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ELECTRONIC SUPPLEMENTARY INFORMATION

Features of noncovalent interactions in the group of highly polymorphic benzenesulfonamide derivatives

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In the following crystal structures coordinates of several H atoms were corrected to improve the geometry of the molecule, as well as several missing H atoms were added in geometrically calculated positions.

Sulfapyridine, polymorph IV

Crystal structure {BEWKUJ05}

CORRECTED COORDINATES:

H1 from (0.1620; 0.8830; 0.6280) to (0.1700; 0.8780; 0.6360)

H2 from (0.0650; 0.2740; 0.6690) to (0.0590; 0.2730; 0.6640)

H4 from (0.6870; 0.1760; 0.6540) to (0.6850; 0.1586; 0.6648)

H5 from (0.4530; 0.0990; 0.7070) to (0.4518; 0.8417; 0.6958)

H6 from (0.3350; 0.0510; 0.5980) to (0.3350; 0.0584; 0.5870)

H7 from (0.5850; 0.4440; 0.6030) to (0.5659; 0.3702; 0.5586)

ADDED ATOMS:

H8 (0.6384; 0.8851; 0.7362)

H9 (0.1250; 0.1496; 0.5315)

H10 (0.0389; 0.5600; 0.7574)

H11 (0.0786; 0.7693; 0.7521)

Sulfapyridine, polymorph II

Crystal structure {BEWKUJ11}

CORRECTED COORDINATES:

H2 from (0.1260; 0.6200; 0.4480) to (0.0887; 0.6050; 0.4561)

Sulfapyridine, polymorph V

Crystal structure {BEWKUJ13}

CORRECTED COORDINATES:

H1 from (0.5740; 0.5080; –0.0340) to (0.5780; 0.5140; –0.0500)

H2 from (0.5390; 0.5730; –0.0310) to (0.5316; 0.5605; –0.1104)

H5 from (0.5520; 0.7040; –0.1550) to (0.5480; 0.7040; –0.1660)

H6 from (0.5730; 0.8390; –0.0870) to (0.5739; 0.8397; –0.1124)

H8 from (0.8410; 0.9070; –0.0940) to (0.8466; 0.8947; –0.1079)

H9 from (0.8130; 0.9110; –0.2750) to (0.8087; 0.9060; –0.2835)

H10 from (0.7170; 0.9360; –0.3000) to (0.7165; 0.9240; –0.3018)

H11 from (0.6590; 0.9210; –0.1430) to (0.6590; 0.9220; –0.1430)

H12 from (0.5100; 0.0620; 0.3310) to (0.5311; 0.0128; 0.2089)

H14 from (0.5510; 0.3160; 0.3470) to (0.5500; 0.3220; 0.3530)

H15 from (0.5220; 0.1850; 0.3830) to (0.5152; 0.1935; 0.3853)

H16 from (0.5580; 0.1170; 0.0960) to (0.5678; 0.1114; 0.0846)

H17 from (0.5990; 0.2460; 0.0590) to (0.6030; 0.2460; 0.0590)

H18 from (0.7710; 0.3880; 0.2040) to (0.7710; 0.3696; 0.2009)

H19 from (0.8170; 0.3570; 0.3410) to (0.8234; 0.3363; 0.3532)

H20 from (0.7850; 0.3070; 0.5250) to (0.7864; 0.3175; 0.5252)

H21 from (0.6910; 0.3500; 0.5470) to (0.6895; 0.3326; 0.5492)

H22 from (0.6460; 0.3830; 0.3710) to (0.6368; 0.3664; 0.3966)

Sulfamerazine, *Pbca* polymorph

Crystal structure {SLFNMA01}

CORRECTED COORDINATES:

H2 from (0.4800; 0.4910; 0.1320) to (0.4877; 0.4961; 0.1349)

H10 from (0.0540; 0.1890; 0.3810) to (0.0473; 0.1850; 0.3690)

H11 from (0.1830; 0.1450; 0.3470) to (0.1880; 0.1500; 0.3520)

H12 from (0.1580; 0.0830; 0.3980) to (0.1202; 0.1026; 0.4047)

Characteristics of atomic interactions in the polymorphs of six benzenesulfonamide derivatives calculated within the MVDP method

The following Tables S1–S3 include these characteristics of atomic interactions:

- k – the number of pyramids representing interatomic contacts;
- d_{min} and d_{max} (Å) – distances for the shortest and the longest contact respectively;
- S (Å^2) – the total surface area of all faces corresponding to the given type of contacts;
- V (Å^3) – the total volume of all pyramids corresponding to the given type of contacts;
- Δ_S (%) – partial contribution of contacts to the total surface area of the corresponding faces;
- Δ_V (%) – partial contribution of contacts to the total volume of the corresponding pyramids.

The last column Σ shows the cumulative values for each molecule.

Table S1.1. Characteristics of chemical bonds in sulfapyridine polymorphs (VD polyhedra faces with RF = 1). The temperature at which X-ray diffraction experiments were conducted (as stated in respective .cif files) is provided below the refcodes.

Form	Refcode		H–C	H–N	C–C	C–N	C–S	N–S	O–S	Σ
II	BEWKUJ11	*k*	16	6	20	8	2	2	4	58
	295 K	d_{min}	0.84	1.02	1.35	1.35	1.76	1.60	1.44	0.84
		d_{max}	1.08	1.08	1.40	1.38	1.76	1.60	1.46	1.76
		S	121.13	38.48	156.99	56.81	9.82	10.18	23.43	416.82
		V	19.80	6.77	36.11	12.94	2.88	2.72	5.66	86.87
		Δ_S	29.06	9.23	37.66	13.63	2.35	2.44	5.62	100.00
		Δ_V	22.80	7.80	41.56	14.89	3.31	3.13	6.51	100.00
III	BEWKUJ15	*k*	16	6	20	8	2	2	4	58
	173 K	d_{min}	0.95	0.84	1.35	1.34	1.75	1.61	1.44	0.84
		d_{max}	0.95	0.88	1.42	1.37	1.75	1.61	1.46	1.75
		S	118.85	37.84	147.26	56.75	10.08	10.38	24.41	405.56
		V	18.82	5.42	34.10	12.86	2.94	2.78	5.89	82.82
		Δ_S	29.31	9.33	36.31	13.99	2.48	2.56	6.02	100.00
		Δ_V	22.72	6.55	41.18	15.52	3.55	3.36	7.12	100.00
IV	BEWKUJ05	*k*	16	6	20	8	2	2	4	58
	295 K	d_{min}	0.85	0.85	1.35	1.35	1.77	1.63	1.42	0.85
		d_{max}	1.08	0.87	1.43	1.37	1.77	1.63	1.43	1.77
		S	117.70	38.84	136.35	53.44	9.83	9.82	23.64	389.62
		V	19.27	5.55	31.53	12.11	2.89	2.66	5.61	79.62
		Δ_S	30.21	9.97	35.00	13.72	2.52	2.52	6.07	100.00
		Δ_V	24.20	6.97	39.60	15.21	3.63	3.34	7.04	100.00
V	BEWKUJ13	*k*	16	6	20	8	2	2	4	58
	295 K	d_{min}	0.94	0.86	1.31	1.33	1.74	1.61	1.42	0.86
		d_{max}	1.03	1.05	1.41	1.39	1.78	1.62	1.44	1.78
		S	119.09	39.80	141.62	57.61	9.82	10.17	23.50	401.61
		V	19.67	6.28	32.24	13.10	2.88	2.74	5.60	82.51
		Δ_S	29.65	9.91	35.26	14.35	2.44	2.53	5.85	100.00
		Δ_V	23.84	7.62	39.07	15.88	3.49	3.32	6.79	100.00
V*a*		*k*	16	6	20	8	2	2	4	58
		d_{min}	0.97	0.90	1.33	1.36	1.78	1.62	1.43	0.90
		d_{max}	1.03	1.05	1.40	1.39	1.78	1.62	1.43	1.78
		S	118.75	40.30	138.66	58.42	10.13	10.17	24.10	400.51
		V	19.77	6.48	31.61	13.38	3.00	2.75	5.74	82.72
		Δ_S	29.65	10.06	34.62	14.59	2.53	2.54	6.02	100.00
		Δ_V	23.90	7.83	38.21	16.17	3.63	3.32	6.94	100.00
V*b*		*k*	16	6	20	8	2	2	4	58
		d_{min}	0.94	0.86	1.31	1.33	1.74	1.61	1.42	0.86
		d_{max}	1.00	1.02	1.41	1.39	1.74	1.61	1.44	1.74
		S	119.44	39.31	144.58	56.81	9.51	10.18	22.89	402.70
		V	19.58	6.09	32.87	12.83	2.75	2.73	5.46	82.30
		Δ_S	29.66	9.76	35.90	14.11	2.36	2.53	5.68	100.00
		Δ_V	23.79	7.40	39.94	15.59	3.34	3.31	6.63	100.00
VI	BEWKUJ14	*k*	16	6	20	8	2	2	4	58
	120 K	d_{min}	0.95	0.84	1.35	1.34	1.74	1.60	1.43	0.84
		d_{max}	0.95	0.90	1.40	1.41	1.75	1.64	1.45	1.75
		S	121.02	35.56	151.98	53.52	9.92	9.54	23.12	404.65
		V	19.16	5.11	35.04	12.13	2.88	2.58	5.56	82.45
		Δ_S	29.91	8.79	37.56	13.22	2.45	2.36	5.71	100.00
		Δ_V	23.23	6.19	42.50	14.72	3.49	3.12	6.74	100.00

Table S1.1. (continued)

Form	Refcode		H–C	H–N	C–C	C–N	C–S	N–S	O–S	Σ
VI*a*		*k*	16	6	20	8	2	2	4	58
		d_{min}	0.95	0.84	1.35	1.35	1.75	1.60	1.45	0.84
		d_{max}	0.95	0.90	1.40	1.36	1.75	1.60	1.45	1.75
		S	121.31	36.53	154.74	55.08	9.38	9.72	21.63	408.38
		V	19.21	5.25	35.72	12.46	2.73	2.59	5.23	83.17
		Δ_S	29.71	8.94	37.89	13.49	2.30	2.38	5.30	100.00
		Δ_V	23.09	6.31	42.95	14.98	3.28	3.11	6.29	100.00
VI*b*		*k*	16	6	20	8	2	2	4	58
		d_{min}	0.95	0.84	1.37	1.34	1.74	1.64	1.43	0.84
		d_{max}	0.95	0.88	1.40	1.41	1.74	1.64	1.44	1.74
		S	120.73	34.59	149.22	51.95	10.46	9.37	24.61	400.92
		V	19.11	4.97	34.37	11.81	3.03	2.57	5.89	81.74
		Δ_S	30.11	8.63	37.22	12.96	2.61	2.34	6.14	100.00
		Δ_V	23.38	6.07	42.05	14.45	3.71	3.14	7.20	100.00

Table S1.2. Characteristics of chemical bonds in sulfamerazine polymorphs (VD polyhedra faces with RF = 1). The temperature at which X-ray diffraction experiments were conducted (as stated in respective .cif files) is provided below the refcodes.

Form	Refcode		H–C	H–N	C–C	C–N	C–S	N–S	O–S	Σ
$P2_1/c$	SLFNMA03	k	18	6	18	12	2	2	4	62
	150 K	d_{min}	0.95	0.88	1.37	1.33	1.73	1.65	1.43	0.88
		d_{max}	0.98	0.88	1.50	1.39	1.73	1.65	1.44	1.73
		S	109.72	39.41	121.47	90.00	10.26	9.70	24.24	404.80
		V	17.47	5.78	28.20	20.22	2.97	2.67	5.80	83.10
		Δ_S	27.11	9.74	30.01	22.23	2.53	2.40	5.99	100.00
		Δ_V	21.02	6.96	33.94	24.33	3.57	3.22	6.97	100.00
Pbca	SLFNMA01	k	18	6	18	12	2	2	4	62
	295 K	d_{min}	0.87	0.80	1.36	1.32	1.75	1.64	1.43	0.80
		d_{max}	1.05	0.89	1.52	1.38	1.75	1.64	1.44	1.75
		S	106.24	36.69	133.85	82.46	9.91	10.00	23.94	403.09
		V	17.08	5.08	31.05	18.49	2.89	2.74	5.73	83.05
		Δ_S	26.36	9.10	33.21	20.46	2.46	2.48	5.94	100.00
		Δ_V	20.57	6.12	37.38	22.26	3.48	3.30	6.89	100.00
$Pna2_1$	SLFNMA04	k	18	6	18	12	2	2	4	62
	150 K	d_{min}	0.95	0.80	1.37	1.33	1.73	1.66	1.43	0.80
		d_{max}	0.98	0.89	1.50	1.40	1.74	1.66	1.44	1.74
		S	110.37	35.93	118.63	88.02	9.84	8.84	22.96	394.60
		V	17.57	5.08	27.61	19.80	2.85	2.44	5.49	80.84
		Δ_S	27.97	9.11	30.06	22.31	2.49	2.24	5.82	100.00
		Δ_V	21.74	6.28	34.16	24.49	3.52	3.02	6.79	100.00
a		k	18	6	18	12	2	2	4	62
		d_{min}	0.95	0.80	1.38	1.33	1.74	1.66	1.43	0.80
		d_{max}	0.98	0.84	1.49	1.40	1.74	1.66	1.44	1.74
		S	109.53	35.61	113.48	85.70	9.97	8.93	23.12	386.34
		V	17.44	4.89	26.41	19.29	2.89	2.47	5.53	78.89
		Δ_S	28.35	9.22	29.37	22.18	2.58	2.31	5.98	100.00
		Δ_V	22.10	6.19	33.47	24.45	3.66	3.13	7.01	100.00
b		k	18	6	18	12	2	2	4	62
		d_{min}	0.95	0.86	1.37	1.33	1.73	1.66	1.43	0.86
		d_{max}	0.98	0.89	1.50	1.38	1.73	1.66	1.44	1.73
		S	111.21	36.25	123.79	90.35	9.71	8.74	22.81	402.86
		V	17.71	5.27	28.82	20.31	2.81	2.41	5.46	82.78
		Δ_S	27.61	9.00	30.73	22.43	2.41	2.17	5.66	100.00
		Δ_V	21.39	6.37	34.81	24.53	3.39	2.91	6.59	100.00

Table S1.3. Characteristics of chemical bonds in sulfamethoxazole polymorphs (VD polyhedra faces with RF = 1). The temperature at which X-ray diffraction experiments were conducted (as stated in respective .cif files) is provided below the refcodes.

