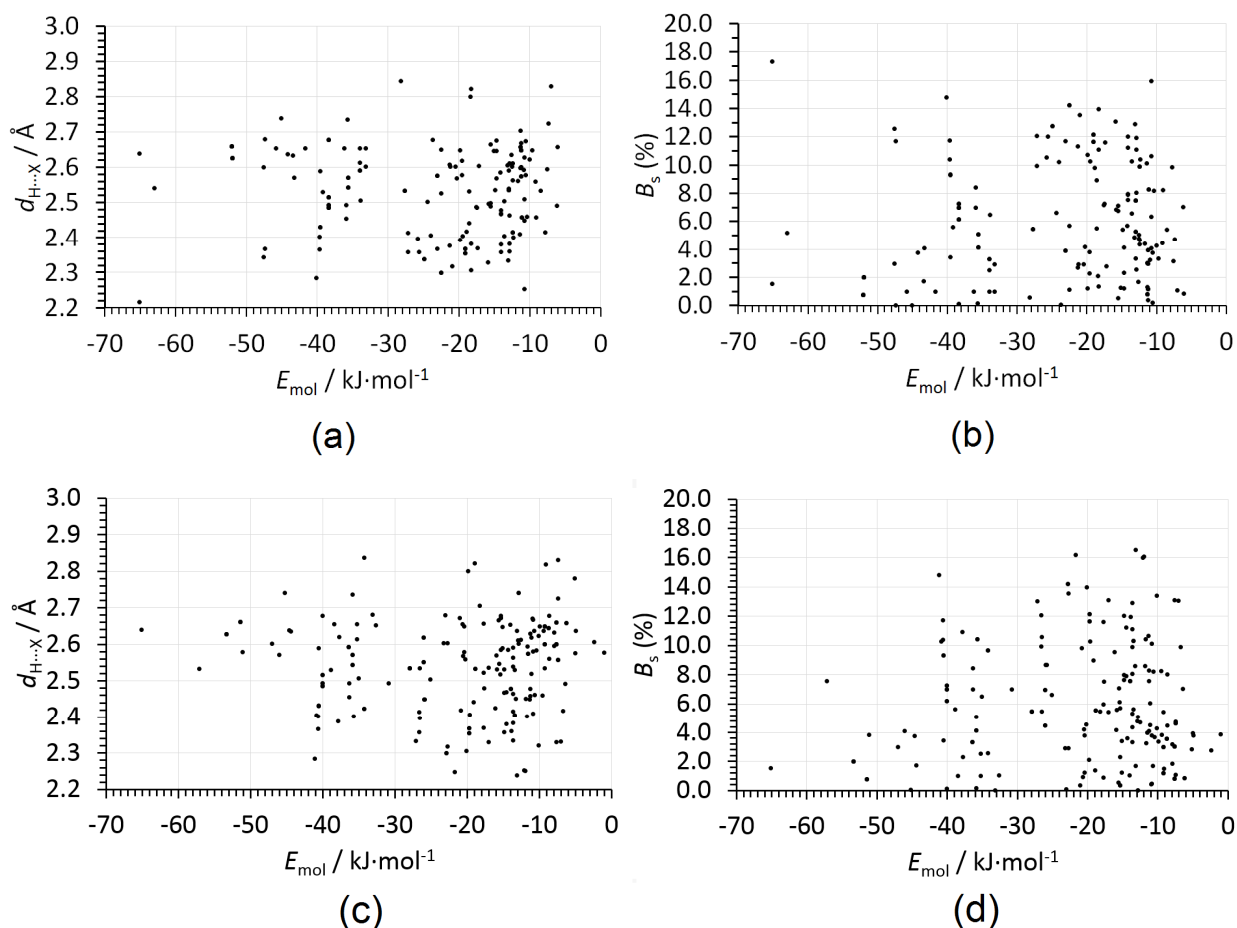


Figure S5. Short hydrogen-bond contacts in AZADAG, FUWFAG and DAKFUQ polymorphs, all characterized by non-conserved interactions. The H···O and H···N contact distances (in Å) are highlighted.

