Electronic Supplementary Material (ESI) for CrystEngComm.

The extensive solid-form landscape of sulfathiazole: hydrogen-bond topology and node shape

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Electronic Supplementary Information

S1. Summary of new sulfathiazole multi-component crystals

The structures considered in this paper are described in:

The extensive solid-form landscape of sulfathiazole: geometrical similarity and interaction energies
David S. Hughes, Ann L. Bingham, Michael B. Hursthouse, Terry L. Threlfall and Andrew D. Bond
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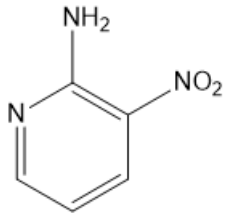
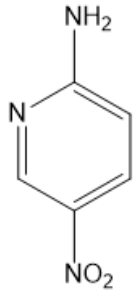
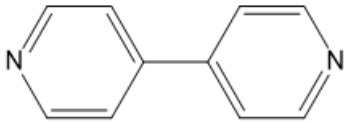
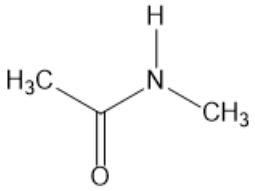
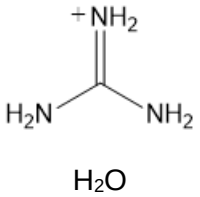
Five new structures are added (3 from the CSD, 2 new structure determinations):

				
92 (co-crystal)	**93 (co-crystal)**	**94 (co-crystal)**	**95 (co-crystal)**	**96 (salt)**

	CSD Refcode	Space Group	Partner		Stoichiometry	Cell dimensions						Z	V
						a	b	c	α	β	γ		
92	TAPCIA	P-1	3-nitropyridine-2-amine	$C_5H_5N_3O_2$	1:1	8.335	9.746	10.535	101.76	93.93	93.84	2	832.9
93	TAPCUM	P-1	5-nitropyridine-2-amine	$C_5H_5N_3O_2$	2:1	8.287	11.542	15.414	79.82	88.64	76.53	2	1410.9
94	TAPDEX	P21/n	4,4′-bipyridine	$C_{10}H_8N_2$	2:1	8.411	31.674	11.638	90	95.11	90	4	3087.9
95	—	Pbca	N-methylacetamide	C_3H_7NO	1:1	10.602	8.164	35.137	90	90	90	8	3041.4
96	—	P-1	guanidinium hydrate	$[CH_6N_3]^+$ / H_2O	1:1:1	7.630	8.777	11.305	101.35	93.00	97.45	2	733.6

S2. Crystallographic information for the new crystal structures

	95	**96**
CCDC number	2189394	2189393
Chemical formula	$C_{12}H_{16}N_4O_3S_2$	$C_{10}H_{16}N_6O_3S_2$
Formula weight	328.41	332.41
Temperature / K	150(2)	150(2)
Crystal system	orthorhombic	triclinic
Space group	P b c a	P –1
a / Å	10.6023(3)	7.6295(2)
b / Å	8.1642(2)	8.7769(5)
c / Å	35.1366(12)	11.3046(6)
alpha / °	90	101.353(2)
beta / °	90	92.999(3)
gamma / °	90	97.446(3)
Unit-cell volume / $Å^3$	3041.40(15)	733.56(6)
Z	8	2
Calc. density / g cm^{-3}	1.434	1.505
F(000)	1376	348
Radiation type	MoKα	MoKα
Absorption coefficient / mm^{-1}	0.365	0.383
Crystal size / mm^3	0.10 x 0.10 x 0.10	0.35 x 0.30 x 0.20
2-Theta range / °	6.02-50.05	6.29-46.55
Completeness to max 2-theta	0.901	0.992
No. of reflections measured	6860	9430
No. of independent reflections	2417	2107
R_{int}	0.0513	0.0468
No. parameters / restraints	210 / 3	230 / 0
Final R1 values (I > 2σ(I))	0.0444	0.0270
Final wR(F^2) values (all data)	0.1109	0.0706
Goodness-of-fit on F^2	1.031	1.064
Largest difference peak & hole / e $Å^{-3}$	0.308, –0.340	0.252, –0.338
Flack parameter	—	—

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

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1p

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10.5340 12.9360 17.1910 90.000 107.770 90.000 V = 2230.81

Space group: P 21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 2
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.7561 0.7992 0.3688
Molecule 02 = C9 H9 N3 O2 S2
Centroid = 0.8066 0.2131 0.0481

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01	---> 2_645_01]	1.03	1.92	2.917	161.3
N11---H11...O12	[1_555_01	---> 4_564_01]	1.02	2.12	2.930	133.9
N13---H17...O11	[1_555_01	---> 3_776_01]	1.06	2.60	3.277	121.5
N13---H17...N12	[1_555_01	---> 3_776_01]	1.06	1.77	2.819	172.0
N21---H20...N11	[1_555_02	---> 1_555_01]	1.03	2.09	3.116	176.0
N21---H21...O21	[1_555_02	---> 2_755_02]	1.02	2.16	3.043	142.9
N23---H27...N22	[1_555_02	---> 3_755_02]	1.06	1.75	2.808	173.7

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2p

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10.3990 15.1320 14.2800 90.000 91.210 90.000 V = 2246.57

Space group: P 21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 2
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.7461 0.4793 0.6110
Molecule 02 = C9 H9 N3 O2 S2
Centroid = 0.2234 0.4496 0.8943

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O22	[1_555_01	---> 2_646_02]	1.03	1.98	2.987	166.5
N11---H11...O11	[1_555_01	---> 2_646_01]	1.03	2.49	3.242	129.3
N11---H11...N12	[1_555_01	---> 2_646_01]	1.03	1.95	2.954	165.4
N13---H17...O21	[1_555_01	---> 1_555_02]	1.04	1.82	2.853	171.2
N21---H20...O12	[1_555_02	---> 2_646_01]	1.03	2.04	3.011	156.8
N21---H21...O21	[1_555_02	---> 2_546_02]	1.03	2.08	3.028	152.6
N21---H21...N22	[1_555_02	---> 2_546_02]	1.03	2.48	3.335	140.6
N23---H27...O11	[1_555_02	---> 1_455_01]	1.05	1.74	2.780	174.3

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3p

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17.4480 8.4980 15.5110 90.000 112.810 90.000 V = 2120.00

Space group: P 21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 2
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.7272 0.2737 0.9869
Molecule 02 = C9 H9 N3 O2 S2
Centroid = 0.7807 0.7848 0.7766

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...N22	[1_555_01	---> 3_767_02]	1.03	2.18	3.159	156.8
N11---H11...O21	[1_555_01	---> 1_555_02]	1.04	1.95	2.955	162.7
N13---H17...N21	[1_555_01	---> 1_555_02]	1.07	1.75	2.804	166.7
N21---H20...O11	[1_555_02	---> 2_656_01]	1.03	1.96	2.972	166.4
N21---H21...O11	[1_555_02	---> 1_565_01]	1.03	1.98	2.942	154.2
N23---H27...N11	[1_555_02	---> 1_565_01]	1.06	1.84	2.874	164.5

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

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4p

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8.1930 8.5380 15.4370 90.000 94.010 90.000 V = 1077.20

Space group: P 21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.0515 0.7261 0.3686

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	1_455_01]	1.03	1.94	2.954	165.6
N11---H11...O11	[1_555_01 --->	2_545_01]	1.03	1.99	2.967	155.6
N13---H17...N11	[1_555_01 --->	2_545_01]	1.07	1.78	2.826	166.0

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5p

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10.7740 8.4670 11.3670 90.000 91.650 90.000 V = 1036.51