Form	Refcode		H–C	H–N	C–C	C–N	C–O	C–S	N–O	N–S	O–S	Σ
I	SLFNMB01	k	16	6	18	6	2	2	2	2	4	58
	295 K	d_{min}	0.86	0.83	1.33	1.29	1.35	1.74	1.41	1.65	1.43	0.83
		d_{max}	0.97	0.86	1.47	1.40	1.35	1.74	1.41	1.65	1.44	1.74
		S	88.81	33.44	108.14	33.18	12.29	10.38	13.67	8.21	24.18	332.30
		V	13.38	4.72	24.94	7.50	2.77	3.01	3.22	2.25	5.78	67.56
		Δ_S	26.73	10.06	32.54	9.98	3.70	3.12	4.11	2.47	7.28	100.00
		Δ_V	19.80	6.98	36.91	11.10	4.10	4.46	4.76	3.34	8.55	100.00
II	SLFNMB02	k	16	6	18	6	2	2	2	2	4	58
	295 K	d_{min}	0.89	0.90	1.33	1.30	1.35	1.74	1.41	1.65	1.43	0.89
		d_{max}	0.99	1.00	1.48	1.39	1.35	1.74	1.41	1.65	1.44	1.74
		S	91.51	35.57	118.61	38.30	11.71	10.63	14.53	9.22	24.69	354.76
		V	14.58	5.52	27.39	8.64	2.62	3.09	3.43	2.53	5.91	73.71
		Δ_S	25.80	10.03	33.43	10.80	3.30	3.00	4.10	2.60	6.96	100.00
		Δ_V	19.78	7.49	37.16	11.72	3.56	4.19	4.65	3.43	8.02	100.00
III	SLFNMB05	k	16	6	18	6	2	2	2	2	4	58
	153 K	d_{min}	0.95	0.83	1.34	1.30	1.35	1.75	1.43	1.64	1.43	0.83
		d_{max}	0.98	0.99	1.50	1.40	1.35	1.75	1.43	1.64	1.44	1.75
		S	96.29	33.67	115.98	36.51	11.60	10.84	15.17	9.41	25.30	354.74
		V	15.34	5.12	27.05	8.25	2.61	3.15	3.60	2.56	6.06	73.74
		Δ_S	27.14	9.49	32.69	10.29	3.27	3.05	4.27	2.65	7.13	100.00
		Δ_V	20.80	6.94	36.68	11.19	3.54	4.27	4.89	3.48	8.21	100.00
IV	SLFNMB06	k	16	6	18	6	2	2	2	2	4	58
	153 K	d_{min}	0.95	0.81	1.34	1.30	1.35	1.74	1.41	1.64	1.43	0.81
		d_{max}	0.98	0.89	1.48	1.39	1.35	1.74	1.41	1.64	1.44	1.74
		S	91.03	38.53	116.43	36.89	13.03	10.74	13.86	9.38	24.19	354.07
		V	14.51	5.43	27.02	8.30	2.93	3.11	3.26	2.56	5.79	72.90
		Δ_S	25.71	10.88	32.88	10.42	3.68	3.03	3.91	2.65	6.83	100.00
		Δ_V	19.90	7.45	37.07	11.39	4.02	4.26	4.47	3.51	7.94	100.00

Table S1.4. Characteristics of chemical bonds in sulfathiazole polymorphs (VD polyhedra faces with RF = 1). The temperature at which X-ray diffraction experiments were conducted (as stated in respective .cif files) is provided below the refcodes.

Form	Refcode		H–C	H–N	C–C	C–N	C–S	N–S	O–S	Σ
I	SUTHAZ29	*k*	12	6	14	8	6	2	4	52
	105 K	d_{min}	1.08	1.02	1.35	1.33	1.74	1.61	1.44	1.02
		d_{max}	1.08	1.06	1.41	1.38	1.75	1.62	1.45	1.75
		S	94.74	36.58	104.42	55.29	39.84	10.58	24.69	366.13
		V	17.10	6.32	24.20	12.48	11.56	2.84	5.95	80.46
		Δ_S	25.88	9.99	28.52	15.10	10.88	2.89	6.74	100.00
		Δ_V	21.25	7.85	30.08	15.51	14.37	3.53	7.40	100.00
I*a*		*k*	12	6	14	8	6	2	4	52
		d_{min}	1.08	1.02	1.35	1.33	1.74	1.61	1.45	1.02
		d_{max}	1.08	1.06	1.41	1.38	1.75	1.61	1.45	1.75
		S	94.21	36.62	96.29	54.26	39.24	10.74	24.61	355.96
		V	17.00	6.33	22.32	12.26	11.39	2.88	5.94	78.10
		Δ_S	26.47	10.29	27.05	15.24	11.02	3.02	6.91	100.00
		Δ_V	21.77	8.10	28.57	15.69	14.58	3.68	7.60	100.00
I*b*		*k*	12	6	14	8	6	2	4	52
		d_{min}	1.08	1.02	1.35	1.33	1.74	1.62	1.44	1.02
		d_{max}	1.08	1.06	1.41	1.38	1.75	1.62	1.45	1.75
		S	95.27	36.55	112.55	56.31	40.44	10.42	24.76	376.30
		V	17.20	6.31	26.09	12.71	11.73	2.81	5.97	82.82
		Δ_S	25.32	9.71	29.91	14.96	10.75	2.77	6.58	100.00
		Δ_V	20.77	7.62	31.51	15.34	14.17	3.39	7.21	100.00
II	SUTHAZ31	*k*	12	6	14	8	6	2	4	52
	100 K	d_{min}	1.07	1.02	1.35	1.33	1.74	1.60	1.45	1.02
		d_{max}	1.10	1.06	1.41	1.41	1.76	1.60	1.45	1.76
		S	91.98	32.50	97.86	51.78	38.26	10.46	23.32	346.16
		V	16.62	5.61	22.66	11.74	11.15	2.78	5.64	76.21
		Δ_S	26.57	9.39	28.27	14.96	11.05	3.02	6.74	100.00
		Δ_V	21.81	7.36	29.74	15.40	14.64	3.65	7.40	100.00
III	SUTHAZ34	*k*	12	6	14	8	6	2	4	52
	100 K	d_{min}	1.08	1.02	1.35	1.33	1.74	1.59	1.44	1.02
		d_{max}	1.10	1.06	1.41	1.41	1.76	1.60	1.45	1.76
		S	91.19	32.39	96.64	50.85	38.88	10.30	23.30	343.54
		V	16.52	5.60	22.37	11.52	11.33	2.74	5.62	75.70
		Δ_S	26.55	9.43	28.13	14.80	11.32	3.00	6.78	100.00
		Δ_V	21.82	7.40	29.55	15.22	14.96	3.62	7.42	100.00
III*a*		*k*	12	6	14	8	6	2	4	52
		d_{min}	1.08	1.02	1.35	1.33	1.74	1.59	1.45	1.02
		d_{max}	1.10	1.06	1.41	1.41	1.76	1.59	1.45	1.76
		S	90.86	32.23	95.76	50.19	38.21	10.39	23.35	341.00
		V	16.46	5.59	22.17	11.37	11.14	2.76	5.64	75.12
		Δ_S	26.65	9.45	28.08	14.72	11.21	3.05	6.85	100.00
		Δ_V	21.91	7.44	29.51	15.13	14.83	3.67	7.50	100.00
III*b*		*k*	12	6	14	8	6	2	4	52
		d_{min}	1.08	1.02	1.35	1.33	1.74	1.60	1.44	1.02
		d_{max}	1.10	1.05	1.41	1.41	1.76	1.60	1.45	1.76
		S	91.52	32.54	97.51	51.51	39.54	10.20	23.24	346.07
		V	16.57	5.62	22.58	11.67	11.51	2.73	5.60	76.28
		Δ_S	26.45	9.40	28.18	14.88	11.43	2.95	6.72	100.00
		Δ_V	21.73	7.36	29.60	15.30	15.09	3.58	7.34	100.00

Table S1.4. (continued)

Form	Refcode		H–C	H–N	C–C	C–N	C–S	N–S	O–S	Σ
IV	SUTHAZ37	*k*	12	6	14	8	6	2	4	52
	100 K	d_{min}	1.08	1.01	1.35	1.33	1.74	1.61	1.44	1.01
		d_{max}	1.09	1.05	1.41	1.41	1.77	1.61	1.45	1.77
		S	91.48	31.86	96.75	51.33	39.02	10.20	23.17	343.81
		V	16.55	5.49	22.41	11.64	11.38	2.73	5.59	75.78
		Δ_S	26.61	9.27	28.14	14.93	11.35	2.97	6.74	100.00
		Δ_V	21.84	7.24	29.58	15.36	15.01	3.60	7.38	100.00
V	SUTHAZ05	*k*	12	6	14	8	6	2	4	52
	150 K	d_{min}	0.93	0.86	1.33	1.32	1.73	1.59	1.44	0.86
		d_{max}	0.93	0.94	1.41	1.38	1.75	1.60	1.45	1.75
		S	91.46	38.89	95.27	58.53	40.37	10.45	24.43	359.38
		V	14.18	5.77	21.94	13.16	11.70	2.78	5.89	75.43
		Δ_S	25.45	10.82	26.51	16.29	11.23	2.91	6.80	100.00
		Δ_V	18.79	7.65	29.09	17.45	15.52	3.69	7.81	100.00
V*a*		*k*	12	6	14	8	6	2	4	52
		d_{min}	0.93	0.86	1.33	1.33	1.73	1.59	1.44	0.86
		d_{max}	0.93	0.94	1.41	1.38	1.74	1.59	1.45	1.74
		S	87.14	41.15	92.55	59.11	39.92	10.89	24.69	355.45
		V	13.51	6.15	21.34	13.28	11.56	2.89	5.95	74.66
		Δ_S	24.52	11.58	26.04	16.63	11.23	3.06	6.95	100.00
		Δ_V	18.09	8.23	28.58	17.78	15.48	3.87	7.97	100.00
V*b*		*k*	12	6	14	8	6	2	4	52
		d_{min}	0.93	0.86	1.33	1.32	1.74	1.60	1.45	0.86
		d_{max}	0.93	0.91	1.41	1.38	1.75	1.60	1.45	1.75
		S	95.78	36.62	97.98	57.95	40.82	10.02	24.16	363.32
		V	14.85	5.39	22.55	13.04	11.85	2.68	5.84	76.19
		Δ_S	26.36	10.08	26.97	15.95	11.23	2.76	6.65	100.00
		Δ_V	19.48	7.07	29.60	17.12	15.56	3.51	7.66	100.00

Table S1.5. Characteristics of chemical bonds in chlorpropamide polymorphs (VD polyhedra faces with RF = 1). The temperature at which X-ray diffraction experiments were conducted (as stated in respective .cif files) is provided below the refcodes.

Form	Refcode		H–C	H–N	C–C	C–N	C–O	C–S	C–Cl	N–S	O–S	Σ
α	BEDMIG10	*k*	22	4	16	6	2	2	2	2	4	60
	295 K	d_{min}	0.93	0.86	1.36	1.33	1.23	1.77	1.74	1.63	1.43	0.86
		d_{max}	0.97	0.86	1.52	1.46	1.23	1.77	1.74	1.63	1.43	1.77
		S	104.61	26.46	104.11	31.16	15.13	10.07	15.24	9.95	24.86	341.59
		V	16.49	3.79	24.05	7.19	3.09	2.97	4.43	2.70	5.91	70.62
		Δ_S	30.63	7.75	30.48	9.12	4.43	2.95	4.46	2.91	7.28	100.00
		Δ_V	23.35	5.37	34.05	10.18	4.38	4.20	6.27	3.82	8.37	100.00
β	BEDMIG01	*k*	22	4	16	6	2	2	2	2	4	60
	295 K	d_{min}	0.93	0.86	1.35	1.33	1.23	1.76	1.73	1.63	1.42	0.86
		d_{max}	0.97	0.86	1.54	1.45	1.23	1.76	1.73	1.63	1.43	1.76
		S	102.39	27.61	105.17	34.03	15.78	10.32	14.05	9.82	25.02	344.18
		V	16.14	3.96	24.18	7.79	3.23	3.02	4.06	2.67	5.94	70.98
		Δ_S	29.75	8.02	30.56	9.89	4.59	3.00	4.08	2.85	7.27	100.00
		Δ_V	22.73	5.57	34.06	10.98	4.55	4.25	5.72	3.76	8.37	100.00
γ	BEDMIG02	*k*	22	4	16	6	2	2	2	2	4	60
	295 K	d_{min}	0.93	0.86	1.35	1.32	1.25	1.76	1.74	1.64	1.43	0.86
		d_{max}	0.97	0.86	1.52	1.46	1.25	1.76	1.74	1.64	1.43	1.76
		S	102.54	28.37	100.65	32.40	14.40	10.40	14.28	9.93	25.64	338.61
		V	16.16	4.07	23.32	7.42	3.00	3.05	4.15	2.71	6.12	70.01
		Δ_S	30.28	8.38	29.73	9.57	4.25	3.07	4.22	2.93	7.57	100.00
		Δ_V	23.09	5.81	33.31	10.60	4.29	4.36	5.93	3.88	8.75	100.00
δ	BEDMIG03	*k*	22	4	16	6	2	2	2	2	4	60
	295 K	d_{min}	0.93	0.86	1.36	1.33	1.22	1.77	1.74	1.63	1.41	0.86
		d_{max}	0.97	0.86	1.48	1.45	1.22	1.77	1.74	1.63	1.42	1.77
		S	100.26	25.46	101.71	31.32	14.68	9.64	14.69	10.03	24.16	331.95
		V	15.80	3.65	23.42	7.22	2.99	2.84	4.27	2.73	5.70	68.62
		Δ_S	30.20	7.67	30.64	9.44	4.42	2.90	4.43	3.02	7.28	100.00
		Δ_V	23.02	5.32	34.13	10.52	4.36	4.13	6.23	3.98	8.31	100.00
ε	BEDMIG04	*k*	22	4	16	6	2	2	2	2	4	60
	295 K	d_{min}	0.93	0.86	1.35	1.30	1.24	1.76	1.74	1.63	1.43	0.86
		d_{max}	0.97	0.86	1.49	1.47	1.24	1.76	1.74	1.63	1.43	1.76
		S	106.71	25.51	108.59	28.55	13.65	9.60	14.37	9.21	25.09	341.27
		V	16.81	3.66	25.02	6.55	2.82	2.82	4.16	2.50	5.98	70.31
		Δ_S	31.27	7.48	31.82	8.36	4.00	2.81	4.21	2.70	7.35	100.00
		Δ_V	23.91	5.20	35.59	9.32	4.01	4.00	5.91	3.55	8.50	100.00

Table S1.6. Characteristics of chemical bonds in tolbutamide polymorphs (VD polyhedra faces with RF = 1). The temperature at which X-ray diffraction experiments were conducted (as stated in respective .cif files) is provided below the refcodes.