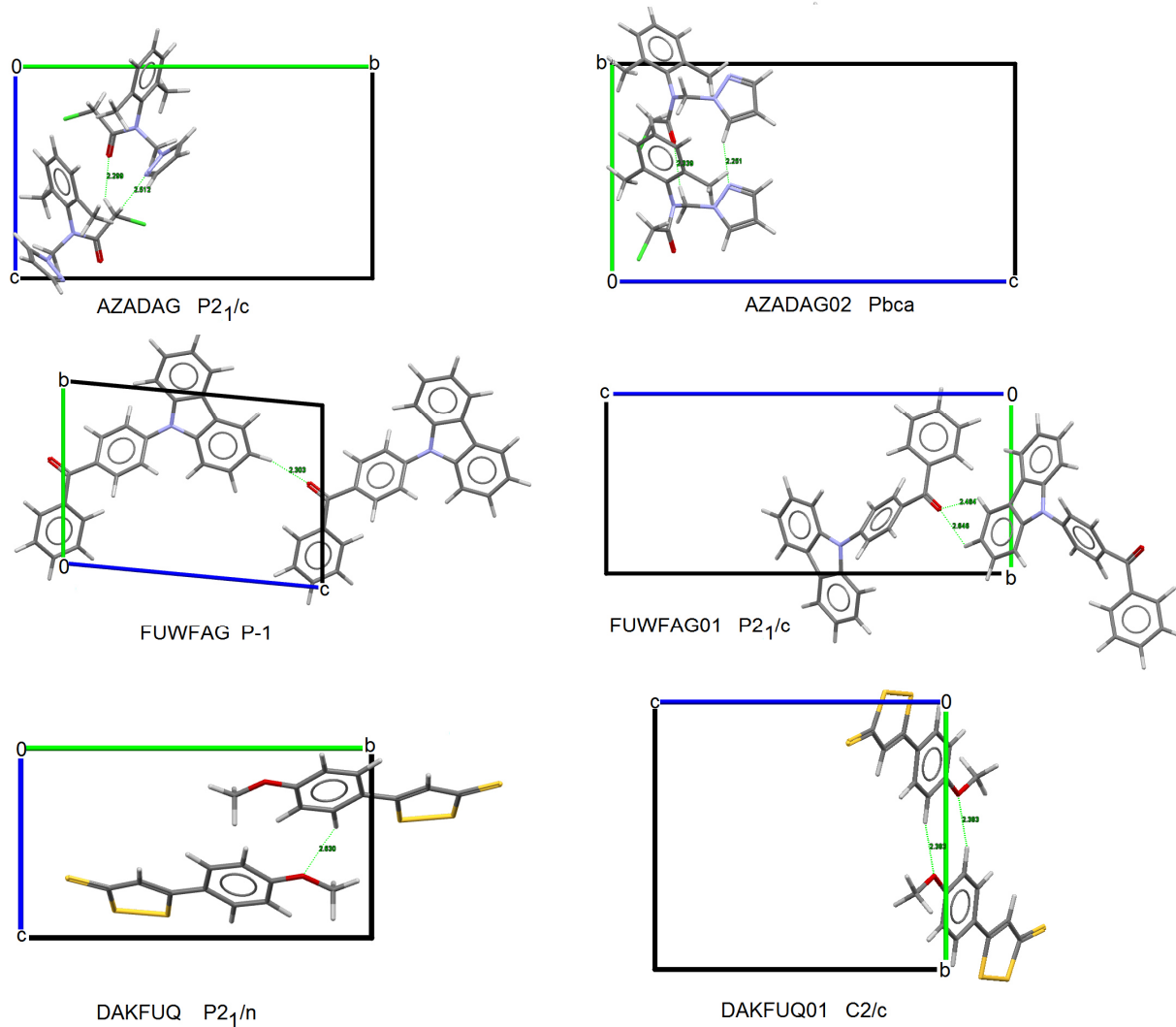


Table S8. Interaction geometries and AA–CLP molecular interaction energies^a for close neighbours of crystal forms shown in Figure S4. Values in Å, deg and kJ·mol⁻¹.

Crystal	$d_{H\cdots X}$	$d_{C\cdots X}$	$\alpha_{CH\cdots X}$	d_{CM}^b	Symmetry ^c	Donor– Acceptor	E_c	E_p	E_d	E_r	E_{mol}
AZADAG	2.299	3.235	144.0	6.1	$x, \frac{1}{2}-y, -\frac{1}{2}+z$	$CH_2\cdots O=C$	-15.5	-5.5	-43.5	26.3	-38.1
	2.512	3.441	143.5	6.1		$CH_2\cdots N=C$					
AZADAG02	2.338	3.395	165.8	6.4	$-\frac{1}{2}-x, \frac{1}{2}+y, z$	$CH_2\cdots O=C$	-9.7	-4.6	-37.4	29.7	-22.0
	2.249	3.246	152.6	6.4		$CH_2\cdots N=C$					
FUWFAG	2.303	3.349	162.6	13.0	$x, y, 1+z$	$Ph-H\cdots O=C$	-4.2	-1.2	-7.0	10.9	-1.4
FUWFAG01	2.484	3.216	124.1	12.9	$1+x, 3/2-y, \frac{1}{2}+z$	$Ph-H\cdots O=C$	-2.7	-1.7	-13.9	11.3	-7.0
	2.645	3.293	118.0	12.9		$Ph-H\cdots O=C$					
DAKFUQ	2.640	3.515	137.8	9.5	$\frac{1}{2}+x, -\frac{1}{2}-y, \frac{1}{2}+z$	$Ph-H\cdots OC_2$	0.3	-1.9	-13.9	8.2	-7.3
DAKFUQ01	2.383	3.432	163.4	10.8	$2-x, 1-y, -z$	$Ph-H\cdots OC_2$	-2.7	-1.9	-13.7	15.4	-2.9

^a The total molecule–molecule interaction energy, E_{mol} , is decomposed into Coulomb (E_c), polarization (E_p), dispersion (E_d) and repulsion (E_r) contributions.

^b Centre of mass distance, in Å.

^c Symmetry operation generating the HB acceptor.