Space group: P 21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.3948 0.7109 0.8431

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...N12	[1_555_01 --->	4_465_01]	1.03	2.15	3.129	156.1
N11---H11...O11	[1_555_01 --->	2_546_01]	1.04	1.97	2.955	158.0
N11---H11...O11	[1_555_01 --->	4_465_01]	1.04	2.69	3.147	106.7
N13---H17...N11	[1_555_01 --->	2_546_01]	1.06	1.84	2.869	164.9

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1_SLFZ

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8.0510 11.4920 15.5520 77.450 88.640 88.640 V = 1403.87

Space group: P-1
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,-y,-z

Z(prime) = 2
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.4052 0.2079 0.8001
Molecule 02 = C9 H9 N3 O2 S2
Centroid = 0.4312 0.7538 0.5957

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O21	[1_555_01 --->	2_566_02]	1.03	2.55	2.954	102.5
N11---H10...O21	[1_555_01 --->	1_555_02]	1.03	1.93	2.923	160.7
N11---H11...O21	[1_555_01 --->	2_566_02]	1.03	2.55	2.954	102.8
N11---H11...N22	[1_555_01 --->	2_566_02]	1.03	2.37	3.279	147.2
N13---H17...O11	[1_555_01 --->	2_657_01]	1.06	2.46	3.141	121.6
N13---H17...N12	[1_555_01 --->	2_657_01]	1.06	1.76	2.802	169.1
N21---H21...N11	[1_555_02 --->	1_655_01]	1.02	2.50	3.358	140.7
N23---H27...O12	[1_555_02 --->	2_666_01]	1.04	1.80	2.835	176.3

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2_SLFZ

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8.5410 12.4010 8.8360 90.000 102.960 90.000 V = 912.04

Space group: P21
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z

Z(prime) = 1

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.6852 0.1458 0.6981

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...N12	[1_555_01 --->	1_455_01]	1.03	2.02	3.047	175.2
N11---H11...O12	[1_555_01 --->	2_646_01]	1.03	1.98	3.001	170.0

3_SLFZ

8.4090 16.6400 11.2740 90.000 101.370 90.000 V = 1546.56

Space group: Pc
Symmetry operators read from CIF:
[1] x,y,z
[2] x,-y,z+0.50

Z(prime) = 2
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.5346 0.3843 0.4393
Molecule 02 = C9 H9 N3 O2 S2
Centroid = 0.4795 0.1493 0.8057

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	1_655_01]	1.02	1.97	2.954	160.2
N11---H11...O12	[1_555_01 --->	2_665_01]	1.02	2.46	2.975	110.2
N13---H17...N22	[1_555_01 --->	1_555_02]	1.06	1.76	2.819	174.8
N21---H20...O21	[1_555_02 --->	2_655_02]	1.02	2.66	3.064	103.6
N21---H21...O21	[1_555_02 --->	2_655_02]	1.02	2.68	3.064	102.4
N21---H21...O22	[1_555_02 --->	1_655_02]	1.02	2.16	3.121	156.2
N23---H27...N12	[1_555_02 --->	1_555_01]	1.06	1.75	2.810	175.9

4_SLFZ

16.6160 16.0880 12.6300 90.000 110.690 90.000 V = 3158.48

Space group: Cc

Symmetry operators read from CIF:
[1] x,y,z
[2] x,-y,z+0.50
[3] x+0.50,y+0.50,z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 2
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.6061 0.8578 0.7320
Molecule 02 = C9 H9 N3 O2 S2
Centroid = 0.6024 0.6359 0.2832

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O22	[1_555_01 --->	4_465_02]	1.02	2.03	3.021	160.7
N11---H11...O21	[1_555_01 --->	3_455_02]	1.03	1.91	2.923	167.6
N13---H17...N22	[1_555_01 --->	1_555_02]	1.06	1.76	2.823	175.1
N21---H20...O12	[1_555_02 --->	3_444_01]	1.02	2.32	3.152	138.0
N21---H21...O11	[1_555_02 --->	4_464_01]	1.03	1.97	3.001	179.0
N23---H27...N12	[1_555_02 --->	1_555_01]	1.06	1.72	2.779	175.5

5_SLFZ

8.3220 16.0200 11.3520 90.000 100.290 90.000 V = 1489.09

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.2042 0.6423 0.0863

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	1_455_01]	1.02	2.04	2.998	155.6
N13---H17...N12	[1_555_01 --->	3_665_01]	1.06	1.77	2.823	171.5

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

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6_SLFZ

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8.4160 17.3940 10.3420 90.000 104.700 90.000 V = 1464.39

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.1854 0.3984 0.2771

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O12	[1_555_01 --->	4_655_01]	1.02	2.41	3.359	153.3
N11---H11...O11	[1_555_01 --->	4_655_01]	1.02	2.47	2.988	110.4
N11---H11...O12	[1_555_01 --->	1_655_01]	1.02	2.41	3.362	154.2
N13---H17...O11	[1_555_01 --->	3_565_01]	1.06	2.53	3.234	123.1
N13---H17...N12	[1_555_01 --->	3_565_01]	1.06	1.79	2.838	170.6

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7_SLFZ

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8.6360 19.1870 9.3540 90.000 91.030 90.000 V = 1549.70

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.8685 0.8273 0.4721

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H11...O12	[1_555_01 --->	1_455_01]	1.02	2.05	3.066	169.4
N13---H17...N12	[1_555_01 --->	3_776_01]	1.06	1.73	2.791	173.4

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8_SLFZ

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8.3920 21.2070 9.3020 90.000 93.120 90.000 V = 1653.02

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.3361 0.1604 0.5456

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	4_455_01]	1.03	2.02	3.007	161.1
N11---H11...O12	[1_555_01 --->	1_455_01]	1.02	2.00	2.982	159.5
N13---H17...N12	[1_555_01 --->	3_656_01]	1.06	1.74	2.795	175.1

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9_SLFZ

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11.4480 14.2240 15.3230 90.000 111.600 90.000 V = 2319.92

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

Centroid = 0.6526 0.6524 0.8792

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O12	[1_555_01 --->	2_656_01]	1.03	1.94	2.957	171.3
N13---H17...N12	[1_555_01 --->	3_667_01]	1.06	1.74	2.793	173.1

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10_SLFZ

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6.0360 21.0200 12.7910 90.000 94.440 90.000 V = 1618.01

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.1213 0.3553 0.1873

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	4_455_01]	1.03	2.00	3.007	166.9
N11---H10...N12	[1_555_01 --->	4_455_01]	1.03	2.58	3.339	130.0
N11---H11...O11	[1_555_01 --->	4_555_01]	1.02	2.48	3.248	131.6
N11---H11...O12	[1_555_01 --->	4_555_01]	1.02	2.53	3.394	142.1
N13---H17...O12	[1_555_01 --->	1_655_01]	1.04	1.79	2.816	168.3

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11_SLFZ

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8.3660 21.3530 9.0970 90.000 93.370 90.000 V = 1622.27

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.3702 0.1571 0.5487

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	4_455_01]	1.03	2.04	3.030	161.7
N11---H11...O12	[1_555_01 --->	1_455_01]	1.02	2.04	2.995	155.0
N13---H17...O11	[1_555_01 --->	3_656_01]	1.06	2.66	3.347	121.9
N13---H17...N12	[1_555_01 --->	3_656_01]	1.06	1.75	2.811	175.2