Form	Refcode		H–C	H–N	C–C	C–N	C–O	C–S	N–S	O–S	Σ
I	ZZZPUS20	*k*	32	4	20	6	2	2	2	4	72
	100 K	d_{min}	0.95	0.78	1.39	1.33	1.24	1.76	1.65	1.43	0.78
		d_{max}	0.99	0.79	1.53	1.46	1.24	1.76	1.65	1.44	1.76
		S	135.88	24.19	109.69	27.60	13.17	9.58	8.97	24.20	353.28
		V	21.98	3.17	25.92	6.39	2.72	2.81	2.47	5.79	71.23
		Δ_S	38.46	6.85	31.05	7.81	3.73	2.71	2.54	6.85	100.00
		Δ_V	30.85	4.45	36.38	8.97	3.82	3.94	3.46	8.12	100.00
II	ZZZPUS21	*k*	32	4	20	6	2	2	2	4	72
	100 K	d_{min}	0.95	0.88	1.37	1.32	1.23	1.75	1.64	1.42	0.88
		d_{max}	0.99	0.88	1.57	1.47	1.24	1.76	1.64	1.44	1.76
		S	135.29	25.70	104.09	30.66	13.65	9.91	9.69	24.38	353.37
		V	21.89	3.77	24.48	7.09	2.81	2.91	2.65	5.81	71.40
		Δ_S	38.29	7.27	29.46	8.68	3.86	2.80	2.74	6.90	100.00
		Δ_V	30.66	5.28	34.29	9.93	3.93	4.07	3.70	8.14	100.00
II*a*		*k*	32	4	20	6	2	2	2	4	72
		d_{min}	0.95	0.88	1.37	1.32	1.23	1.76	1.64	1.43	0.88
		d_{max}	0.99	0.88	1.53	1.47	1.23	1.76	1.64	1.43	1.76
		S	135.33	24.17	106.65	29.45	13.50	9.84	9.45	24.87	353.27
		V	21.90	3.55	25.04	6.81	2.78	2.89	2.58	5.93	71.47
		Δ_S	38.31	6.84	30.19	8.34	3.82	2.78	2.68	7.04	100.00
		Δ_V	30.64	4.96	35.03	9.52	3.88	4.05	3.61	8.30	100.00
II*b*		*k*	32	4	20	6	2	2	2	4	72
		d_{min}	0.95	0.88	1.37	1.33	1.24	1.75	1.64	1.42	0.88
		d_{max}	0.99	0.88	1.53	1.47	1.24	1.75	1.64	1.43	1.75
		S	133.20	24.12	107.11	29.49	13.82	9.89	9.67	24.88	352.16
		V	21.55	3.54	25.18	6.82	2.85	2.89	2.65	5.91	71.38
		Δ_S	37.82	6.85	30.41	8.37	3.92	2.81	2.75	7.06	100.00
		Δ_V	30.19	4.96	35.27	9.55	3.99	4.05	3.71	8.28	100.00
II*c*		*k*	32	4	20	6	2	2	2	4	72
		d_{min}	0.95	0.88	1.37	1.33	1.24	1.76	1.64	1.43	0.88
		d_{max}	0.99	0.88	1.53	1.46	1.24	1.76	1.64	1.43	1.76
		S	133.89	27.27	102.63	31.49	13.25	9.99	9.52	23.28	351.33
		V	21.66	4.00	24.15	7.28	2.73	2.94	2.60	5.54	70.89
		Δ_S	38.11	7.76	29.21	8.96	3.77	2.84	2.71	6.63	100.00
		Δ_V	30.55	5.65	34.06	10.26	3.85	4.14	3.67	7.81	100.00
II*d*		*k*	32	4	20	6	2	2	2	4	72
		d_{min}	0.95	0.88	1.38	1.33	1.23	1.76	1.64	1.43	0.88
		d_{max}	0.99	0.88	1.57	1.46	1.23	1.76	1.64	1.44	1.76
		S	138.74	27.22	99.98	32.21	14.04	9.93	10.10	24.49	356.71
		V	22.44	3.99	23.57	7.44	2.88	2.91	2.75	5.86	71.84
		Δ_S	38.90	7.63	28.03	9.03	3.94	2.78	2.83	6.87	100.00
		Δ_V	31.23	5.55	32.80	10.36	4.01	4.05	3.83	8.15	100.00
III	ZZZPUS12	*k*	32	4	20	6	2	2	2	4	72
	150 K	d_{min}	0.95	0.88	1.37	1.32	1.23	1.76	1.63	1.43	0.88
		d_{max}	0.99	0.88	1.53	1.46	1.23	1.76	1.63	1.43	1.76
		S	130.95	25.99	103.95	28.81	12.13	10.34	9.83	25.37	347.38
		V	21.19	3.81	24.36	6.66	2.49	3.03	2.68	6.04	70.27
		Δ_S	37.70	7.48	29.92	8.29	3.49	2.98	2.83	7.30	100.00
		Δ_V	30.16	5.43	34.67	9.48	3.54	4.32	3.81	8.60	100.00

Table S1.6. (continued)

Form	Refcode		H–C	H–N	C–C	C–N	C–O	C–S	N–S	O–S	Σ
IV	ZZZPUS07	k	32	4	20	6	2	2	2	4	72
	298 K	d_{min}	0.93	0.83	1.38	1.32	1.25	1.76	1.64	1.43	0.83
		d_{max}	0.97	0.89	1.54	1.47	1.25	1.76	1.64	1.43	1.76
		S	139.40	27.81	113.62	32.15	15.15	10.47	10.58	25.97	375.14
		V	22.07	4.03	26.72	7.39	3.15	3.06	2.90	6.20	75.51
		Δ_S	37.16	7.41	30.29	8.57	4.04	2.79	2.82	6.92	100.00
		Δ_V	29.23	5.33	35.38	9.78	4.17	4.06	3.84	8.21	100.00
V	ZZZPUS10	k	32	4	20	6	2	2	2	4	72
	298 K	d_{min}	0.93	0.72	1.29	1.32	1.22	1.74	1.64	1.41	0.72
		d_{max}	0.97	0.76	1.54	1.44	1.22	1.74	1.64	1.42	1.74
		S	133.74	25.85	117.22	32.46	15.33	10.54	8.76	25.21	369.10
		V	21.17	3.16	27.02	7.38	3.13	3.06	2.39	5.95	73.27
		Δ_S	36.23	7.00	31.76	8.79	4.15	2.86	2.37	6.83	100.00
		Δ_V	28.90	4.32	36.88	10.08	4.27	4.17	3.26	8.12	100.00

Table S2.1. Characteristics of intramolecular noncovalent interactions in sulfapyridine polymorphs (VD polyhedra faces with RF > 1). The temperature at which X-ray diffraction experiments were conducted (as stated in respective .cif files) is provided below the refcodes.

Form	Refcode		H···H	H···C	H···N	H···O	H···S	C···C	C···N	C···O	C···S	N···N	N···O	N···S	O···O	O···S	S···S	Σ
II	BEWKUJ11	k	20	32	12	6	6	18	8	8			4		2			116
	295 K	d_{min}	1.80	1.91	2.01	2.36	2.79	2.35	2.35	2.59			2.40		2.47			1.80
		d_{max}	2.81	3.32	3.02	2.74	2.86	4.03	3.23	3.05			2.56		2.47			4.03
		S	51.14	16.49	8.99	18.57	1.83	3.55	4.02	3.01			3.43		2.56			113.58
		V	20.24	6.26	3.93	7.76	0.86	1.88	1.81	1.33			1.41		1.05			46.54
		Δ_S	45.03	14.52	7.91	16.35	1.61	3.12	3.54	2.65			3.02		2.25			100.00
		Δ_V	43.49	13.46	8.44	16.67	1.85	4.04	3.90	2.87			3.04		2.26			100.00
III	BEWKUJ15	k	22	44	14	6	6	18	14	6			4		2			136
	173 K	d_{min}	1.49	1.89	2.01	2.20	2.68	2.37	2.35	2.59			2.44		2.46			1.49
		d_{max}	3.96	3.16	3.25	2.70	2.87	3.79	3.45	3.02			2.54		2.46			3.96
		S	58.28	14.38	4.83	17.19	1.98	2.07	6.20	3.65			6.09		2.00			116.65
		V	22.19	4.99	2.27	7.05	0.90	1.06	3.03	1.58			2.51		0.82			46.39
		Δ_S	49.96	12.32	4.14	14.74	1.69	1.78	5.32	3.13			5.22		1.71			100.00
		Δ_V	47.83	10.76	4.90	15.20	1.94	2.28	6.52	3.40			5.41		1.77			100.00
IV	BEWKUJ05	k	20	34	6	6	4	24	8	8			4		2			116
	295 K	d_{min}	1.47	1.92	2.41	2.49	2.76	2.35	2.38	2.57			2.40		2.45			1.47
		d_{max}	2.70	3.14	3.11	2.70	2.86	3.47	3.32	3.01			2.51		2.45			3.47
		S	51.89	15.74	8.19	19.16	1.92	0.82	3.06	4.01			4.87		2.58			112.23
		V	19.99	5.96	3.72	8.17	0.90	0.33	1.43	1.80			1.98		1.05			45.33
		Δ_S	46.23	14.02	7.29	17.07	1.71	0.73	2.72	3.58			4.34		2.30			100.00
		Δ_V	44.10	13.15	8.21	18.02	1.99	0.73	3.14	3.98			4.37		2.32			100.00
V	BEWKUJ13	k	20	38	12	6	6	20	8	7	1	1	4		2			125
	295 K	d_{min}	1.55	1.89	2.03	2.46	2.77	2.29	2.32	2.55	2.61	2.25	2.40		2.45			1.55
		d_{max}	2.76	3.14	3.27	2.69	2.97	4.01	3.38	3.08	2.61	2.25	2.53		2.45			4.01
		S	61.57	17.94	6.47	20.89	1.92	2.96	2.98	4.44	<0.01	0.25	4.55		1.98			125.94
		V	23.89	6.65	2.88	9.03	0.90	1.42	1.35	1.94	<0.01	0.10	1.87		0.81			50.84
		Δ_S	48.88	14.24	5.13	16.59	1.53	2.35	2.36	3.53	<0.01	0.20	3.61		1.57			100.00
		Δ_V	46.99	13.09	5.67	17.77	1.77	2.78	2.66	3.82	<0.01	0.19	3.68		1.59			100.00
V*a*		k	20	36	12	6	6	18	10	6	2	2	4		2			124
		d_{min}	1.55	1.98	2.05	2.46	2.77	2.29	2.35	2.59	2.61	2.25	2.40		2.45			1.55
		d_{max}	2.76	3.14	3.27	2.69	2.97	3.58	3.38	3.04	2.61	2.25	2.53		2.45			3.58
		S	63.52	17.44	5.93	21.36	1.93	2.59	2.59	5.14	<0.01	0.51	4.80		1.95			127.76
		V	24.75	6.46	2.58	9.23	0.90	1.20	1.18	2.26	<0.01	0.19	1.98		0.80			51.53
		Δ_S	49.72	13.65	4.64	16.72	1.51	2.03	2.03	4.03	<0.01	0.40	3.76		1.53			100.00
		Δ_V	48.03	12.54	5.01	17.90	1.75	2.33	2.30	4.39	<0.01	0.37	3.84		1.55			100.00

Table S2.1. (continued)

Form	Refcode		H···H	H···C	H···N	H···O	H···S	C···C	C···N	C···O	C···S	N···N	N···O	N···S	O···O	O···S	S···S	Σ
V*b*		*k*	20	40	12	6	6	22	6	8			4		2			126
		d_{min}	1.55	1.89	2.03	2.52	2.78	2.31	2.32	2.55			2.41		2.45			1.55
		d_{max}	2.61	2.95	3.23	2.69	2.85	4.01	3.32	3.08			2.50		2.45			4.01
		S	59.61	18.45	7.00	20.42	1.92	3.32	3.36	3.74			4.30		2.01			124.12
		V	23.02	6.84	3.18	8.84	0.89	1.63	1.52	1.63			1.77		0.82			50.14
		Δ_S	48.02	14.86	5.64	16.45	1.55	2.67	2.71	3.01			3.47		1.62			100.00
		Δ_V	45.92	13.65	6.35	17.63	1.78	3.24	3.03	3.24			3.52		1.63			100.00
VI	BEWKUJ14	*k*	21	42	8	7	6	20	5	8	2		4		2			125
	120 K	d_{min}	1.51	1.84	1.97	2.35	2.16	2.29	2.34	2.58	2.58		2.41		2.46			1.51
		d_{max}	4.13	3.99	3.05	2.95	2.90	3.74	2.74	3.13	2.70		2.53		2.48			4.13
		S	67.53	20.36	8.37	22.83	2.24	3.43	2.31	3.99	0.03		4.21		2.19			137.49
		V	26.40	7.92	3.46	9.84	1.01	1.77	1.04	1.83	0.01		1.73		0.90			55.90
		Δ_S	49.12	14.81	6.09	16.61	1.63	2.49	1.68	2.90	0.02		3.06		1.59			100.00
		Δ_V	47.22	14.17	6.18	17.60	1.80	3.17	1.85	3.27	0.02		3.10		1.61			100.00
VI*a*		*k*	20	38	10	6	4	14	8	10	2		4		2			118
		d_{min}	1.51	1.88	2.01	2.51	2.82	2.35	2.34	2.58	2.58		2.41		2.46			1.51
		d_{max}	2.79	2.93	3.05	2.95	2.83	3.34	2.74	3.13	2.58		2.53		2.46			3.34
		S	68.56	22.12	7.70	17.48	2.19	0.76	2.35	4.90	<0.01		3.72		2.61			132.38
		V	26.33	8.82	3.46	7.84	1.03	0.33	1.04	2.33	<0.01		1.53		1.07			53.77
		Δ_S	51.79	16.71	5.82	13.20	1.66	0.57	1.77	3.70	<0.01		2.81		1.97			100.00
		Δ_V	48.97	16.41	6.44	14.57	1.92	0.61	1.93	4.33	<0.01		2.84		1.99			100.00
VI*b*		*k*	22	46	6	8	8	26	2	6	2		4		2			132
		d_{min}	1.60	1.84	1.97	2.35	2.16	2.29	2.73	2.58	2.70		2.43		2.48			1.60
		d_{max}	4.13	3.99	2.69	2.69	2.90	3.74	2.73	3.00	2.70		2.49		2.48			4.13
		S	66.51	18.61	9.03	28.19	2.29	6.10	2.28	3.08	0.05		4.70		1.77			142.61
		V	26.47	7.02	3.45	11.84	0.98	3.21	1.04	1.33	0.02		1.94		0.73			58.03
		Δ_S	46.64	13.05	6.33	19.77	1.60	4.28	1.60	2.16	0.04		3.29		1.24			100.00
		Δ_V	45.60	12.10	5.95	20.41	1.69	5.54	1.78	2.29	0.04		3.35		1.26			100.00

Table S2.2. Characteristics of intramolecular noncovalent interactions in sulfamerazine polymorphs (VD polyhedra faces with RF > 1). The temperature at which X-ray diffraction experiments were conducted (as stated in respective .cif files) is provided below the refcodes.

Form	Refcode		H···H	H···C	H···N	H···O	H···S	C···C	C···N	C···O	C···S	N···N	N···O	N···S	O···O	O···S	S···S	Σ
$P2_1/c$	SLFNMA03	*k*	28	30	12	6	6	24	10	6		4	6	2	2			136
	150 K	d_{min}	1.52	1.95	1.98	2.44	2.20	2.25	2.41	2.59		2.29	2.41	3.01	2.48			1.52
		d_{max}	3.90	2.05	3.45	2.63	2.83	3.35	3.46	3.15		2.33	2.97	3.01	2.48			3.90
		S	78.32	23.04	23.00	18.23	0.91	3.13	6.26	2.51		1.06	7.42	0.67	3.53			168.07
		V	29.42	7.80	9.90	7.79	0.43	1.29	3.09	1.10		0.41	3.42	0.34	1.45			66.43
		Δ_S	46.60	13.71	13.69	10.84	0.54	1.86	3.72	1.49		0.63	4.42	0.40	2.10			100.00
		Δ_V	44.29	11.73	14.91	11.73	0.64	1.93	4.66	1.65		0.62	5.14	0.50	2.19			100.00
Pbca	SLFNMA01	*k*	26	40	14	6	6	18	8	10		2	6	2	2			140
	295 K	d_{min}	1.38	1.88	1.96	2.44	2.19	2.25	2.43	2.59		2.35	2.41	3.06	2.47			1.38
		d_{max}	3.55	2.85	3.37	2.67	2.82	3.47	3.55	3.15		2.35	2.98	3.06	2.47			3.55
		S	71.15	22.41	19.08	17.33	1.46	3.33	5.39	2.09		1.14	7.07	0.58	3.60			154.60
		V	24.77	7.57	8.24	7.30	0.64	1.35	2.81	0.91		0.44	3.25	0.30	1.48			59.06
		Δ_S	46.02	14.49	12.34	11.21	0.94	2.15	3.49	1.35		0.74	4.57	0.38	2.33			100.00
		Δ_V	41.95	12.82	13.94	12.37	1.09	2.29	4.75	1.54		0.75	5.50	0.50	2.51			100.00
$Pna2_1$	SLFNMA04	*k*	28	39	13	6	6	19	8	5		4	6	2	2			138
	150 K	d_{min}	1.44	1.87	1.98	2.36	2.12	2.26	2.41	2.59		2.28	2.41	3.00	2.47			1.44
		d_{max}	3.88	3.65	2.92	2.65	2.84	3.31	3.30	2.98		2.34	3.01	3.01	2.47			3.88
		S	87.72	23.94	18.84	18.89	1.67	3.31	5.89	1.93		1.34	5.25	0.73	3.23			172.73
		V	33.43	8.16	7.97	8.08	0.68	1.41	2.95	0.84		0.52	2.40	0.37	1.33			68.13
		Δ_S	50.78	13.86	10.91	10.94	0.97	1.92	3.41	1.12		0.77	3.04	0.42	1.87			100.00
		Δ_V	49.07	11.98	11.69	11.86	1.00	2.07	4.33	1.23		0.76	3.53	0.54	1.95			100.00
a		*k*	28	38	12	6	6	18	8	6		4	6	2	2			136
		d_{min}	1.44	1.87	1.98	2.44	2.14	2.26	2.41	2.59		2.29	2.41	3.01	2.47			1.44
		d_{max}	3.86	3.63	2.92	2.65	2.84	3.27	3.26	2.98		2.34	3.01	3.01	2.47			3.86
		S	89.46	23.60	18.22	19.71	1.51	3.40	6.08	2.23		1.22	4.84	0.74	3.56			174.56
		V	34.16	8.01	7.66	8.50	0.62	1.45	3.05	0.97		0.48	2.21	0.37	1.47			68.93
		Δ_S	51.25	13.52	10.44	11.29	0.86	1.95	3.48	1.28		0.70	2.77	0.42	2.04			100.00
		Δ_V	49.56	11.62	11.11	12.32	0.91	2.11	4.42	1.40		0.69	3.20	0.54	2.13			100.00
b		*k*	28	40	14	6	6	20	8	4		4	6	2	2			140
		d_{min}	1.44	1.95	1.98	2.36	2.12	2.26	2.42	2.59		2.28	2.42	3.00	2.47			1.44
		d_{max}	3.88	3.65	2.85	2.62	2.84	3.31	3.30	2.60		2.33	3.00	3.00	2.47			3.88
		S	85.98	24.27	19.46	18.07	1.84	3.22	5.70	1.64		1.45	5.65	0.72	2.90			170.89
		V	32.70	8.31	8.28	7.67	0.74	1.37	2.85	0.71		0.56	2.60	0.36	1.19			67.33
		Δ_S	50.31	14.20	11.39	10.58	1.08	1.88	3.33	0.96		0.85	3.30	0.42	1.70			100.00
		Δ_V	48.57	12.34	12.29	11.39	1.10	2.04	4.23	1.05		0.83	3.86	0.54	1.77			100.00

Table S2.3. Characteristics of intramolecular noncovalent interactions in sulfamethoxazole polymorphs (VD polyhedra faces with RF > 1). The temperature at which X-ray diffraction experiments were conducted (as stated in respective .cif files) is provided below the refcodes.

Form	Refcode		H···H	H···C	H···N	H···O	H···S	C···C	C···N	C···O	C···S	N···N	N···O	N···S	O···O	O···S	S···S	Σ
I	SLFNMB01	k	22	42	8	12	8	18	2	10	2		4		2			130
	295 K	d_{min}	1.38	1.84	2.30	2.51	2.09	2.17	2.73	2.14	2.65		2.43		2.47			1.38
		d_{max}	2.96	3.65	2.84	2.68	3.16	3.69	2.73	3.07	2.65		2.49		2.47			3.69
		S	67.65	30.04	7.56	35.07	2.42	3.47	0.74	3.30	0.47		4.71		1.62			157.03
		V	24.29	10.58	2.98	15.21	0.95	1.82	0.34	1.38	0.21		1.93		0.67			60.36
		Δ_S	43.08	19.13	4.81	22.33	1.54	2.21	0.47	2.10	0.30		3.00		1.03			100.00
		Δ_V	40.24	17.53	4.94	25.20	1.58	3.02	0.56	2.28	0.34		3.20		1.10			100.00
II	SLFNMB02	k	24	42	10	12	8	16	4	8	2		4		2			132
	295 K	d_{min}	1.48	1.97	2.44	2.48	2.20	2.18	2.73	2.16	2.66		2.42		2.49			1.48
		d_{max}	3.53	3.63	3.38	2.70	3.09	3.70	3.42	2.61	2.66		2.49		2.49			3.70
		S	76.64	25.88	6.25	36.77	1.80	3.12	2.88	3.46	0.27		3.54		1.84			162.44
		V	28.12	9.08	2.59	15.71	0.79	1.63	1.32	1.46	0.12		1.46		0.76			63.03
		Δ_S	47.18	15.93	3.85	22.64	1.11	1.92	1.77	2.13	0.17		2.18		1.13			100.00
		Δ_V	44.61	14.41	4.11	24.92	1.25	2.58	2.10	2.31	0.19		2.31		1.21			100.00
III	SLFNMB05	k	22	40	8	12	8	18	4	10	2		4		2			130
	153 K	d_{min}	1.51	1.87	2.43	2.52	2.28	2.19	2.72	2.17	2.67		2.41		2.49			1.51
		d_{max}	3.15	3.59	3.27	2.80	3.16	3.70	3.35	3.08	2.67		2.48		2.49			3.70
		S	74.74	24.50	5.77	36.01	1.37	3.45	2.72	3.90	0.25		4.08		1.97			158.73
		V	27.79	8.40	2.41	15.65	0.63	1.79	1.28	1.66	0.11		1.67		0.82			62.19
		Δ_S	47.08	15.43	3.63	22.68	0.86	2.17	1.71	2.45	0.15		2.57		1.24			100.00
		Δ_V	44.68	13.50	3.88	25.16	1.01	2.87	2.05	2.66	0.18		2.69		1.32			100.00
IV	SLFNMB06	k	22	38	8	12	8	14	4	12	2		4		2			126
	153 K	d_{min}	1.49	1.90	2.43	2.43	2.11	2.17	2.72	2.15	2.68		2.41		2.48			1.49
		d_{max}	3.15	3.50	3.26	2.75	3.12	3.68	3.36	3.06	2.68		2.49		2.48			3.68
		S	65.83	24.59	5.82	33.17	1.93	1.53	2.52	3.86	0.10		2.43		1.35			143.14
		V	24.37	8.41	2.42	14.33	0.85	0.72	1.15	1.62	0.04		1.00		0.56			55.47
		Δ_S	45.99	17.18	4.07	23.18	1.34	1.07	1.76	2.70	0.07		1.70		0.95			100.00
		Δ_V	43.93	15.16	4.36	25.84	1.52	1.30	2.07	2.93	0.08		1.80		1.01			100.00

Table S2.4. Characteristics of intramolecular noncovalent interactions in sulfathiazole polymorphs (VD polyhedra faces with RF > 1). The temperature at which X-ray diffraction experiments were conducted (as stated in respective .cif files) is provided below the refcodes.

Form	Refcode		H···H	H···C	H···N	H···O	H···S	C···C	C···N	C···O	C···S	N···N	N···O	N···S	O···O	O···S	S···S	Σ
I	SUTHAZ29	*k*	14	27	9	4	8	18	6	9	6	1	4		2	2	2	112
	105 K	d_{min}	1.72	2.02	2.09	2.47	2.43	2.30	2.27	2.58	2.56	2.32	2.41		2.48	2.97	3.28	1.72
		d_{max}	2.75	2.59	3.38	2.69	3.32	3.44	3.42	2.99	3.79	2.32	2.53		2.48	2.99	3.29	3.79
		S	39.00	8.91	4.86	14.91	12.17	2.54	4.10	5.30	2.10	<0.01	3.44		1.22	6.44	0.27	105.24
		V	15.46	3.14	2.14	6.39	6.14	1.26	1.86	2.41	1.22	<0.01	1.42		0.50	3.19	0.15	45.27
		Δ_S	37.06	8.46	4.62	14.17	11.56	2.41	3.89	5.03	2.00	<0.01	3.27		1.16	6.12	0.25	100.00
		Δ_V	34.15	6.93	4.73	14.12	13.56	2.78	4.12	5.32	2.69	<0.01	3.13		1.11	7.04	0.32	100.00
I*a*		*k*	14	26	10	4	8	18	6	8	6	2	4		2	2	2	112
		d_{min}	1.72	2.02	2.09	2.47	2.49	2.30	2.28	2.58	2.56	2.32	2.41		2.48	2.99	3.29	1.72
		d_{max}	2.72	2.18	3.25	2.69	3.32	3.44	2.72	2.99	3.79	2.32	2.53		2.48	2.99	3.29	3.79
		S	42.19	10.34	5.49	13.92	11.10	1.85	3.40	3.75	2.12	<0.01	2.87		1.56	3.84	0.30	102.73
		V	16.74	3.63	2.42	5.96	5.84	0.90	1.51	1.69	1.26	<0.01	1.18		0.64	1.91	0.17	43.84
		Δ_S	41.07	10.07	5.35	13.55	10.80	1.80	3.31	3.65	2.06	<0.01	2.79		1.52	3.74	0.29	100.00
		Δ_V	38.17	8.27	5.51	13.59	13.32	2.06	3.45	3.86	2.86	<0.01	2.70		1.46	4.36	0.38	100.00
I*b*		*k*	14	28	8	4	8	18	6	10	6		4		2	2	2	112
		d_{min}	1.78	2.05	2.12	2.53	2.43	2.41	2.27	2.59	2.57		2.42		2.48	2.97	3.28	1.78
		d_{max}	2.75	2.59	3.38	2.69	3.09	3.37	3.42	2.98	3.72		2.52		2.48	2.97	3.28	3.72
		S	35.82	7.47	4.23	15.90	13.23	3.23	4.79	6.85	2.09		4.01		0.87	9.03	0.23	107.75
		V	14.19	2.65	1.87	6.83	6.44	1.61	2.22	3.12	1.18		1.65		0.36	4.47	0.13	46.70
		Δ_S	33.24	6.93	3.92	14.75	12.28	3.00	4.44	6.36	1.94		3.72		0.81	8.38	0.22	100.00
		Δ_V	30.38	5.67	4.00	14.62	13.78	3.45	4.74	6.68	2.52		3.53		0.77	9.57	0.27	100.00
II	SUTHAZ31	*k*	14	28	10	4	6	16	6	8	6		4		2	2	2	108
	100 K	d_{min}	1.65	2.02	2.13	2.53	2.48	2.41	2.28	2.60	2.53		2.43		2.46	2.91	3.27	1.65
		d_{max}	2.71	3.84	2.96	2.98	3.88	3.80	3.11	3.15	4.11		2.56		2.46	2.91	3.27	4.11
		S	35.00	10.21	15.92	8.52	3.79	3.57	3.33	4.39	2.06		4.09		3.02	6.93	0.09	100.91
		V	13.32	3.60	7.19	3.82	1.93	1.83	1.53	1.99	1.16		1.70		1.24	3.37	0.05	42.71
		Δ_S	34.69	10.12	15.78	8.44	3.76	3.54	3.30	4.35	2.04		4.05		2.99	6.87	0.09	100.00
		Δ_V	31.19	8.42	16.84	8.94	4.52	4.28	3.58	4.65	2.72		3.97		2.90	7.88	0.11	100.00
III	SUTHAZ34	*k*	16	27	9	4	6	16	6	8	6	1	4		2	2	2	109
	100 K	d_{min}	1.64	2.00	2.11	2.54	2.46	2.41	2.27	2.59	2.53	2.32	2.43		2.46	2.87	3.27	1.64
		d_{max}	4.15	3.81	2.91	3.02	3.98	3.84	3.12	3.17	4.13	2.32	2.55		2.47	2.93	3.28	4.15
		S	33.08	10.36	12.79	8.72	4.14	3.53	2.96	4.50	2.10	<0.01	4.11		3.29	6.89	0.07	96.53
		V	12.81	3.67	5.73	3.95	2.03	1.79	1.33	2.04	1.20	<0.01	1.70		1.35	3.33	0.04	40.98
		Δ_S	34.26	10.73	13.25	9.04	4.29	3.65	3.07	4.66	2.18	<0.01	4.26		3.41	7.13	0.07	100.00
		Δ_V	31.26	8.96	13.97	9.64	4.96	4.37	3.25	4.98	2.94	<0.01	4.16		3.30	8.12	0.09	100.00

Table S2.4. (continued)