==========

12_SLFZ

==========

8.1940 21.1110 9.5700 90.000 94.200 90.000 V = 1651.01

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.3876 0.1590 0.5641

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	4_455_01]	1.03	1.96	2.954	161.1
N11---H11...O12	[1_555_01 --->	1_455_01]	1.02	2.08	3.008	150.3
N13---H17...O11	[1_555_01 --->	3_656_01]	1.06	2.62	3.306	122.3
N13---H17...N12	[1_555_01 --->	3_656_01]	1.06	1.77	2.826	173.7

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

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13_SLFZ

==========

8.6280 21.1510 9.1350 90.000 97.700 90.000 V = 1652.02

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.3634 0.1550 0.5687

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	4_455_01]	1.03	1.94	2.949	167.2
N11---H11...O12	[1_555_01 --->	1_455_01]	1.02	1.96	2.963	166.5
N13---H17...O11	[1_555_01 --->	3_656_01]	1.06	2.60	3.295	122.5
N13---H17...N12	[1_555_01 --->	3_656_01]	1.06	1.76	2.818	173.2

==========

14_SLFZ

==========

8.6060 21.6430 8.7350 90.000 98.760 90.000 V = 1608.00

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.3255 0.1523 0.5762

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	4_455_01]	1.03	1.93	2.948	170.3
N11---H11...O12	[1_555_01 --->	1_455_01]	1.02	1.92	2.934	168.9
N13---H17...O11	[1_555_01 --->	3_656_01]	1.06	2.60	3.288	121.7
N13---H17...N12	[1_555_01 --->	3_656_01]	1.06	1.75	2.803	174.0

==========

15_SLFZ

==========

8.5500 21.4910 9.2150 90.000 90.270 90.000 V = 1693.22

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.3184 0.8438 0.4569

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	4_464_01]	1.02	2.31	3.270	155.2
N11---H11...O12	[1_555_01 --->	1_455_01]	1.02	1.99	2.988	165.3
N13---H17...N12	[1_555_01 --->	3_676_01]	1.06	1.73	2.795	175.3

==========

16_SLFZ

==========

6.4870 12.3320 22.2590 90.000 94.190 90.000 V = 1775.91

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.3855 0.6541 0.1344

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O12	[1_555_01 --->	2_555_01]	1.03	1.91	2.936	173.0
N11---H11...O11	[1_555_01 --->	2_655_01]	1.02	2.06	2.977	147.3
N13---H17...N12	[1_555_01 --->	3_665_01]	1.06	1.78	2.835	173.2

==========

17_SLFZ

==========

6.6130 12.0740 22.0850 90.000 93.440 90.000 V = 1760.21

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.3876 0.6550 0.1362

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O12	[1_555_01 --->	2_555_01]	1.03	1.88	2.903	173.6
N11---H11...O11	[1_555_01 --->	2_655_01]	1.02	2.01	2.943	149.4
N13---H17...N12	[1_555_01 --->	3_665_01]	1.06	1.76	2.814	173.0

==========

18_SLFZ

==========

8.4170 20.9750 9.4720 90.000 93.830 90.000 V = 1668.51

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.3874 0.1587 0.5516

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	4_455_01]	1.03	1.99	2.981	162.2
N11---H11...O12	[1_555_01 --->	1_455_01]	1.02	2.10	3.063	156.2
N13---H17...O11	[1_555_01 --->	3_656_01]	1.06	2.66	3.344	122.0
N13---H17...N12	[1_555_01 --->	3_656_01]	1.06	1.75	2.808	173.7

==========

19_SLFZ

==========

6.5720 12.9590 21.5330 90.000 92.480 90.000 V = 1832.17

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.3867 0.6251 0.1453

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O12	[1_555_01 --->	2_555_01]	1.03	1.86	2.882	171.3
N11---H11...O11	[1_555_01 --->	2_655_01]	1.02	2.04	2.958	147.7
N13---H17...N12	[1_555_01 --->	3_665_01]	1.06	1.72	2.787	176.7

==========

20_SLFZ

==========

8.7830 14.7280 23.8000 90.000 98.460 90.000 V = 3045.17

Space group: P21/n

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 2
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.1197 0.6038 0.8759
Molecule 02 = C9 H9 N3 O2 S2
Centroid = 0.5747 0.5141 0.6190

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O21	[1_555_01 --->	1_555_02]	1.03	1.92	2.932	165.3
N11---H11...O12	[1_555_01 --->	1_655_01]	1.03	1.87	2.898	173.8
N13---H17...O11	[1_555_01 --->	3_567_01]	1.06	2.59	3.284	122.4
N13---H17...N12	[1_555_01 --->	3_567_01]	1.06	1.77	2.825	172.6
N21---H20...N11	[1_555_02 --->	2_646_01]	1.03	2.01	3.038	173.9
N21---H21...O22	[1_555_02 --->	1_655_02]	1.03	2.02	3.044	176.0
N23---H27...O11	[1_555_02 --->	4_564_01]	1.04	1.79	2.831	174.5

==========

21_SLFZ

==========

8.4540 20.6990 9.4870 90.000 92.370 90.000 V = 1658.70

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.3882 0.1596 0.5423

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	4_455_01]	1.03	2.05	3.034	159.7
N11---H11...O12	[1_555_01 --->	1_455_01]	1.02	2.08	3.045	156.4
N13---H17...O11	[1_555_01 --->	3_656_01]	1.06	2.67	3.363	122.6
N13---H17...N12	[1_555_01 --->	3_656_01]	1.06	1.76	2.814	173.9

==========

22_SLFZ

==========

8.5830 20.6520 9.5200 90.000 93.660 90.000 V = 1684.04

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.3537 0.1597 0.5549

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	4_455_01]	1.03	1.99	2.979	160.2
N11---H11...O12	[1_555_01 --->	1_455_01]	1.02	1.99	2.993	164.9
N13---H17...O11	[1_555_01 --->	3_656_01]	1.06	2.60	3.278	120.9
N13---H17...N12	[1_555_01 --->	3_656_01]	1.06	1.74	2.794	173.8

==========

23_SLFZ

==========

16.5330 9.9960 19.8100 90.000 112.260 90.000 V = 3029.89

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 2
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.7981 0.1697 0.8802

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

Molecule 02 = C9 H9 N3 O2 S2
Centroid = 0.3898 0.3029 0.8938

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O21	[1_555_01	---> 1_555_02]	1.02	2.15	3.108	155.0
N11---H11...O12	[1_555_01	---> 2_646_01]	1.03	2.07	3.064	163.2
N13---H17...O11	[1_555_01	---> 3_757_01]	1.06	2.66	3.340	121.1
N13---H17...N12	[1_555_01	---> 3_757_01]	1.06	1.74	2.798	176.0
N21---H20...O11	[1_555_02	---> 1_455_01]	1.03	2.01	3.017	166.5
N21---H21...O21	[1_555_02	---> 2_556_02]	1.03	2.00	3.007	164.8

==========

24_SLFZ

==========

20.7050 11.3850 14.1360 90.000 99.020 90.000 V = 3291.02

Space group: C2/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y,-z+0.50
[3] -x,-y,-z
[4] x,-y,z+0.50
[5] x+0.50,y+0.50,z
[6] -x+0.50,y+0.50,-z+0.50
[7] -x+0.50,-y+0.50,-z
[8] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.6072 0.7331 0.4223

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H11...O11	[1_555_01	---> 4_564_01]	1.02	2.11	3.058	152.3
N13---H17...N12	[1_555_01	---> 3_676_01]	1.06	1.78	2.838	175.5

==========

25_SLFZ

==========

9.5150 16.6750 19.2490 90.000 90.000 90.000 V = 3054.10

Space group: P212121
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,-y,z+0.50
[3] x+0.50,-y+0.50,-z
[4] -x,y+0.50,-z+0.50

Z(prime) = 2
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.4842 0.3850 0.3467
Molecule 02 = C9 H9 N3 O2 S2
Centroid = 0.5047 0.6287 0.6388

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O12	[1_555_01	---> 4_645_01]	1.03	1.96	2.935	158.4
N11---H11...O21	[1_555_01	---> 3_556_02]	1.02	2.09	3.032	152.6
N13---H17...O21	[1_555_01	---> 1_555_02]	1.06	2.69	3.371	121.8
N13---H17...N22	[1_555_01	---> 1_555_02]	1.06	1.74	2.797	172.8
N21---H20...O22	[1_555_02	---> 4_656_02]	1.02	2.17	3.025	139.4
N21---H21...O11	[1_555_02	---> 3_466_01]	1.03	2.02	3.043	171.4
N23---H27...N12	[1_555_02	---> 1_555_01]	1.06	1.72	2.784	174.3

==========

26_SLFZ

==========

19.6390 8.8640 24.6120 90.000 90.000 90.000 V = 4284.46

Space group: Aba2
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,-y,z
[3] -x+0.50,y,z+0.50
[4] x+0.50,-y,z+0.50
[5] x,y+0.50,z+0.50
[6] -x,-y+0.50,z+0.50
[7] -x+0.50,y+0.50,z
[8] x+0.50,-y+0.50,z

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

Centroid = 0.1441 0.8820 0.2637

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N13---H17...N12	[1_555_01 ---> 2_575_01]		1.07	1.69	2.758	175.9

==========

27_SLFZ

==========

20.4060 9.0160 20.4940 90.000 90.000 90.000 V = 3770.50

Space group: Pbca
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,-y,z+0.50
[3] x+0.50,-y+0.50,-z
[4] -x,y+0.50,-z+0.50
[5] -x,-y,-z
[6] x+0.50,y,-z+0.50
[7] -x+0.50,y+0.50,z
[8] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.3756 0.7021 0.4303

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N13---H17...N12	[1_555_01 ---> 5_666_01]		1.06	1.79	2.850	175.0

==========

28_SLFZ

==========

8.0100 20.8200 8.9900 90.000 94.650 90.000 V = 1494.31

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.4128 0.1558 0.5665

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 ---> 4_455_01]		1.03	1.96	2.938	158.1
N11---H11...O12	[1_555_01 ---> 1_455_01]		1.02	2.05	2.930	143.0
N13---H17...O11	[1_555_01 ---> 3_656_01]		1.06	2.52	3.220	123.3
N13---H17...N12	[1_555_01 ---> 3_656_01]		1.06	1.77	2.816	169.9

==========

29_SLFZ

==========

8.5230 21.0730 9.0870 90.000 96.540 90.000 V = 1621.45

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.3707 0.1535 0.5756

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 ---> 4_455_01]		1.03	1.94	2.936	163.6
N11---H11...O12	[1_555_01 ---> 1_455_01]		1.03	1.89	2.904	170.2
N13---H17...O11	[1_555_01 ---> 3_656_01]		1.06	2.56	3.241	121.4
N13---H17...N12	[1_555_01 ---> 3_656_01]		1.06	1.75	2.802	173.2

==========

30_SLFZ

==========

8.6785 19.9110 10.0217 90.000 97.776 90.000 V = 1715.80

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.3704 0.1594 0.5702

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 ---> 4_455_01]		1.03	1.89	2.909	168.4
N11---H11...O12	[1_555_01 ---> 1_455_01]		1.02	1.92	2.946	174.1
N13---H17...O11	[1_555_01 ---> 3_656_01]		1.05	2.48	3.180	123.3
N13---H17...N12	[1_555_01 ---> 3_656_01]		1.05	1.82	2.869	170.5

==========

31_SLFZ

==========

8.2478 21.0191 9.0739 90.000 96.534 90.000 V = 1562.85

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.3966 0.1554 0.5637

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 ---> 4_455_01]		1.03	1.94	2.943	163.9
N11---H11...O12	[1_555_01 ---> 1_455_01]		1.02	1.98	2.937	153.6
N13---H17...O11	[1_555_01 ---> 3_656_01]		1.06	2.56	3.256	122.5
N13---H17...N12	[1_555_01 ---> 3_656_01]		1.06	1.76	2.811	171.5

==========

32_SLFZ

==========

8.4758 20.7179 9.6108 90.000 97.840 90.000 V = 1671.89

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.3469 0.1567 0.5811

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 ---> 4_455_01]		1.03	1.88	2.887	166.7
N11---H11...O12	[1_555_01 ---> 1_455_01]		1.03	1.87	2.881	169.4
N13---H17...O11	[1_555_01 ---> 3_656_01]		1.06	2.46	3.147	121.6
N13---H17...N12	[1_555_01 ---> 3_656_01]		1.06	1.78	2.827	171.2

==========

33_SLFZ

==========

9.1120 18.9940 10.5900 90.000 101.370 90.000 V = 1796.88

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.3531 0.1654 0.5476

INTERMOLECULAR HYDROGEN BONDS

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01	---> 4_455_01]	1.03	1.93	2.951	175.3
N11---H11...O12	[1_555_01	---> 1_455_01]	1.02	2.06	3.069	168.2
N13---H17...N12	[1_555_01	---> 3_656_01]	1.06	1.77	2.823	174.8

==========

34_SLFZ

==========

8.3551 18.8800 10.7764 90.000 96.790 90.000 V = 1687.99

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.3637 0.1746 0.5251

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01	---> 4_455_01]	1.03	1.92	2.932	168.3
N11---H11...O12	[1_555_01	---> 1_455_01]	1.02	1.99	2.971	159.3
N13---H17...N12	[1_555_01	---> 3_656_01]	1.06	1.73	2.787	176.8

==========

35_SLFZ

==========

8.3630 21.1460 9.1160 90.000 95.760 90.000 V = 1603.97

Space group: P21
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z

Z(prime) = 2
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.6155 0.1559 0.8217
Molecule 02 = C9 H9 N3 O2 S2
Centroid = 0.8947 -0.1547 0.6814

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O21	[1_555_01	---> 2_657_02]	1.03	1.93	2.927	164.2
N11---H11...O12	[1_555_01	---> 1_455_01]	1.03	1.88	2.884	164.9
N13---H17...O21	[1_555_01	---> 1_555_02]	1.06	2.53	3.203	120.8
N13---H17...N22	[1_555_01	---> 1_555_02]	1.06	1.73	2.786	173.0
N21---H20...O11	[1_555_02	---> 2_746_01]	1.03	1.97	2.956	161.4
N21---H21...O22	[1_555_02	---> 1_655_02]	1.02	1.95	2.924	157.8
N23---H27...O11	[1_555_02	---> 1_555_01]	1.06	2.53	3.207	120.8
N23---H27...N12	[1_555_02	---> 1_555_01]	1.06	1.73	2.788	172.6

==========

36_SLFZ

==========

8.1540 17.3990 10.0770 90.000 101.320 90.000 V = 1401.83

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.6925 0.6284 0.4158

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01	---> 1_455_01]	1.03	2.65	3.240	116.8
N11---H10...O12	[1_555_01	---> 4_464_01]	1.03	2.10	3.013	146.6
N13---H17...O11	[1_555_01	---> 3_766_01]	1.06	2.56	3.274	124.2
N13---H17...N12	[1_555_01	---> 3_766_01]	1.06	1.77	2.815	170.5

==========

37_SLFZ

==========

8.3900 18.8130 9.5400 90.000 102.540 90.000 V = 1469.88

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.8280 0.8256 0.4327

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H11...O12	[1_555_01 --->	1_455_01]	1.02	2.23	3.158	150.2
N13---H17...O11	[1_555_01 --->	3_776_01]	1.07	2.64	3.325	121.7
N13---H17...N12	[1_555_01 --->	3_776_01]	1.07	1.70	2.766	174.0