Form	Refcode		H···H	H···C	H···N	H···O	H···S	C···C	C···N	C···O	C···S	N···N	N···O	N···S	O···O	O···S	S···S	Σ
III*a*		*k*	16	30	10	4	6	16	6	8	6	2	4		2	2	2	114
		d_{min}	1.64	2.01	2.12	2.56	2.46	2.41	2.28	2.60	2.53	2.32	2.43		2.46	2.93	3.28	1.64
		d_{max}	3.95	3.71	2.87	3.02	3.98	3.76	3.10	3.17	4.13	2.32	2.55		2.46	2.93	3.28	4.13
		S	32.11	9.50	15.80	7.80	3.82	3.62	2.69	4.63	2.23	<0.01	4.17		2.93	6.85	0.07	96.22
		V	12.70	3.39	7.06	3.53	1.82	1.85	1.21	2.09	1.28	<0.01	1.73		1.20	3.34	0.04	41.24
		Δ_S	33.37	9.88	16.43	8.11	3.97	3.76	2.80	4.81	2.32	<0.01	4.33		3.04	7.12	0.07	100.00
		Δ_V	30.79	8.23	17.12	8.57	4.40	4.48	2.93	5.07	3.11	<0.01	4.20		2.91	8.10	0.09	100.00
III*b*		*k*	16	24	8	4	6	16	6	8	6		4		2	2	2	104
		d_{min}	1.69	2.00	2.11	2.54	2.48	2.41	2.27	2.59	2.54		2.43		2.47	2.87	3.27	1.69
		d_{max}	4.15	3.81	2.91	2.97	3.84	3.84	3.12	3.12	4.09		2.55		2.47	2.87	3.27	4.15
		S	34.05	11.22	9.78	9.64	4.46	3.44	3.22	4.38	1.97		4.06		3.65	6.92	0.07	96.85
		V	12.92	3.95	4.39	4.36	2.25	1.74	1.45	1.99	1.12		1.68		1.50	3.31	0.04	40.71
		Δ_S	35.15	11.58	10.10	9.96	4.60	3.55	3.33	4.52	2.03		4.19		3.77	7.15	0.07	100.00
		Δ_V	31.74	9.71	10.79	10.72	5.53	4.26	3.57	4.89	2.75		4.12		3.69	8.14	0.09	100.00
IV	SUTHAZ37	*k*	16	26	8	4	6	18	6	8	6		4		2	2	2	108
	100 K	d_{min}	1.66	2.01	2.11	2.55	2.46	2.41	2.28	2.60	2.54		2.44		2.47	2.89	3.28	1.66
		d_{max}	4.12	3.76	2.88	2.99	3.87	3.82	3.11	3.14	4.12		2.55		2.47	2.89	3.28	4.12
		S	30.88	9.65	9.97	9.27	5.51	3.46	2.99	4.39	1.92		4.15		3.21	6.96	0.07	92.43
		V	11.96	3.43	4.47	4.21	2.72	1.74	1.34	1.99	1.09		1.71		1.32	3.35	0.04	39.36
		Δ_S	33.41	10.44	10.79	10.02	5.96	3.74	3.24	4.75	2.08		4.49		3.47	7.53	0.07	100.00
		Δ_V	30.37	8.70	11.35	10.69	6.91	4.43	3.41	5.05	2.78		4.35		3.35	8.51	0.09	99.99
V	SUTHAZ05	*k*	15	26	8	6	7	13	6	8	4		4		2	2	1	102
	150 K	d_{min}	1.48	1.93	2.50	2.54	2.38	2.40	2.24	2.58	2.54		2.42		2.45	2.82	3.26	1.48
		d_{max}	4.32	2.56	2.84	3.76	4.04	3.83	3.12	3.20	4.17		2.54		2.46	2.91	3.26	4.32
		S	42.52	11.47	14.33	10.46	5.16	2.19	2.57	6.83	1.33		3.34		2.30	9.37	0.10	111.97
		V	15.69	3.82	6.38	4.78	2.43	1.02	1.11	3.08	0.75		1.38		0.94	4.48	0.06	45.91
		Δ_S	37.98	10.25	12.80	9.34	4.61	1.95	2.30	6.10	1.18		2.98		2.06	8.37	0.09	100.00
		Δ_V	34.18	8.31	13.89	10.40	5.30	2.23	2.42	6.71	1.62		3.01		2.05	9.75	0.12	100.00
V*a*		*k*	14	26	8	6	6	14	6	8	2		4		2	2		98
		d_{min}	1.52	1.94	2.50	2.54	2.38	2.41	2.25	2.58	2.56		2.42		2.45	2.82		1.52
		d_{max}	2.51	2.04	2.78	3.69	2.85	3.51	3.06	2.90	2.56		2.54		2.45	2.82		3.69
		S	40.99	9.54	11.86	7.81	4.45	1.54	2.68	7.05	0.30		3.14		3.03	9.55		101.92
		V	15.14	3.20	5.28	3.60	1.86	0.66	1.16	3.16	0.13		1.30		1.24	4.48		41.20
		Δ_S	40.21	9.36	11.63	7.66	4.36	1.51	2.63	6.91	0.29		3.08		2.97	9.37		100.00
		Δ_V	36.75	7.76	12.81	8.74	4.50	1.59	2.83	7.68	0.31		3.15		3.00	10.88		100.00

Table S2.4. (continued)

Form	Refcode		H···H	H···C	H···N	H···O	H···S	C···C	C···N	C···O	C···S	N···N	N···O	N···S	O···O	O···S	S···S	Σ
V*b*		*k*	16	26	8	6	8	12	6	8	6		4		2	2	2	106
		d_{min}	1.48	1.93	2.50	2.55	2.38	2.40	2.24	2.59	2.54		2.42		2.46	2.91	3.26	1.48
		d_{max}	4.32	2.56	2.84	3.76	4.04	3.83	3.12	3.20	4.17		2.54		2.46	2.91	3.26	4.32
		S	44.06	13.41	16.80	13.11	5.88	2.83	2.46	6.61	2.35		3.53		1.58	9.20	0.21	122.01
		V	16.25	4.44	7.48	5.95	3.01	1.39	1.06	3.00	1.36		1.46		0.65	4.47	0.11	50.63
		Δ_S	36.11	10.99	13.77	10.74	4.82	2.32	2.01	5.42	1.93		2.89		1.29	7.54	0.17	100.00
		Δ_V	32.09	8.76	14.78	11.76	5.95	2.75	2.09	5.92	2.69		2.89		1.28	8.82	0.22	100.00

Table S2.5. Characteristics of intramolecular noncovalent interactions in chlorpropamide polymorphs (VD polyhedra faces with RF > 1). The temperature at which X-ray diffraction experiments were conducted (as stated in respective .cif files) is provided below the refcodes.

Form	Refcode		H···H	H···C	H···N	H···O	H···S	H···Cl	C···C	C···N	C···O	C···S	C···Cl	N···N	N···O	N···S	N···Cl	O···O	O···S	O···Cl	S···S	S···Cl	Cl···Cl	Σ
α	BEDMIG10	*k*	40	50	12	12	6	4	12	4	6				8			4	2					160
	295 K	d_{min}	1.57	1.90	2.00	2.46	2.16	2.78	2.37	2.46	2.58				2.27			2.48	3.01					1.57
		d_{max}	3.66	3.79	3.39	3.40	2.81	2.79	3.65	2.71	2.98				2.50			2.84	3.01					3.79
		S	85.97	20.84	9.30	31.90	1.51	15.36	0.82	4.22	2.94				2.91			5.65	0.25					181.64
		V	30.17	7.46	3.58	14.02	0.65	7.12	0.40	1.90	1.27				1.18			2.50	0.13					70.37
		Δ_S	47.33	11.47	5.12	17.56	0.83	8.45	0.45	2.32	1.62				1.60			3.11	0.14					100.00
		Δ_V	42.87	10.61	5.08	19.92	0.93	10.12	0.57	2.70	1.80				1.67			3.55	0.18					100.00
β	BEDMIG01	*k*	40	50	14	12	6	4	16	6	14				8			4	2					176
	295 K	d_{min}	1.57	1.89	1.99	2.46	2.18	2.74	2.35	2.48	2.59				2.26			2.47	2.94					1.57
		d_{max}	3.44	5.09	3.30	3.18	2.82	2.79	4.01	3.37	3.29				2.51			2.92	2.94					5.09
		S	96.49	21.96	10.67	36.00	0.87	10.31	2.79	3.19	8.24				4.12			5.64	0.76					201.03
		V	34.00	7.94	4.32	16.29	0.39	4.76	1.42	1.45	4.12				1.69			2.55	0.37					79.32
		Δ_S	47.99	10.92	5.31	17.91	0.43	5.13	1.39	1.59	4.10				2.05			2.81	0.38					100.00
		Δ_V	42.87	10.01	5.45	20.54	0.49	6.00	1.79	1.83	5.20				2.13			3.22	0.47					100.00
γ	BEDMIG02	*k*	40	48	12	12	6	4	16	6	14				8			4	2					172
	295 K	d_{min}	1.57	1.89	2.00	2.47	2.17	2.76	2.37	2.47	2.59				2.27			2.49	3.00					1.57
		d_{max}	3.61	3.05	3.55	3.02	2.85	2.78	3.65	3.51	3.45				2.51			2.88	3.00					3.65
		S	89.09	21.79	8.74	38.32	1.18	14.40	2.40	4.77	4.66				2.83			6.84	0.43					195.44
		V	30.84	7.87	3.52	17.06	0.52	6.65	1.32	2.14	2.14				1.15			3.00	0.22					76.40
		Δ_S	45.58	11.15	4.47	19.61	0.60	7.37	1.23	2.44	2.38				1.45			3.50	0.22					100.00
		Δ_V	40.36	10.30	4.61	22.32	0.68	8.70	1.72	2.80	2.79				1.50			3.92	0.28					100.00
δ	BEDMIG03	*k*	42	56	16	14	6	4	18	6	6				6			4	2					180
	295 K	d_{min}	1.56	1.90	1.99	2.42	2.17	2.76	2.36	2.45	2.58				2.28			2.46	3.01					1.56
		d_{max}	3.90	3.86	3.32	3.75	2.81	2.79	3.61	3.39	3.01				2.50			2.81	3.01					3.90
		S	94.51	23.15	9.07	32.51	1.41	14.08	0.86	4.37	2.32				3.36			4.99	0.19					190.80
		V	32.43	8.73	3.55	14.23	0.60	6.51	0.40	1.96	1.00				1.36			2.24	0.09					73.10
		Δ_S	49.53	12.13	4.75	17.04	0.74	7.38	0.45	2.29	1.21				1.76			2.61	0.10					100.00
		Δ_V	44.37	11.95	4.85	19.46	0.82	8.90	0.54	2.68	1.37				1.86			3.07	0.13					100.00
ε	BEDMIG04	*k*	50	56	14	12	6	4	16	4	14	2			8			4	2					192
	295 K	d_{min}	1.57	1.87	2.01	2.48	2.18	2.77	2.37	2.48	2.60	2.65			2.27			2.47	2.93					1.57
		d_{max}	4.65	4.87	3.54	3.74	2.81	2.79	3.37	2.67	3.72	2.65			2.52			2.95	2.93					4.87
		S	110.56	28.01	15.08	28.01	2.00	10.77	2.48	1.04	11.28	<0.01			4.06			6.09	0.79					220.17
		V	40.85	12.02	6.29	12.69	0.88	4.99	1.28	0.46	5.72	<0.01			1.65			2.72	0.39					89.94
		Δ_S	50.22	12.72	6.85	12.72	0.91	4.89	1.13	0.47	5.12	<0.01			1.84			2.77	0.36					100.00
		Δ_V	45.42	13.36	6.99	14.11	0.98	5.55	1.43	0.51	6.36	<0.01			1.83			3.03	0.43					100.00

Table S2.6. Characteristics of intramolecular noncovalent interactions in tolbutamide polymorphs (VD polyhedra faces with RF > 1). The temperature at which X-ray diffraction experiments were conducted (as stated in respective .cif files) is provided below the refcodes.

Form	Refcode		H···H	H···C	H···N	H···O	H···S	C···C	C···N	C···O	C···S	N···N	N···O	N···S	O···O	O···S	S···S	Σ
I	ZZZPUS20	*k*	82	84	14	12	6	20	4	12	2		8		4	2		250
	100 K	d_{min}	1.60	1.83	2.02	2.45	2.10	2.40	2.48	2.59	2.64		2.28		2.47	2.95		1.60
		d_{max}	4.61	4.28	3.24	3.69	2.84	3.24	2.70	3.84	2.64		2.54		2.96	2.95		4.61
		S	157.04	41.38	9.29	21.49	2.14	2.82	0.83	8.58	0.06		2.74		4.56	0.77		251.68
		V	57.60	16.81	3.64	9.50	0.92	1.39	0.37	4.18	0.03		1.12		2.03	0.38		97.94
		Δ_S	62.39	16.44	3.69	8.54	0.85	1.12	0.33	3.41	0.02		1.09		1.81	0.30		100.00
		Δ_V	58.81	17.16	3.71	9.70	0.94	1.42	0.37	4.27	0.03		1.14		2.08	0.38		100.00
II	ZZZPUS21	*k*	67	75	13	13	6	17	5	12			7		4	2		221
	100 K	d_{min}	1.60	1.91	2.02	2.46	2.18	2.37	2.47	2.58			2.27		2.46	2.95		1.60
		d_{max}	3.97	3.73	3.55	4.10	2.86	3.81	3.45	4.08			2.53		2.93	3.01		4.10
		S	147.10	29.39	9.81	26.52	1.50	1.15	3.19	5.71			3.05		5.40	0.54		233.36
		V	52.68	10.49	4.04	11.77	0.67	0.53	1.44	2.76			1.24		2.43	0.27		88.31
		Δ_S	63.04	12.59	4.20	11.36	0.64	0.49	1.37	2.45			1.31		2.31	0.23		100.00
		Δ_V	59.65	11.88	4.57	13.33	0.76	0.59	1.63	3.13			1.40		2.75	0.31		100.00
II*a*		*k*	66	72	12	12	6	16	6	14			6		4	2		216
		d_{min}	1.60	1.91	2.02	2.46	2.19	2.37	2.49	2.58			2.27		2.48	2.95		1.60
		d_{max}	3.11	3.65	2.88	3.26	2.86	3.81	3.15	3.93			2.53		2.93	2.95		3.93
		S	147.68	29.40	11.91	23.38	1.52	1.08	1.91	9.27			2.95		4.30	0.76		234.16
		V	52.70	10.59	4.94	10.36	0.70	0.45	0.86	4.51			1.19		1.96	0.38		88.63
		Δ_S	63.07	12.56	5.09	9.98	0.65	0.46	0.82	3.96			1.26		1.84	0.33		100.00
		Δ_V	59.46	11.95	5.57	11.69	0.79	0.51	0.97	5.08			1.34		2.21	0.42		100.00
II*b*		*k*	68	70	14	14	6	20	4	12			6		4	2		220
		d_{min}	1.60	1.92	2.02	2.46	2.20	2.38	2.48	2.59			2.29		2.46	2.99		1.60
		d_{max}	3.97	3.47	2.81	4.10	2.86	3.70	2.71	4.08			2.52		2.91	2.99		4.10
		S	152.62	29.85	11.93	23.50	1.55	1.50	1.61	8.05			2.84		6.40	0.74		240.60
		V	55.22	10.65	4.98	10.52	0.73	0.72	0.72	4.09			1.16		2.90	0.37		92.05
		Δ_S	63.43	12.41	4.96	9.77	0.65	0.62	0.67	3.34			1.18		2.66	0.31		100.00
		Δ_V	59.99	11.57	5.40	11.43	0.79	0.78	0.78	4.44			1.26		3.15	0.40		100.00
II*c*		*k*	66	82	12	12	6	12	6	10			8		4	2		220
		d_{min}	1.60	1.92	2.02	2.47	2.19	2.37	2.48	2.59			2.27		2.48	3.01		1.60
		d_{max}	3.59	3.73	3.43	2.90	2.84	3.76	3.45	3.01			2.50		2.80	3.01		3.76
		S	139.04	28.91	7.50	29.92	1.59	0.87	4.43	2.71			3.22		5.13	0.23		223.53
		V	49.48	10.37	3.09	13.25	0.69	0.37	2.00	1.19			1.31		2.30	0.12		84.14
		Δ_S	62.20	12.93	3.35	13.38	0.71	0.39	1.98	1.21			1.44		2.29	0.10		100.00
		Δ_V	58.80	12.32	3.67	15.74	0.82	0.44	2.38	1.41			1.55		2.73	0.14		100.00

Table S2.6. (continued)

Form	Refcode		H···H	H···C	H···N	H···O	H···S	C···C	C···N	C···O	C···S	N···N	N···O	N···S	O···O	O···S	S···S	Σ
II*d*		*k*	66	76	14	12	6	18	4	12			6		4	2		220
		d_{min}	1.60	1.92	2.02	2.46	2.18	2.39	2.47	2.59			2.29		2.49	3.00		1.60
		d_{max}	3.57	3.07	3.55	3.20	2.86	3.77	2.72	3.52			2.51		2.86	3.00		3.77
		S	149.06	29.39	7.90	29.26	1.32	1.14	4.82	2.83			3.20		5.78	0.45		235.12
		V	53.32	10.34	3.14	12.95	0.58	0.56	2.18	1.27			1.30		2.56	0.22		88.42
		Δ_S	63.40	12.50	3.36	12.44	0.56	0.48	2.05	1.20			1.36		2.46	0.19		100.00
		Δ_V	60.31	11.69	3.55	14.64	0.65	0.64	2.46	1.44			1.47		2.89	0.25		100.00
III	ZZZPUS12	*k*	74	80	12	14	6	14	6	6			6		4	2		224
	150 K	d_{min}	1.60	1.91	2.02	2.48	2.18	2.37	2.48	2.59			2.30		2.47	3.02		1.60
		d_{max}	4.19	3.59	3.05	3.28	2.86	2.76	3.24	3.19			2.50		2.84	3.02		4.19
		S	171.77	34.20	10.51	36.64	1.83	0.95	3.06	4.55			2.53		4.09	0.15		270.27
		V	63.40	12.61	4.26	15.96	0.82	0.38	1.38	1.97			1.02		1.85	0.07		103.72
		Δ_S	63.55	12.65	3.89	13.56	0.68	0.35	1.13	1.68			0.93		1.51	0.05		100.00
		Δ_V	61.13	12.16	4.11	15.38	0.79	0.37	1.33	1.90			0.99		1.78	0.07		100.00
IV	ZZZPUS07	*k*	68	80	16	12	6	16	6	8			8		4	2		226
	298 K	d_{min}	1.57	1.86	2.01	2.46	2.21	2.38	2.49	2.59			2.27		2.48	3.06		1.57
		d_{max}	4.39	4.56	3.59	3.21	2.82	3.61	3.55	3.00			2.51		2.93	3.06		4.56
		S	144.21	35.69	10.19	39.33	1.14	3.14	4.49	3.02			4.40		5.03	0.27		250.91
		V	51.27	13.09	3.98	17.52	0.52	1.74	2.04	1.31			1.79		2.29	0.14		95.68
		Δ_S	57.48	14.22	4.06	15.67	0.45	1.25	1.79	1.21			1.76		2.01	0.11		100.00
		Δ_V	53.58	13.68	4.16	18.31	0.55	1.82	2.13	1.37			1.87		2.39	0.14		100.00
V	ZZZPUS10	*k*	68	84	10	12	6	20	4	12			8		4	2		230
	298 K	d_{min}	1.57	1.82	1.98	2.37	2.01	2.27	2.44	2.57			2.25		2.45	2.97		1.57
		d_{max}	4.52	4.90	2.66	2.97	2.85	3.64	2.70	3.36			2.49		2.89	2.97		4.90
		S	159.22	36.27	8.38	37.93	1.96	4.20	3.29	5.66			4.07		5.31	0.57		266.87
		V	56.37	13.51	3.07	16.78	0.75	2.02	1.48	2.64			1.65		2.40	0.28		100.95
		Δ_S	59.66	13.59	3.14	14.21	0.74	1.57	1.23	2.12			1.52		1.99	0.21		100.00
		Δ_V	55.84	13.38	3.05	16.63	0.74	2.00	1.46	2.62			1.63		2.38	0.28		100.00

Table S3.1. Characteristics of intermolecular noncovalent interactions in sulfapyridine polymorphs (VD polyhedra faces with RF = 0). The temperature at which X-ray diffraction experiments were conducted (as stated in respective .cif files) is provided below the refcodes.

Form	Refcode		H···H	H···C	H···N	H···O	H···S	C···C	C···N	C···O	C···S	N···N	N···O	N···S	O···O	O···S	S···S	Σ
II	BEWKUJ11	k	75	64	26	28	4	51	14	8		2						272
	295 K	d_{min}	2.06	2.78	1.90	2.09	3.63	3.66	3.56	3.19		4.02						1.90
		d_{max}	4.26	4.38	4.12	3.68	3.63	4.95	4.54	3.60		4.02						4.95
		S	130.41	40.48	30.60	68.01	0.96	23.14	6.26	3.29		0.14						303.29
		V	65.12	23.12	14.34	30.76	0.58	15.69	3.81	1.86		0.09						155.37
		Δ_S	43.00	13.35	10.09	22.42	0.32	7.63	2.06	1.08		0.05						100.00
		Δ_V	41.91	14.88	9.23	19.80	0.38	10.10	2.45	1.20		0.06						100.00
III	BEWKUJ15	k	70	90	30	28	8	37	12						2			277
	173 K	d_{min}	2.49	2.83	2.23	2.12	3.40	3.52	3.38						2.99			2.12
		d_{max}	4.56	4.68	4.60	4.30	4.46	4.85	4.61						3.78			4.85
		S	124.11	51.55	30.94	68.83	0.40	18.52	6.12						1.99			302.47
		V	62.66	29.07	15.30	31.00	0.25	12.24	3.98						1.23			155.73
		Δ_S	41.03	17.04	10.23	22.76	0.13	6.12	2.02						0.66			100.00
		Δ_V	40.24	18.67	9.83	19.90	0.16	7.86	2.56						0.79			100.00
IV	BEWKUJ05	k	70	78	16	32	4	25	18	10		1	4	2				260
	295 K	d_{min}	2.22	2.93	2.04	2.31	3.69	3.57	3.61	3.33		4.09	3.07	3.92				2.04
		d_{max}	4.23	4.40	4.41	4.61	3.70	3.94	4.07	3.75		4.09	3.75	3.92				4.61
		S	122.72	61.95	25.76	72.42	0.78	13.91	6.57	1.72		0.12	2.32	0.02				308.29
		V	61.77	34.51	12.05	35.22	0.48	8.56	4.10	1.00		0.09	1.30	0.02				159.07
		Δ_S	39.81	20.09	8.36	23.49	0.25	4.51	2.13	0.56		0.04	0.75	0.01				100.00
		Δ_V	38.83	21.70	7.57	22.14	0.30	5.38	2.57	0.63		0.05	0.81	0.01				100.00
V	BEWKUJ13	k	75	89	27	34	5	25	13	6			3		1			278
	295 K	d_{min}	2.34	2.77	1.83	2.11	2.88	3.44	3.49	3.50			3.00		3.39			1.83
		d_{max}	5.26	4.66	4.56	4.77	3.65	4.44	4.59	4.05			4.36		3.39			5.26
		S	121.55	61.56	26.62	75.08	0.70	12.15	7.74	0.67			1.32		2.35			309.73
		V	61.77	34.96	12.24	36.55	0.41	8.01	5.11	0.42			0.71		1.33			161.51
		Δ_S	39.24	19.88	8.59	24.24	0.23	3.92	2.50	0.22			0.43		0.76			100.00
		Δ_V	38.25	21.65	7.58	22.63	0.26	4.96	3.16	0.26			0.44		0.82			100.00
V*a*		k	77	86	30	36	6	25	13	10			3		1			287
		d_{min}	2.34	2.77	1.83	2.11	2.88	3.44	3.49	3.50			3.24		3.39			1.83
		d_{max}	4.62	4.66	4.56	4.77	3.65	4.44	4.59	4.05			4.36		3.39			4.77
		S	120.17	61.30	29.40	75.47	0.89	12.15	7.74	1.02			2.53		2.35			313.02
		V	60.98	34.86	13.80	37.50	0.53	8.01	5.11	0.64			1.36		1.33			164.13
		Δ_S	38.39	19.58	9.39	24.11	0.29	3.88	2.47	0.33			0.81		0.75			100.00
		Δ_V	37.16	21.24	8.41	22.85	0.32	4.88	3.11	0.39			0.83		0.81			100.00

Table S3.1. (continued)

Form	Refcode		H···H	H···C	H···N	H···O	H···S	C···C	C···N	C···O	C···S	N···N	N···O	N···S	O···O	O···S	S···S	Σ
V*b*		*k*	73	92	24	32	4	25	13	2			3		1			269
		d_{min}	2.34	2.77	1.83	2.11	2.88	3.44	3.49	3.54			3.00		3.39			1.83
		d_{max}	5.26	4.66	4.56	4.77	3.62	4.44	4.59	3.91			4.36		3.39			5.26
		S	122.93	61.83	23.84	74.68	0.51	12.15	7.74	0.31			0.11		2.35			306.44
		V	62.56	35.06	10.67	35.60	0.30	8.01	5.11	0.19			0.06		1.33			158.90
		Δ_S	40.11	20.18	7.78	24.37	0.17	3.96	2.52	0.10			0.04		0.77			100.00
		Δ_V	39.37	22.07	6.72	22.41	0.19	5.04	3.22	0.12			0.04		0.84			100.00
VI	BEWKUJ14	*k*	71	83	27	30	5	34	8	2		2	1		2			265
	120 K	d_{min}	2.29	2.71	2.07	2.03	3.09	3.50	3.38	3.80		3.28	3.71		3.87			2.03
		d_{max}	4.89	4.64	4.40	5.01	3.99	4.60	4.78	4.23		3.29	3.71		4.34			5.01
		S	111.48	60.64	32.99	73.04	0.95	13.85	2.66	1.14		0.13	1.20		0.54			298.62
		V	56.99	35.56	15.86	33.92	0.54	9.20	1.63	0.73		0.07	0.74		0.35			155.59
		Δ_S	37.33	20.31	11.05	24.46	0.32	4.64	0.89	0.38		0.04	0.40		0.18			100.00
		Δ_V	36.63	22.86	10.19	21.80	0.35	5.91	1.05	0.47		0.05	0.47		0.22			100.00
VI*a*		*k*	73	85	25	33	5	34	8	2		2	1		2			270
		d_{min}	2.29	2.71	2.09	2.03	3.09	3.50	3.38	3.80		3.28	3.71		3.87			2.03
		d_{max}	4.89	4.64	4.40	5.01	3.99	4.60	4.78	4.23		3.29	3.71		4.34			5.01
		S	110.11	63.13	29.92	78.13	0.95	13.85	2.66	1.14		0.13	1.20		0.54			301.76
		V	56.50	37.22	14.25	35.17	0.54	9.20	1.63	0.73		0.07	0.74		0.35			156.38
		Δ_S	36.49	20.92	9.92	25.89	0.31	4.59	0.88	0.38		0.04	0.40		0.18			100.00
		Δ_V	36.13	23.80	9.11	22.49	0.34	5.88	1.04	0.46		0.05	0.47		0.22			100.00
VI*b*		*k*	69	81	29	27	5	34	8	2		2	1		2			260
		d_{min}	2.29	2.71	2.07	2.46	3.09	3.50	3.38	3.80		3.28	3.71		3.87			2.07
		d_{max}	4.89	4.64	4.40	5.01	3.99	4.60	4.78	4.23		3.29	3.71		4.34			5.01
		S	112.85	58.16	36.05	67.95	0.95	13.85	2.66	1.14		0.13	1.20		0.54			295.47
		V	57.49	33.91	17.47	32.67	0.54	9.20	1.63	0.73		0.07	0.74		0.35			154.80
		Δ_S	38.19	19.68	12.20	23.00	0.32	4.69	0.90	0.39		0.05	0.40		0.18			100.00
		Δ_V	37.14	21.91	11.29	21.10	0.35	5.94	1.05	0.47		0.05	0.48		0.23			100.00

Table S3.2. Characteristics of intermolecular noncovalent interactions in sulfamerazine polymorphs (VD polyhedra faces with RF = 0). The temperature at which X-ray diffraction experiments were conducted (as stated in respective .cif files) is provided below the refcodes.

Form	Refcode		H···H	H···C	H···N	H···O	H···S	C···C	C···N	C···O	C···S	N···N	N···O	N···S	O···O	O···S	S···S	Σ
$P2_1/c$	SLFNMA03	k	76	60	52	22	2	21	20	12					3	2		270
	150 K	d_{min}	2.42	2.71	2.08	2.14	3.35	3.36	3.68	3.27					3.76	3.75		2.08
		d_{max}	4.62	4.70	4.90	3.93	3.35	4.70	4.79	4.06					3.80	3.75		4.90
		S	137.12	52.71	48.39	56.97	0.46	8.96	4.14	11.39					2.46	0.67		323.26
		V	69.81	29.58	26.29	24.58	0.26	6.33	2.99	6.53					1.55	0.42		168.33
		Δ_S	42.42	16.31	14.97	17.62	0.14	2.77	1.28	3.52					0.76	0.21		100.00
		Δ_V	41.47	17.57	15.62	14.60	0.15	3.76	1.78	3.88					0.92	0.25		100.00
$Pbca$	SLFNMA01	k	72	102	36	28	2	22	14	10	2	2	2					292
	295 K	d_{min}	2.34	2.90	2.06	2.30	3.36	3.71	3.50	3.17	3.98	4.26	3.80					2.06
		d_{max}	4.34	4.92	4.70	3.91	3.36	4.86	4.47	4.46	3.98	4.26	3.80					4.92
		S	122.38	64.50	47.06	67.87	0.87	7.47	5.27	6.63	0.09	1.05	0.92					324.11
		V	58.38	37.69	22.57	30.94	0.49	5.18	3.54	3.89	0.06	0.75	0.59					164.06
		Δ_S	37.76	19.90	14.52	20.94	0.27	2.30	1.63	2.05	0.03	0.32	0.28					100.00
		Δ_V	35.59	22.97	13.76	18.86	0.30	3.16	2.16	2.37	0.04	0.46	0.36					100.00
$Pna2_1$	SLFNMA04	k	76	68	46	26	5	24	12	3		1	1		1			263
	150 K	d_{min}	2.51	2.74	2.02	2.25	3.25	3.40	3.99	3.35		3.45	3.54		3.65			2.02
		d_{max}	4.89	4.75	4.89	4.33	3.38	4.79	4.82	3.54		3.45	3.54		3.65			4.89
		S	122.38	61.94	54.93	73.03	1.46	10.64	0.92	1.86		0.31	0.30		0.86			328.63
		V	66.01	34.59	29.22	33.38	0.81	7.34	0.68	1.07		0.18	0.18		0.52			173.98
		Δ_S	37.24	18.85	16.72	22.22	0.44	3.24	0.28	0.57		0.09	0.09		0.26			100.00
		Δ_V	37.94	19.88	16.80	19.19	0.46	4.22	0.39	0.62		0.10	0.10		0.30			100.00
a		k	77	68	46	25	5	24	12	3			1		1			262
		d_{min}	2.55	2.74	2.02	2.25	3.25	3.40	3.99	3.35			3.54		3.65			2.02
		d_{max}	4.89	4.75	4.89	4.33	3.37	4.79	4.82	3.54			3.54		3.65			4.89
		S	124.91	62.10	55.23	70.99	1.47	10.64	0.92	1.86			0.30		0.86			329.28
		V	67.17	34.66	29.09	32.52	0.81	7.34	0.68	1.07			0.18		0.52			174.04
		Δ_S	37.94	18.86	16.77	21.56	0.45	3.23	0.28	0.57			0.09		0.26			100.00
		Δ_V	38.59	19.92	16.72	18.68	0.47	4.21	0.39	0.62			0.10		0.30			100.00
b		k	75	68	46	27	5	24	12	3		2	1		1			264
		d_{min}	2.51	2.74	2.02	2.29	3.25	3.40	3.99	3.35		3.45	3.54		3.65			2.02
		d_{max}	4.89	4.75	4.89	4.33	3.38	4.79	4.82	3.54		3.45	3.54		3.65			4.89
		S	119.86	61.77	54.64	75.07	1.45	10.64	0.92	1.86		0.62	0.30		0.86			327.98
		V	64.86	34.52	29.35	34.24	0.80	7.34	0.68	1.07		0.36	0.18		0.52			173.92
		Δ_S	36.54	18.83	16.66	22.89	0.44	3.24	0.28	0.57		0.19	0.09		0.26			100.00
		Δ_V	37.29	19.85	16.88	19.69	0.46	4.22	0.39	0.62		0.21	0.10		0.30			100.00

Table S3.3. Characteristics of intermolecular noncovalent interactions in sulfamethoxazole polymorphs (VD polyhedra faces with RF = 0). The temperature at which X-ray diffraction experiments were conducted (as stated in respective .cif files) is provided below the refcodes.