==========

38_SLFZ

==========

8.1670 12.4430 15.6320 90.000 96.880 90.000 V = 1577.12

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.2645 0.4202 0.1526

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	1_455_01]	1.02	2.20	3.062	141.2
N13---H17...N12	[1_555_01 --->	3_665_01]	1.06	1.75	2.811	174.5

==========

39_SLFZ

==========

9.0450 16.8640 39.4210 90.000 90.000 90.000 V = 6013.08

Space group: Pbca
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,-y,z+0.50
[3] x+0.50,-y+0.50,-z
[4] -x,y+0.50,-z+0.50
[5] -x,-y,-z
[6] x+0.50,y,-z+0.50
[7] -x+0.50,y+0.50,z
[8] x,-y+0.50,z+0.50

Z(prime) = 2
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.5601 0.7022 0.8035
Molecule 02 = C9 H9 N3 O2 S2
Centroid = 0.5580 0.6687 0.9519

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O12	[1_555_01 --->	4_656_01]	1.03	1.96	2.929	156.7
N11---H11...O11	[1_555_01 --->	7_555_01]	1.03	1.97	2.970	163.1
N13---H17...O21	[1_555_01 --->	1_555_02]	1.06	2.63	3.331	123.1
N13---H17...N22	[1_555_01 --->	1_555_02]	1.06	1.72	2.774	172.3
N21---H20...O21	[1_555_02 --->	3_467_02]	1.03	2.09	3.104	169.5
N21---H21...O22	[1_555_02 --->	7_655_02]	1.03	1.90	2.916	169.1
N23---H27...O11	[1_555_02 --->	1_555_01]	1.06	2.62	3.337	124.3
N23---H27...N12	[1_555_02 --->	1_555_01]	1.06	1.76	2.808	170.3

==========

40_SLFZ

==========

9.1790 16.9070 39.2020 90.000 90.000 90.000 V = 6083.73

Space group: Pbca
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,-y,z+0.50
[3] x+0.50,-y+0.50,-z
[4] -x,y+0.50,-z+0.50

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

[5] -x,-y,-z
[6] x+0.50,y,-z+0.50
[7] -x+0.50,y+0.50,z
[8] x,-y+0.50,z+0.50

Z(prime) = 2
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.5556 0.7023 0.8025
Molecule 02 = C9 H9 N3 O2 S2
Centroid = 0.5708 0.6715 0.9516

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O12	[1_555_01 ---> 4_656_01]		1.03	2.01	2.986	158.9
N11---H11...O11	[1_555_01 ---> 7_555_01]		1.03	2.02	3.019	163.0
N13---H17...N22	[1_555_01 ---> 1_555_02]		1.06	1.73	2.788	172.5
N21---H20...O21	[1_555_02 ---> 3_467_02]		1.03	2.11	3.126	169.1
N21---H21...O22	[1_555_02 ---> 7_655_02]		1.03	1.85	2.873	170.5
N23---H27...O11	[1_555_02 ---> 1_555_01]		1.06	2.64	3.337	122.8
N23---H27...N12	[1_555_02 ---> 1_555_01]		1.06	1.74	2.792	171.7

==========

41_SLFZ

==========

12.2130 20.5500 13.5830 90.000 97.030 90.000 V = 3383.39

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 2
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.9055 0.1596 0.9527
Molecule 02 = C9 H9 N3 O2 S2
Centroid = 0.4295 0.1585 0.4659

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O21	[1_555_01 ---> 4_555_02]		1.02	2.42	3.311	144.6
N11---H11...O22	[1_555_01 ---> 1_555_02]		1.02	2.19	3.163	159.1
N13---H17...O11	[1_555_01 ---> 3_757_01]		1.06	2.57	3.245	120.7
N13---H17...N12	[1_555_01 ---> 3_757_01]		1.06	1.72	2.782	173.6
N21---H20...O11	[1_555_02 ---> 4_454_01]		1.02	2.17	3.111	151.2
N21---H21...O12	[1_555_02 ---> 1_454_01]		1.02	2.24	3.224	161.4
N23---H27...O21	[1_555_02 ---> 3_656_02]		1.06	2.57	3.263	123.0
N23---H27...N22	[1_555_02 ---> 3_656_02]		1.06	1.78	2.828	171.3

==========

42_SLFZ

==========

8.3850 9.2720 20.7040 90.000 100.100 90.000 V = 1584.70

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.5137 0.3011 0.3895

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 ---> 1_655_01]		1.03	1.96	2.970	166.7
N11---H11...O11	[1_555_01 ---> 2_655_01]		1.02	2.24	3.216	159.4

==========

43_SLFZ

==========

8.6514 8.6514 20.5380 90.000 90.000 90.000 V = 1537.20

Space group: P43
Symmetry operators read from CIF:
[1] x,y,z
[2] -y,x,z+0.75
[3] -x,-y,z+0.50
[4] y,-x,z+0.25

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.2244 0.8556 0.1884

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 ---> 1_545_01]		1.03	1.86	2.890	173.2
N11---H11...O12	[1_555_01 ---> 2_654_01]		1.02	2.28	2.973	123.5

==========

44_SLFZ

==========

10.7410 7.5920 16.7480 90.000 103.990 90.000 V = 1325.22

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.8035 0.5458 0.6326

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O12	[1_555_01 ---> 2_746_01]		1.02	2.25	3.097	139.2
N11---H11...O12	[1_555_01 ---> 4_565_01]		1.02	1.90	2.907	167.9
N13---H17...O11	[1_555_01 ---> 3_666_01]		1.06	2.56	3.268	123.6
N13---H17...N12	[1_555_01 ---> 3_666_01]		1.06	1.76	2.803	169.7

==========

45_SLFZ

==========

10.5390 12.1890 13.9810 95.290 107.380 90.630 V = 1705.30

Space group: P-1
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,-y,-z

Z(prime) = 2
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.7707 0.6571 0.2511
Molecule 02 = C9 H9 N3 O2 S2
Centroid = 0.2871 0.7528 0.3388

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N13---H17...N22	[1_555_01 ---> 1_555_02]		1.06	1.77	2.822	173.0
N23---H27...O11	[1_555_02 ---> 1_555_01]		1.06	2.64	3.315	121.1
N23---H27...N12	[1_555_02 ---> 1_555_01]		1.06	1.73	2.788	172.7

==========

46_SLFZ

==========

6.6309 15.0142 17.7082 90.000 94.551 90.000 V = 1757.43

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.1344 0.2002 0.3872

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O12	[1_555_01 ---> 2_555_01]		1.03	1.95	2.953	165.8
N11---H11...O11	[1_555_01 ---> 2_455_01]		1.02	2.14	3.017	142.7
N13---H17...N12	[1_555_01 ---> 3_556_01]		1.06	1.77	2.825	174.2

==========

47_SLFZ

==========

9.4240 17.1950 19.5600 90.000 90.000 90.000 V = 3169.61

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

Space group: Pbca
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,-y,z+0.50
[3] x+0.50,-y+0.50,-z
[4] -x,y+0.50,-z+0.50
[5] -x,-y,-z
[6] x+0.50,y,-z+0.50
[7] -x+0.50,y+0.50,z
[8] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.4932 0.3827 0.3521

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O12	[1_555_01 --->	4_645_01]	1.02	2.07	2.972	145.0
N11---H11...O11	[1_555_01 --->	7_645_01]	1.03	2.08	3.074	162.8
N13---H17...N12	[1_555_01 --->	5_666_01]	1.06	1.72	2.787	176.8

==========

48_SLFZ

==========

8.3550 40.1040 9.3390 90.000 111.130 90.000 V = 2918.82

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.0524 0.8231 0.4178

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	1_455_01]	1.03	1.97	2.972	165.8
N11---H10...N12	[1_555_01 --->	1_455_01]	1.03	2.67	3.434	131.0
N11---H11...O11	[1_555_01 --->	4_465_01]	1.03	1.94	2.940	164.2

==========

49_SLFZ

==========

10.1706 10.8646 16.1335 90.000 105.054 90.000 V = 1721.56

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.7426 0.1862 0.1835

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O12	[1_555_01 --->	4_555_01]	1.03	2.28	3.249	156.8
N11---H11...O12	[1_555_01 --->	2_645_01]	1.03	1.96	2.902	151.1

==========

50_SLFZ

==========

8.8854 13.3231 14.7403 90.000 101.159 90.000 V = 1711.98

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.2737 0.9065 0.1164

INTERMOLECULAR HYDROGEN BONDS

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	1_455_01]	1.02	2.00	2.985	161.1
N11---H11...O12	[1_555_01 --->	2_555_01]	1.02	2.12	3.080	156.2
N13---H17...N12	[1_555_01 --->	3_675_01]	1.06	1.76	2.819	177.0

==========

51_SLFZ

==========

10.5317 8.5508 21.7500 90.000 91.055 90.000 V = 1958.35

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.9268 0.6037 0.7431

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H11...O11	[1_555_01 --->	2_756_01]	1.03	1.99	3.001	167.6

==========

52_SLFZ

==========

8.2576 12.1531 16.5609 90.000 98.785 90.000 V = 1642.48

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.2590 0.4039 0.6327

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	1_455_01]	1.02	2.05	2.997	153.6
N13---H17...N12	[1_555_01 --->	3_666_01]	1.06	1.75	2.802	170.9

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53_SLFZ

==========

9.1350 5.3790 36.6330 90.000 91.170 90.000 V = 1799.67

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.1959 0.1322 0.4407

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N13---H17...N12	[1_555_01 --->	3_656_01]	1.06	1.74	2.800	175.8

==========

54_SLFZ

==========

11.0200 9.0100 20.1860 90.000 113.680 90.000 V = 1835.52

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.2188 0.4017 0.1777

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N13---H17...N12	[1_555_01 ---> 3_565_01]		1.06	1.75	2.804	173.9

55_SLFZ

8.8109 12.7222 13.1696 66.227 73.797 88.068 V = 1292.09

Space group: P-1
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,-y,-z

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.2252 0.1192 1.0460

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A

56_SLFZ

8.5007 18.8407 10.5066 90.000 104.507 90.000 V = 1629.08

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.5898 0.3682 0.6642

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 ---> 1_655_01]		1.03	1.93	2.946	171.4
N11---H11...O12	[1_555_01 ---> 4_554_01]		1.03	1.93	2.955	172.7

57_SLFZ

8.3577 19.2806 10.9972 90.000 105.064 90.000 V = 1711.21

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.6026 0.3693 0.6601

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 ---> 1_655_01]		1.03	1.99	2.994	164.7
N11---H11...O12	[1_555_01 ---> 4_554_01]		1.03	2.00	3.010	167.4

58_SLFZ

8.4031 19.2762 10.9624 90.000 106.229 90.000 V = 1704.93

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.6003 0.3686 0.6603

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	1_655_01]	1.03	1.96	2.972	167.5
N11---H11...O12	[1_555_01 --->	4_554_01]	1.03	1.98	2.981	165.2

59_SLFZ

8.3786 19.6447 11.1172 90.000 106.885 90.000 V = 1750.95

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.5986 0.3691 0.6506

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	1_655_01]	1.03	1.95	2.965	168.3
N11---H11...O12	[1_555_01 --->	4_554_01]	1.03	2.01	3.006	163.5

60_SLFZ

13.9430 9.2600 12.6980 90.000 90.000 90.000 V = 1639.47

Space group: Pna21
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,-y,z+0.50
[3] -x+0.50,y+0.50,z+0.50
[4] x+0.50,-y+0.50,z

Z(prime) = 1
Molecule 01 = C9 H8 N3 O2 S2
Centroid = 0.6445 0.8381 0.5772

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O12	[1_555_01 --->	3_655_01]	1.03	1.94	2.947	166.9
N11---H11...O11	[1_555_01 --->	2_675_01]	1.03	2.39	3.176	133.2
N11---H11...N12	[1_555_01 --->	2_675_01]	1.03	2.37	3.334	156.4

61_SLFZ

15.8070 10.1260 10.7540 90.000 90.000 90.000 V = 1721.30

Space group: Pna21
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,-y,z+0.50
[3] -x+0.50,y+0.50,z+0.50
[4] x+0.50,-y+0.50,z

Z(prime) = 1
Molecule 01 = C9 H8 N3 O2 S2
Centroid = 0.3997 0.3469 0.3684

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...N12	[1_555_01 --->	2_664_01]	1.03	2.04	3.065	173.5
N11---H11...O11	[1_555_01 --->	3_554_01]	1.03	1.94	2.936	161.1

62_SLFZ

6.9480 14.8680 15.9580 90.000 90.000 90.000 V = 1648.51

Space group: P212121
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,-y,z+0.50
[3] x+0.50,-y+0.50,-z
[4] -x,y+0.50,-z+0.50

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

Z(prime) = 1
Molecule 01 = C9 H8 N3 O2 S2
Centroid = 0.2044 0.2572 0.3162

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O12	[1_555_01 --->	4_545_01]	1.03	1.92	2.935	165.9
N11---H11...O11	[1_555_01 --->	4_645_01]	1.03	2.38	3.329	152.4
N11---H11...N12	[1_555_01 --->	4_645_01]	1.03	2.34	3.231	143.3

==========

63_SLFZ

==========

6.5920 15.1550 15.6890 90.000 90.000 90.000 V = 1567.36

Space group: P212121
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,-y,z+0.50
[3] x+0.50,-y+0.50,-z
[4] -x,y+0.50,-z+0.50

Z(prime) = 1
Molecule 01 = C9 H8 N3 O2 S2
Centroid = 0.2001 0.2691 0.3180

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O12	[1_555_01 --->	4_545_01]	1.04	1.87	2.896	171.6
N11---H11...O11	[1_555_01 --->	4_645_01]	1.03	2.24	3.202	154.4
N11---H11...N12	[1_555_01 --->	4_645_01]	1.03	2.39	3.211	135.9

==========

64_SLFZ

==========

17.5620 42.7200 8.2910 90.000 90.000 90.000 V = 6220.31

Space group: Fdd2
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,-y,z
[3] -x+0.25,y+0.25,z+0.25
[4] x+0.75,-y+0.75,z+0.25
[5] x,y+0.50,z+0.50
[6] -x,-y+0.50,z+0.50
[7] -x+0.25,y+0.75,z+0.75
[8] x+0.75,-y+0.25,z+0.75
[9] x+0.50,y,z+0.50
[10] -x+0.50,-y,z+0.50
[11] -x+0.75,y+0.25,z+0.75
[12] x+0.25,-y+0.75,z+0.75
[13] x+0.50,y+0.50,z
[14] -x+0.50,-y+0.50,z
[15] -x+0.75,y+0.75,z+0.25
[16] x+0.25,-y+0.25,z+0.25

Z(prime) = 1
Molecule 01 = C9 H8 N3 O2 S2
Centroid = 0.3074 0.4368 0.5624

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	1_556_01]	1.03	2.03	2.989	153.8
N11---H11...O11	[1_555_01 --->	12_555_01]	1.03	1.92	2.954	174.7