Form	Refcode		H···H	H···C	H···N	H···O	H···S	C···C	C···N	C···O	C···S	N···N	N···O	N···S	O···O	O···S	S···S	Σ
I	SLFNMB01	k	67	72	28	42	4	6	6	10		3	2		3			243
	295 K	d_{min}	2.56	2.88	2.42	2.39	3.47	3.40	3.52	3.57		3.35	3.59		3.81			2.39
		d_{max}	4.24	4.25	3.86	4.50	3.92	3.84	3.91	4.27		3.62	3.59		3.85			4.50
		S	82.46	66.75	37.23	95.62	0.88	0.12	2.37	5.58		3.44	1.28		2.60			298.32
		V	43.02	36.28	18.30	46.33	0.54	0.07	1.45	3.41		1.98	0.77		1.66			153.80
		Δ_S	27.64	22.37	12.48	32.05	0.29	0.04	0.79	1.87		1.15	0.43		0.87			100.00
		Δ_V	27.97	23.59	11.90	30.12	0.35	0.05	0.94	2.22		1.29	0.50		1.08			100.00
II	SLFNMB02	k	66	70	24	44	6	12	6	14		1	4		8	2		257
	295 K	d_{min}	2.65	3.06	2.06	2.11	3.19	3.47	3.66	3.57		3.38	3.47		3.57	4.13		2.06
		d_{max}	4.74	4.14	4.15	4.20	3.76	3.92	3.90	4.24		3.38	3.70		4.26	4.13		4.74
		S	96.83	58.54	42.16	94.16	0.94	5.72	1.12	4.97		<0.01	1.61		4.96	0.04		311.05
		V	49.76	34.10	19.72	45.05	0.56	3.43	0.69	3.11		<0.01	0.98		3.05	0.03		160.46
		Δ_S	31.13	18.82	13.55	30.27	0.30	1.84	0.36	1.60		<0.01	0.52		1.59	0.01		100.00
		Δ_V	31.01	21.25	12.29	28.07	0.35	2.13	0.43	1.94		<0.01	0.61		1.90	0.02		100.00
III	SLFNMB05	k	64	70	22	48	6	13	6	14			8		5			256
	153 K	d_{min}	2.40	2.90	1.95	2.14	3.49	3.52	3.58	3.34			3.31		3.88			1.95
		d_{max}	4.58	4.33	4.27	4.42	4.20	3.99	3.92	3.89			3.98		3.94			4.58
		S	100.30	53.71	38.06	91.45	0.81	5.84	1.78	10.16			3.36		1.95			307.41
		V	49.78	30.95	17.01	44.50	0.52	3.50	1.07	5.96			1.94		1.27			156.49
		Δ_S	32.63	17.47	12.38	29.75	0.26	1.90	0.58	3.31			1.09		0.63			100.00
		Δ_V	31.81	19.78	10.87	28.44	0.33	2.24	0.68	3.81			1.24		0.81			100.00
IV	SLFNMB06	k	62	78	28	44	8	13	8	10			8	2	3			264
	153 K	d_{min}	2.62	3.01	2.36	2.13	3.15	3.52	3.40	3.84			3.18	3.59	3.22			2.13
		d_{max}	4.23	4.43	3.89	4.28	3.73	4.41	4.21	4.43			4.07	3.59	3.45			4.43
		S	89.85	62.01	39.01	95.19	0.69	7.37	2.01	2.15			1.19	0.25	3.16			302.86
		V	46.69	34.03	18.91	45.36	0.37	4.53	1.29	1.47			0.66	0.15	1.74			155.19
		Δ_S	29.67	20.47	12.88	31.43	0.23	2.43	0.66	0.71			0.39	0.08	1.04			100.00
		Δ_V	30.08	21.93	12.18	29.23	0.24	2.92	0.83	0.94			0.42	0.10	1.12			100.00

Table S3.4. Characteristics of intermolecular noncovalent interactions in sulfathiazole polymorphs (VD polyhedra faces with RF = 0). The temperature at which X-ray diffraction experiments were conducted (as stated in respective .cif files) is provided below the refcodes.

Form	Refcode		H···H	H···C	H···N	H···O	H···S	C···C	C···N	C···O	C···S	N···N	N···O	N···S	O···O	O···S	S···S	Σ
I	SUTHAZ29	k	57	76	19	32	22	14	16	4	5	3		4	1	1		254
	105 K	d_{min}	2.20	2.57	1.81	1.95	2.88	3.54	3.11	3.39	3.41	3.31		3.62	4.43	3.62		1.81
		d_{max}	4.81	4.74	4.21	5.09	4.67	4.89	4.34	4.36	4.53	4.79		4.52	4.43	3.62		5.09
		S	87.43	65.05	26.97	70.60	21.82	5.84	7.67	0.90	3.46	0.89		2.85	0.60	4.33		298.40
		V	44.04	36.44	10.90	31.72	12.73	3.75	4.80	0.59	2.12	0.51		1.79	0.45	2.61		152.44
		Δ_S	29.30	21.80	9.04	23.66	7.31	1.96	2.57	0.30	1.16	0.30		0.96	0.20	1.45		100.00
		Δ_V	28.89	23.91	7.15	20.81	8.35	2.46	3.15	0.39	1.39	0.33		1.17	0.29	1.71		100.00
I*a*		k	56	72	17	33	23	14	16	3	5	3		4				246
		d_{min}	2.20	2.57	1.84	1.95	2.94	3.54	3.11	3.39	3.41	3.31		3.62				1.84
		d_{max}	4.81	4.74	4.21	5.09	4.67	4.89	4.34	4.36	4.53	4.79		4.52				5.09
		S	83.78	60.25	25.08	83.45	28.64	5.84	7.67	0.90	3.46	0.89		2.85				302.81
		V	43.31	33.98	10.12	36.47	16.13	3.75	4.80	0.58	2.12	0.51		1.79				153.56
		Δ_S	27.67	19.90	8.28	27.56	9.46	1.93	2.53	0.30	1.14	0.29		0.94				100.00
		Δ_V	28.20	22.13	6.59	23.75	10.51	2.44	3.12	0.38	1.38	0.33		1.16				100.00
I*b*		k	57	80	21	31	21	14	16	5	5	3		4	1	2		260
		d_{min}	2.20	2.57	1.81	2.23	2.88	3.54	3.11	3.39	3.41	3.31		3.62	4.43	3.62		1.81
		d_{max}	4.81	4.74	4.21	5.09	4.67	4.89	4.34	4.36	4.53	4.79		4.52	4.43	3.62		5.09
		S	91.07	69.85	28.85	57.74	15.00	5.84	7.67	0.90	3.46	0.89		2.85	1.21	8.66		293.99
		V	44.77	38.91	11.67	26.97	9.33	3.75	4.80	0.59	2.12	0.51		1.79	0.89	5.22		151.32
		Δ_S	30.98	23.76	9.81	19.64	5.10	1.98	2.61	0.31	1.18	0.30		0.97	0.41	2.94		100.00
		Δ_V	29.58	25.71	7.71	17.82	6.17	2.48	3.17	0.39	1.40	0.34		1.18	0.59	3.45		100.00
II	SUTHAZ31	k	51	60	22	26	26	23	14	2	4	3			1			232
	100 K	d_{min}	2.17	2.54	1.82	2.02	2.83	3.44	3.41	3.35	4.03	3.20			4.05			1.82
		d_{max}	4.40	4.48	4.47	4.44	4.27	4.45	4.44	3.35	4.09	3.80			4.05			4.48
		S	79.07	72.68	29.35	71.68	33.05	3.39	4.71	0.21	4.58	1.46			1.90			302.09
		V	38.30	38.71	14.08	30.61	18.43	2.19	2.77	0.12	3.10	0.78			1.29			150.37
		Δ_S	26.17	24.06	9.72	23.73	10.94	1.12	1.56	0.07	1.51	0.48			0.63			100.00
		Δ_V	25.47	25.74	9.37	20.36	12.25	1.46	1.84	0.08	2.06	0.52			0.85			100.00
III	SUTHAZ34	k	54	58	22	27	23	17	11	6	5	2	1	1	1	2		230
	100 K	d_{min}	2.15	2.48	1.80	1.98	2.94	3.42	3.39	3.33	3.74	3.18	3.35	3.86	2.97	4.03		1.80
		d_{max}	4.56	4.52	4.28	4.51	4.29	4.39	4.47	4.11	4.09	3.78	3.35	3.86	4.02	4.38		4.56
		S	77.69	71.39	30.28	65.71	32.24	2.44	3.18	4.18	5.34	0.78	2.08	0.02	1.90	0.28		297.51
		V	37.40	37.60	13.63	28.18	18.23	1.60	1.86	2.49	3.59	0.41	1.16	0.02	1.13	0.19		147.47
		Δ_S	26.11	23.99	10.18	22.09	10.84	0.82	1.07	1.41	1.79	0.26	0.70	0.01	0.64	0.09		100.00
		Δ_V	25.36	25.50	9.24	19.11	12.36	1.09	1.26	1.69	2.43	0.28	0.79	0.01	0.76	0.13		100.00

Table S3.4. (continued)

Form	Refcode		H···H	H···C	H···N	H···O	H···S	C···C	C···N	C···O	C···S	N···N	N···O	N···S	O···O	O···S	S···S	Σ
III*a*		k	55	62	24	24	24	18	13	1	4	2		1	1			229
		d_{min}	2.15	2.48	1.80	1.98	2.94	3.42	3.39	3.33	4.00	3.18		3.86	4.02			1.80
		d_{max}	4.56	4.52	4.28	4.51	4.29	4.39	4.48	3.33	4.09	3.78		3.86	4.02			4.56
		S	75.62	74.91	32.54	65.27	31.80	2.94	4.31	0.20	5.08	1.56		0.02	2.13			296.39
		V	36.09	39.62	14.87	27.86	17.93	1.89	2.51	0.11	3.43	0.83		0.02	1.43			146.58
		Δ_S	25.51	25.27	10.98	22.02	10.73	0.99	1.45	0.07	1.72	0.53		0.01	0.72			100.00
		Δ_V	24.62	27.03	10.14	19.01	12.23	1.29	1.71	0.08	2.34	0.56		0.01	0.97			100.00
III*b*		k	52	54	20	30	22	16	9	11	6	1	2	1	1	4		229
		d_{min}	2.15	2.48	1.80	1.98	2.96	3.51	3.39	3.33	3.74	3.78	3.35	3.86	2.97	4.03		1.80
		d_{max}	4.56	4.52	4.28	4.51	4.29	4.39	4.48	4.11	4.09	3.78	3.35	3.86	2.97	4.38		4.56
		S	79.75	67.86	28.03	66.15	32.68	1.94	2.05	8.16	5.59	<0.01	4.15	0.02	1.67	0.56		298.62
		V	38.70	35.59	12.38	28.49	18.52	1.32	1.21	4.87	3.74	<0.01	2.32	0.02	0.83	0.38		148.37
		Δ_S	26.71	22.72	9.38	22.15	10.94	0.65	0.69	2.73	1.87	<0.01	1.39	0.01	0.56	0.19		100.00
		Δ_V	26.08	23.99	8.34	19.20	12.48	0.89	0.81	3.28	2.52	<0.01	1.56	0.01	0.56	0.26		100.00
IV	SUTHAZ37	k	52	62	22	26	20	19	10	12	6		2	2	1	4		238
	100 K	d_{min}	2.08	2.54	1.89	2.00	2.98	3.52	3.37	3.33	3.72		3.35	4.60	2.93	4.09		1.89
		d_{max}	4.03	4.60	4.33	3.77	4.39	4.50	4.54	4.06	4.15		3.35	4.60	2.93	4.36		4.60
		S	76.99	70.13	30.58	60.92	31.30	1.57	2.36	7.89	6.16		3.75	<0.01	1.96	0.24		293.85
		V	36.34	36.81	13.03	26.93	17.90	1.08	1.37	4.71	4.17		2.09	<0.01	0.96	0.17		145.56
		Δ_S	26.20	23.86	10.41	20.73	10.65	0.53	0.80	2.69	2.10		1.27	<0.01	0.67	0.08		100.00
		Δ_V	24.97	25.29	8.95	18.50	12.29	0.74	0.94	3.24	2.86		1.44	<0.01	0.66	0.11		100.00
V	SUTHAZ05	k	59	70	22	26	19	11	13	3	11	1	4	4		3	1	247
	150 K	d_{min}	2.36	2.91	2.14	1.94	3.12	3.63	3.72	3.65	3.53	3.79	3.21	3.95		3.79	4.22	1.94
		d_{max}	4.88	4.93	4.71	4.40	4.80	4.24	4.32	4.06	4.36	3.79	3.67	4.68		4.94	4.22	4.94
		S	88.30	58.93	26.06	75.51	30.27	5.85	5.18	2.03	4.87	0.30	0.71	0.62		1.89	2.03	302.54
		V	47.14	32.93	12.65	33.12	18.21	3.74	3.34	1.31	3.31	0.19	0.41	0.42		1.29	1.43	159.48
		Δ_S	29.19	19.48	8.61	24.96	10.00	1.93	1.71	0.67	1.61	0.10	0.23	0.20		0.63	0.67	100.00
		Δ_V	29.56	20.65	7.93	20.76	11.42	2.35	2.09	0.82	2.07	0.12	0.26	0.27		0.81	0.89	100.00
V*a*		k	61	67	21	28	19	9	15	3	10	1	5	4		3	1	247
		d_{min}	2.36	2.91	2.14	1.94	3.12	3.63	3.72	3.65	3.53	3.79	3.21	3.95		3.79	4.22	1.94
		d_{max}	4.88	4.93	4.71	4.40	4.80	4.24	4.32	4.06	4.36	3.79	3.67	4.68		4.94	4.22	4.94
		S	91.47	57.68	25.02	80.02	30.80	5.74	5.43	2.03	3.54	0.60	0.72	0.39		1.89	2.03	307.36
		V	48.56	32.04	11.79	35.38	18.14	3.59	3.48	1.31	2.45	0.38	0.42	0.26		1.29	1.43	160.51
		Δ_S	29.76	18.77	8.14	26.04	10.02	1.87	1.77	0.66	1.15	0.19	0.23	0.13		0.62	0.66	100.00
		Δ_V	30.25	19.96	7.35	22.04	11.30	2.23	2.17	0.82	1.53	0.23	0.26	0.16		0.80	0.89	100.00

Table S3.4. (continued)

Form	Refcode		H···H	H···C	H···N	H···O	H···S	C···C	C···N	C···O	C···S	N···N	N···O	N···S	O···O	O···S	S···S	Σ
V*b*		k	57	73	23	24	19	12	11	3	12		3	4		3	1	245
		d_{min}	2.50	2.94	2.44	1.94	3.12	3.64	3.74	3.65	3.53		3.46	4.10		3.79	4.22	1.94
		d_{max}	4.88	4.93	4.71	4.23	4.80	4.24	4.32	4.06	4.36		3.67	4.68		4.94	4.22	4.94
		S	85.12	60.18	27.09	71.01	29.73	5.97	4.92	2.03	6.20		0.69	0.85		1.89	2.03	297.72
		V	45.73	33.82	13.50	30.85	18.29	3.90	3.19	1.31	4.17		0.40	0.58		1.29	1.43	158.44
		Δ_S	28.59	20.22	9.10	23.85	9.99	2.00	1.65	0.68	2.08		0.23	0.28		0.64	0.68	100.00
		Δ_V	28.86	21.35	8.52	19.47	11.54	2.46	2.01	0.83	2.63		0.25	0.37		0.81	0.90	100.00

Table S3.5. Characteristics of intermolecular noncovalent interactions in chlorpropamide polymorphs (VD polyhedra faces with RF = 0). The temperature at which X-ray diffraction experiments were conducted (as stated in respective .cif files) is provided below the refcodes.