==========

65_SLFZ

==========

10.4490 13.3310 13.6640 90.000 110.380 90.000 V = 1784.19

Space group: P21
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z

Z(prime) = 2
Molecule 01 = C9 H8 N3 O2 S2
Centroid = 0.6668 0.8420 0.4395
Molecule 02 = C9 H8 N3 O2 S2
Centroid = 0.3113 0.3231 0.0805

INTERMOLECULAR HYDROGEN BONDS

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

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D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O12	[1_555_01 --->	2_646_01]	1.03	1.98	2.991	168.6
N11---H11...O21	[1_555_01 --->	1_555_02]	1.03	1.94	2.964	172.3
N21---H20...O22	[1_555_02 --->	2_645_02]	1.03	2.04	3.023	158.7
N21---H21...O11	[1_555_02 --->	1_545_01]	1.03	1.91	2.913	164.9

==========

66_SLFZ

==========

8.0810 16.6760 13.1690 90.000 104.560 90.000 V = 1717.65

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H8 N3 O2 S2
Centroid = 0.1193 0.8625 0.7004

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	4_564_01]	1.03	1.99	2.966	156.6
N11---H11...N13	[1_555_01 --->	2_546_01]	1.03	1.98	3.009	172.2

==========

67_SLFZ

==========

20.6230 8.3200 18.1570 90.000 115.640 90.000 V = 2808.66

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 2
Molecule 01 = C9 H8 N3 O2 S2
Centroid = 0.0914 0.4719 0.6692
Molecule 02 = C9 H8 N3 O2 S2
Centroid = 0.4023 0.9766 0.5681

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	1_565_01]	1.03	1.91	2.929	169.5
N11---H11...O22	[1_555_01 --->	1_555_02]	1.03	2.40	3.337	151.6
N21---H20...O21	[1_555_02 --->	1_565_02]	1.03	1.82	2.839	169.4
N21---H21...O11	[1_555_02 --->	4_564_01]	1.03	2.00	3.025	174.6

==========

68_SLFZ

==========

10.8380 11.8260 22.3210 90.000 90.140 90.000 V = 2860.88

Space group: C2/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y,-z+0.50
[3] -x,-y,-z
[4] x,-y,z+0.50
[5] x+0.50,y+0.50,z
[6] -x+0.50,y+0.50,-z+0.50
[7] -x+0.50,-y+0.50,-z
[8] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H8 N3 O2 S2
Centroid = 0.5389 0.7346 0.5353

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	3_676_01]	1.03	2.06	3.019	153.4
N11---H11...N13	[1_555_01 --->	7_666_01]	1.04	2.02	3.059	176.7

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69_SLFZ

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S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

8.4010 11.1420 17.7460 90.000 90.000 90.000 V = 1661.10

Space group: P212121
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,-y,z+0.50
[3] x+0.50,-y+0.50,-z
[4] -x,y+0.50,-z+0.50

Z(prime) = 1
Molecule 01 = C9 H8 N3 O2 S2
Centroid = 0.5452 0.5642 0.3903

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	1_455_01]	1.04	1.95	2.977	173.2
N11---H11...O12	[1_555_01 --->	4_645_01]	1.03	2.50	3.394	145.7

==========

70_SLFZ

==========

13.9493 8.3273 16.9440 90.000 113.288 90.000 V = 1807.86

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H8 N3 O2 S2
Centroid = 0.8360 0.5287 0.5691

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...N11	[1_555_01 --->	3_776_01]	1.02	2.56	3.069	110.3
N11---H11...O12	[1_555_01 --->	1_565_01]	1.03	1.94	2.931	161.8

==========

71_SLFZ

==========

17.7230 11.6840 11.9380 90.000 91.780 90.000 V = 2470.87

Space group: C2/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y,-z+0.50
[3] -x,-y,-z
[4] x,-y,z+0.50
[5] x+0.50,y+0.50,z
[6] -x+0.50,y+0.50,-z+0.50
[7] -x+0.50,-y+0.50,-z
[8] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H10 N3 O2 S2
Centroid = 0.3837 0.4982 0.5869

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H11...N12	[1_555_01 --->	3_666_01]	1.07	1.82	2.854	160.4

==========

72_SLFZ

==========

6.6200 15.3490 17.1480 90.000 90.000 90.000 V = 1742.41

Space group: P212121
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,-y,z+0.50
[3] x+0.50,-y+0.50,-z
[4] -x,y+0.50,-z+0.50

Z(prime) = 1
Molecule 01 = C9 H8 N3 O2 S2
Centroid = 0.1911 0.2876 0.3449

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

N11---H10...O12 [1_555_01 ---> 4_545_01] 1.03 1.88 2.909 175.2
N11---H11...O11 [1_555_01 ---> 4_645_01] 1.03 1.95 2.942 162.3

==========

73_SLFZ

==========

8.4158 10.1810 17.9410 90.000 90.000 90.000 V = 1537.21

Space group: P212121
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,-y,z+0.50
[3] x+0.50,-y+0.50,-z
[4] -x,y+0.50,-z+0.50

Z(prime) = 1
Molecule 01 = C9 H8 N3 O2 S2
Centroid = 0.5234 0.5544 0.3960

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 ---> 1_455_01]		1.03	2.08	3.082	165.4
N11---H11...O11	[1_555_01 ---> 4_645_01]		1.02	2.24	3.263	175.5
N11---H11...O12	[1_555_01 ---> 4_645_01]		1.02	2.68	3.332	121.7

==========

74_SLFZ

==========

12.1060 10.4210 8.2840 102.980 90.030 107.720 V = 967.39

Space group: P-1
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,-y,-z

Z(prime) = 1
Molecule 01 = C9 H8 N3 O2 S2
Centroid = 0.3129 0.3338 0.1730

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A

==========

75_SLFZ

==========

8.0392 19.9339 8.6360 90.000 97.715 90.000 V = 1371.41

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H10 N3 O2 S2
Centroid = -0.1295 0.6115 0.1502

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...N12	[1_555_01 ---> 1_455_01]		1.06	1.95	2.999	170.0
N11---H11...O11	[1_555_01 ---> 4_464_01]		1.04	2.31	2.790	106.5

==========

76_SLFZ

==========

10.6915 10.5459 13.2126 90.000 112.410 90.000 V = 1377.23

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H10 N3 O2 S2
Centroid = 0.0511 0.7303 0.1311

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

---
N13---H17...O12 [1_555_01 ---> 4_564_01] 1.04 1.83 2.805 155.4

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77_SLFZ
==========
7.8774 12.1090 16.2492 90.000 105.532 90.000 V = 1493.37

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H8 N3 O2 S2
Centroid = 0.7578 0.5305 0.6129

INTERMOLECULAR HYDROGEN BONDS

D---H...A ARU1 ARU2 D-H H...A D...A D-H...A

N11---H11...N13 [1_555_01 ---> 3_666_01] 1.03 2.04 3.070 173.8

==========
78_SLFZ
==========
8.9763 11.4441 17.3672 90.000 99.299 90.000 V = 1760.61

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H8 N3 O2 S2
Centroid = 0.2107 0.6386 0.3662

INTERMOLECULAR HYDROGEN BONDS

D---H...A ARU1 ARU2 D-H H...A D...A D-H...A

N11---H10...O11 [1_555_01 ---> 2_545_01] 1.03 1.97 2.963 160.9
N11---H11...N12 [1_555_01 ---> 4_564_01] 1.03 2.12 3.145 174.6

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79_SLFZ
==========
8.0122 12.7431 16.7992 90.000 102.200 90.000 V = 1676.47