Form	Refcode		H···H	H···C	H···N	H···O	H···S	H···Cl	C···C	C···N	C···O	C···S	C···Cl	N···N	N···O	N···S	N···Cl	O···O	O···S	O···Cl	S···S	S···Cl	Cl···Cl	Σ
α	BEDMIG10	*k*	72	38	10	36	6	24	6		20	2	18		6	2		2					2	244
	295 K	d_{min}	2.54	3.12	2.85	1.95	3.62	3.13	3.95		3.38	3.81	3.82		3.56	3.90		3.27					4.80	1.95
		d_{max}	4.75	4.74	3.89	4.44	3.90	4.32	4.13		3.86	3.81	4.79		3.81	3.90		3.27					4.80	4.80
		S	131.69	29.18	5.18	77.62	0.29	48.76	1.99		17.98	0.47	12.53		4.66	0.13		4.31					0.44	335.22
		V	65.98	17.47	2.69	35.29	0.17	27.90	1.33		10.83	0.30	8.35		2.84	0.09		2.35					0.35	175.93
		Δ_S	39.28	8.70	1.55	23.15	0.09	14.55	0.59		5.36	0.14	3.74		1.39	0.04		1.29					0.13	100.00
		Δ_V	37.50	9.93	1.53	20.06	0.10	15.86	0.75		6.15	0.17	4.75		1.61	0.05		1.33					0.20	100.00
β	BEDMIG01	*k*	75	54	12	34	2	22	15		10	4	2				4	3		6				243
	295 K	d_{min}	2.54	3.14	2.90	1.95	3.38	3.03	3.91		3.21	3.90	3.68				3.57	3.57		3.45				1.95
		d_{max}	4.53	4.79	4.50	4.18	3.38	4.30	4.46		4.32	4.13	3.68				3.97	3.98		3.89				4.79
		S	136.68	30.71	8.01	83.19	0.42	42.71	6.75		8.64	0.34	3.89				0.94	2.03		14.62				338.94
		V	70.89	18.15	4.77	39.28	0.24	24.09	4.66		5.12	0.23	2.39				0.62	1.33		8.73				180.50
		Δ_S	40.33	9.06	2.36	24.55	0.12	12.60	1.99		2.55	0.10	1.15				0.28	0.60		4.31				100.00
		Δ_V	39.27	10.06	2.64	21.76	0.13	13.35	2.58		2.83	0.13	1.32				0.35	0.74		4.84				100.00
γ	BEDMIG02	*k*	74	44	16	36	2	20			22	2	6		2			2		6		2	2	236
	295 K	d_{min}	2.60	2.92	2.94	1.97	3.55	3.15			3.29	3.92	3.88		4.99			4.36		3.80		4.19	4.55	1.97
		d_{max}	4.81	4.51	4.57	4.68	3.55	4.43			4.89	3.92	4.42		4.99			4.36		4.26		4.19	4.55	4.99
		S	127.73	32.81	9.05	85.47	0.37	48.67			18.84	0.17	8.02		0.04			0.62		4.25		0.23	0.05	336.31
		V	66.94	18.76	4.97	39.36	0.22	27.56			11.53	0.11	5.21		0.03			0.45		2.75		0.16	0.04	178.08
		Δ_S	37.98	9.76	2.69	25.41	0.11	14.47			5.60	0.05	2.38		0.01			0.18		1.26		0.07	0.01	100.00
		Δ_V	37.59	10.53	2.79	22.10	0.12	15.47			6.47	0.06	2.93		0.02			0.25		1.54		0.09	0.02	100.00
δ	BEDMIG03	*k*	64	66	10	40	6	26			8		12		4			4					2	242
	295 K	d_{min}	2.31	2.86	2.99	1.96	3.29	3.10			3.34		4.34		3.46			3.25					4.68	1.96
		d_{max}	4.85	4.24	3.92	3.86	3.87	4.55			3.86		4.80		3.47			3.66					4.68	4.85
		S	108.04	52.22	6.71	87.90	1.20	57.59			6.87		4.76		2.41			4.13					0.29	332.11
		V	54.44	30.11	3.81	40.68	0.68	33.05			3.92		3.56		1.39			2.27					0.23	174.13
		Δ_S	32.53	15.72	2.02	26.47	0.36	17.34			2.07		1.43		0.72			1.24					0.09	100.00
		Δ_V	31.26	17.29	2.19	23.36	0.39	18.98			2.25		2.04		0.80			1.30					0.13	100.00
ε	BEDMIG04	*k*	60	66	10	38	2	24			4		8				2			6		2		222
	295 K	d_{min}	2.54	2.87	2.97	2.02	3.83	3.19			3.84		3.51				4.27			3.67		3.99		2.02
		d_{max}	4.52	5.31	3.71	4.30	3.83	4.32			3.84		4.34				4.27			3.85		3.99		5.31
		S	113.22	37.70	6.38	103.91	0.20	50.85			5.98		4.32				0.03			7.44		0.19		330.22
		V	58.51	23.38	3.40	47.67	0.13	29.67			3.82		2.63				0.02			4.59		0.13		173.93
		Δ_S	34.29	11.42	1.93	31.47	0.06	15.40			1.81		1.31				0.01			2.25		0.06		100.00
		Δ_V	33.64	13.44	1.96	27.41	0.07	17.06			2.20		1.51				0.01			2.64		0.07		100.00

Table S3.6. Characteristics of intermolecular noncovalent interactions in tolbutamide polymorphs (VD polyhedra faces with RF = 0). The temperature at which X-ray diffraction experiments were conducted (as stated in respective .cif files) is provided below the refcodes.

Form	Refcode		H···H	H···C	H···N	H···O	H···S	C···C	C···N	C···O	C···S	N···N	N···O	N···S	O···O	O···S	S···S	Σ
I	ZZZPUS20	k	102	64	14	50	4			4								238
	100 K	d_{min}	2.36	2.95	2.90	1.99	3.41			4.02								1.99
		d_{max}	4.05	4.47	3.73	4.31	3.80			4.06								4.47
		S	176.98	44.45	13.17	109.84	0.74			0.30								345.47
		V	89.18	25.46	7.18	50.50	0.44			0.20								172.97
		Δ_S	51.23	12.87	3.81	31.79	0.21			0.09								100.00
		Δ_V	51.56	14.72	4.15	29.20	0.26			0.12								100.00
II	ZZZPUS21	k	121	80	16	53	6	3		1					1			281
	100 K	d_{min}	2.25	2.69	2.84	1.92	3.27	3.51		3.80					3.79			1.92
		d_{max}	4.69	4.43	4.35	4.47	4.22	3.76		4.43					4.19			4.69
		S	189.30	58.30	8.79	110.48	0.93	0.51		0.29					0.32			368.91
		V	93.62	32.30	4.83	51.44	0.54	0.30		0.21					0.20			183.45
		Δ_S	51.31	15.80	2.38	29.95	0.25	0.14		0.08					0.09			100.00
		Δ_V	51.04	17.61	2.63	28.04	0.29	0.16		0.12					0.11			100.00
II*a*		k	121	72	16	52	8								2			271
		d_{min}	2.44	2.82	3.02	1.92	3.43								3.79			1.92
		d_{max}	4.58	4.43	4.04	4.47	4.01								4.19			4.58
		S	190.50	48.72	8.20	122.66	0.74								0.63			371.46
		V	96.06	27.05	4.39	56.20	0.45								0.40			184.55
		Δ_S	51.28	13.12	2.21	33.02	0.20								0.17			100.00
		Δ_V	52.05	14.66	2.38	30.45	0.24								0.22			100.00
II*b*		k	116	87	14	57	6	6		1								287
		d_{min}	2.25	2.77	2.94	1.94	3.43	3.51		4.43								1.94
		d_{max}	4.69	4.43	4.35	4.37	4.22	3.76		4.43								4.69
		S	179.34	65.74	8.30	110.66	0.91	1.01		0.57								366.52
		V	88.59	36.49	4.48	52.54	0.55	0.60		0.42								183.66
		Δ_S	48.93	17.94	2.27	30.19	0.25	0.28		0.15								100.00
		Δ_V	48.24	19.87	2.44	28.61	0.30	0.33		0.23								100.00
II*c*		k	123	86	17	43	4			2								275
		d_{min}	2.39	2.69	2.84	1.94	3.27			3.80								1.94
		d_{max}	4.69	4.30	4.02	4.47	3.52			4.43								4.69
		S	199.70	65.49	8.63	92.01	0.87			0.57								367.28
		V	97.13	36.18	4.80	41.59	0.49			0.42								180.61
		Δ_S	54.37	17.83	2.35	25.05	0.24			0.16								100.00
		Δ_V	53.78	20.03	2.66	23.02	0.27			0.23								100.00

Table S3.6. (continued)

Form	Refcode		H···H	H···C	H···N	H···O	H···S	C···C	C···N	C···O	C···S	N···N	N···O	N···S	O···O	O···S	S···S	Σ
II*d*		*k*	122	73	17	58	6	6		1					2			285
		d_{min}	2.25	2.79	2.84	1.92	3.27	3.51		3.80					3.79			1.92
		d_{max}	4.61	4.32	4.35	4.37	3.92	3.76		3.80					4.19			4.61
		S	187.66	53.24	10.04	116.58	1.19	1.01		<0.01					0.63			370.37
		V	92.72	29.48	5.63	55.44	0.68	0.60		<0.01					0.40			184.96
		Δ_S	50.67	14.38	2.71	31.48	0.32	0.27		<0.01					0.17			100.00
		Δ_V	50.13	15.94	3.04	29.97	0.37	0.33		<0.01					0.22			100.00
III	ZZZPUS12	*k*	122	74	14	44	10											264
	150 K	d_{min}	2.48	2.78	2.74	1.94	3.30											1.94
		d_{max}	4.73	4.25	3.74	4.30	4.50											4.73
		S	181.89	56.60	9.54	101.65	0.53											350.21
		V	95.48	31.32	5.11	45.78	0.31											178.00
		Δ_S	51.94	16.16	2.72	29.02	0.15											100.00
		Δ_V	53.64	17.60	2.87	25.72	0.17											100.00
IV	ZZZPUS07	*k*	120	62	14	44	8	17		6	4				1			276
	298 K	d_{min}	2.13	2.70	3.17	1.96	3.37	3.89		3.75	4.19				3.93			1.96
		d_{max}	4.63	4.93	3.90	4.71	4.39	4.21		4.22	4.20				3.93			4.93
		S	208.68	38.84	9.23	101.46	0.28	6.83		1.24	0.24				2.47			369.26
		V	104.85	23.59	5.38	48.13	0.16	4.56		0.78	0.17				1.62			189.24
		Δ_S	56.51	10.52	2.50	27.48	0.08	1.85		0.33	0.06				0.67			100.00
		Δ_V	55.41	12.47	2.84	25.44	0.09	2.41		0.41	0.09				0.85			100.00
V	ZZZPUS10	*k*	116	60	18	48	6	17		4	4				1			274
	298 K	d_{min}	2.43	3.03	2.95	2.11	3.50	3.68		3.50	4.19				3.98			2.11
		d_{max}	4.44	4.90	4.31	4.25	3.91	5.25		4.38	4.47				3.98			5.25
		S	201.86	39.10	10.88	102.15	0.26	6.74		1.71	0.16				0.91			363.76
		V	101.86	22.96	6.34	50.26	0.17	4.80		1.07	0.11				0.60			188.16
		Δ_S	55.49	10.75	2.99	28.08	0.07	1.85		0.47	0.04				0.25			100.00
		Δ_V	54.13	12.20	3.37	26.71	0.09	2.55		0.57	0.06				0.32			100.00

Table S4. Average partial contributions of volumes of pyramids (R_V, %), corresponding to covalent (RF = 1), intramolecular noncovalent (RF > 1) and intermolecular (RF = 0) interactions, to the total volume of molecular VD polyhedra in a series of highly polymorphic crystal structures

Refcode family	**Polymorphs**	**Molecules**	**R_V, %**			**Reference (numbering as in the main article)**
			RF = 1	**RF > 1**	**RF = 0**	
BEWKUJ	5	7	28	17	54	This work
SLFNMA	3	4	26	21	54	
SLFNMB	4	4	25	21	54	
SUTHAZ	5	8	28	16	56	
BEDMIG	5	5	22	24	54	
ZZZPUS	5	8	21	27	52	
TOKSAO	4	9	28	15	57	23
BIXGIY	4	4	27	18	55	
KAXXAI	9	11	26	20	54	
MOTNUF	4	17	27	20	53	
QAXMEH	12	14	26	17	57	25
DOR . . .	11	12	28	22	50	22
DORDUM	10	12	28	22	50	21
MELFIT	9	12	21	28	51	20
FPAMCA	8	27	30	10	60	19
SALOXM	4	5	28	13	59	18
GLYCIN	5	5	17	21	62	
PUBMUU	20	21	24	27	49	
SALCAN	3	4	27	15	58	24
RIGHUK	3	4	25	21	54	
ZOGQAN	3	4	28	19	53	
ATIWOP	2	2	23	30	47	
MOPNAH	3	3	22	28	50	
FOGVIG	4	4	22	27	51	17
QAXMEH*	7	7	26	17	57	
SUTHAZ*	6	9	27	17	56	
SULAMD	4	4	26	18	56	
SLFNMB*	4	4	25	21	54	
LILHAP	2	2	29	15	56	
LILHAP*	2	2	29	15	56	16
QAXMEH*	7	7	26	17	57	
SLFNMB*	4	4	25	21	54	
SLFNMA*	3	4	27	20	53	
26 unique refcode families (33 total)	151 unique polymorphs (184 total)	212 unique molecules (249 total)	Average values with standard deviations for unique molecules			
			25(3)	20(5)	54(4)	

* The marked polymorphic compounds were not counted as ‘unique’ and their characteristics were not averaged in the last row as the MVDP data on them were updated in later publications.