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H8 N3 O2 S2
Centroid = 0.7460 0.5316 0.6074

INTERMOLECULAR HYDROGEN BONDS

D---H...A ARU1 ARU2 D-H H...A D...A D-H...A

N11---H11...N13 [1_555_01 ---> 3_666_01] 1.03 2.20 3.217 169.9

==========
80_SLFZ
==========
13.8930 11.7710 22.1910 90.000 91.401 90.000 V = 3627.91

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 2
Molecule 01 = C9 H8 N3 O2 S2
Centroid = 0.2218 0.2435 0.5565
Molecule 02 = C9 H8 N3 O2 S2
Centroid = 0.2934 0.7196 0.7023

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H11...O22	[1_555_01 --->	1_555_02]	1.02	2.06	3.022	155.6
N21---H20...O11	[1_555_02 --->	3_666_01]	1.02	2.15	3.167	169.3
N21---H20...O12	[1_555_02 --->	3_666_01]	1.02	2.67	3.417	129.9
N21---H21...O12	[1_555_02 --->	1_565_01]	1.02	2.13	3.126	164.7

==========

81_SLFZ

==========

12.1917 7.6348 15.3895 90.000 107.466 90.000 V = 1366.43

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H10 N3 O2 S2
Centroid = 0.7962 0.2607 0.4827

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H11...O11	[1_555_01 --->	4_554_01]	1.05	1.84	2.886	172.4
N11---H11...N12	[1_555_01 --->	4_554_01]	1.05	2.45	3.032	113.8

==========

82_SLFZ

==========

12.1790 9.6098 13.3530 90.000 101.920 90.000 V = 1529.11

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H8 N3 O2 S2
Centroid = 0.3678 0.3201 0.5715

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	2_556_01]	1.02	2.14	3.002	140.9
N11---H11...O11	[1_555_01 --->	4_555_01]	1.03	1.90	2.923	171.4

==========

83_SLFZ

==========

14.9484 8.2585 22.9621 90.000 100.818 90.000 V = 2784.33

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 2
Molecule 01 = C9 H10 N3 O2 S2
Centroid = 0.8503 0.4097 0.5663
Molecule 02 = C9 H10 N3 O2 S2
Centroid = 0.5779 0.5844 0.3003

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 --->	1_565_01]	1.05	1.82	2.858	168.4
N11---H10...O21	[1_555_01 --->	1_555_02]	1.05	2.65	3.234	114.5
N11---H10...N12	[1_555_01 --->	1_565_01]	1.05	2.69	3.157	106.4
N21---H20...O21	[1_555_02 --->	1_545_02]	1.05	1.77	2.820	173.3
N21---H20...N22	[1_555_02 --->	1_545_02]	1.05	2.57	3.239	120.7

==========

84_SLFZ

==========

8.0557 9.9422 17.2090 90.000 90.570 90.000 V = 1378.22

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H10 N3 O2 S2
Centroid = 0.4597 0.3989 0.1873

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 ---> 2_655_01]		1.05	2.49	2.921	103.3
N11---H10...N12	[1_555_01 ---> 2_655_01]		1.05	1.96	2.967	158.7
N11---H11...O12	[1_555_01 ---> 1_655_01]		1.05	1.76	2.806	171.7

==========
85_SLFZ
==========
17.4737 11.6240 11.7557 90.000 90.072 90.000 V = 2387.75

Space group: Cc
Symmetry operators read from CIF:
[1] x,y,z
[2] x,-y,z+0.50
[3] x+0.50,y+0.50,z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 2
Molecule 01 = C9 H10 N3 O2 S2
Centroid = 0.3828 0.4878 0.5856
Molecule 02 = C9 H10 N3 O2 S2
Centroid = 0.6165 0.5066 0.4159

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H11...O21	[1_555_01 ---> 1_555_02]		1.06	2.56	3.246	122.1
N11---H11...N22	[1_555_01 ---> 1_555_02]		1.06	1.84	2.828	153.5
N21---H21...O11	[1_555_02 ---> 1_555_01]		1.06	2.66	3.261	115.6
N21---H21...N12	[1_555_02 ---> 1_555_01]		1.06	1.94	2.924	153.0

==========
86_SLFZ
==========
15.5302 8.1448 28.4964 90.000 90.000 90.000 V = 3604.52

Space group: Pna21
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,-y,z+0.50
[3] -x+0.50,y+0.50,z+0.50
[4] x+0.50,-y+0.50,z

Z(prime) = 2
Molecule 01 = C9 H10 N3 O2 S2
Centroid = 0.5558 0.7324 0.3473
Molecule 02 = C9 H10 N3 O2 S2
Centroid = 0.9459 0.7372 0.6523

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 ---> 1_545_01]		1.05	2.65	3.162	109.2
N11---H10...N12	[1_555_01 ---> 1_545_01]		1.05	1.92	2.962	168.1
N21---H20...O21	[1_555_02 ---> 1_545_02]		1.06	2.58	3.088	108.8
N21---H20...N22	[1_555_02 ---> 1_545_02]		1.06	1.87	2.911	168.7

==========
87_SLFZ
==========
14.6389 5.9835 20.9270 90.000 94.783 90.000 V = 1826.65

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H10 N3 O2 S2
Centroid = 0.0975 0.8760 0.4234

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H11...N12	[1_555_01 ---> 3_576_01]		1.06	1.82	2.850	161.8

==========

88_SLFZ

==========

8.8101 17.1707 13.2499 90.000 101.100 90.000 V = 1966.89

Space group: P21/c
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H8 N3 O2 S2
Centroid = 0.2056 0.8747 0.7195

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 ---> 2_646_01]		1.02	2.67	3.286	119.0
N11---H11...O12	[1_555_01 ---> 2_646_01]		1.02	2.62	3.270	121.5

==========

89_SLFZ

==========

16.6760 11.7710 19.0620 90.000 111.710 90.000 V = 3476.33

Space group: P21
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,y+0.50,-z

Z(prime) = 4
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.5547 0.4991 0.5301
Molecule 02 = C9 H9 N3 O2 S2
Centroid = 0.0632 0.2789 0.5285
Molecule [2] = C9 H8 N3 O2 S2
Centroid = 0.4160 0.4781 0.9631
Molecule [3] = C9 H8 N3 O2 S2
Centroid = 0.9187 0.2890 0.9658

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 ---> 2_656_01]		1.03	2.57	3.167	116.3
N11---H10...N12	[1_555_01 ---> 2_656_01]		1.03	2.28	3.291	165.7
N11---H11...O21	[1_555_01 ---> 1_555_02]		1.03	2.12	3.121	163.8
N13---H17...N43	[1_555_01 ---> 1_555_04]		1.09	1.65	2.728	170.4
N21---H20...O21	[1_555_02 ---> 2_546_02]		1.03	2.43	3.174	128.3
N21---H20...N22	[1_555_02 ---> 2_546_02]		1.03	2.45	3.430	159.9
N21---H21...O11	[1_555_02 ---> 1_455_01]		1.03	2.24	3.190	153.1
N23---H27...N33	[1_555_02 ---> 1_555_03]		1.09	1.63	2.719	171.5
N31---H30...O31	[1_555_03 ---> 2_657_03]		1.03	1.99	2.921	148.5
N31---H31...O42	[1_555_03 ---> 1_555_04]		1.03	1.95	2.968	167.2
N41---H40...O41	[1_555_04 ---> 2_747_04]		1.03	1.97	2.908	149.4
N41---H41...O32	[1_555_04 ---> 1_655_03]		1.03	1.90	2.926	170.7

==========

90_SLFZ

==========

8.1838 13.3578 13.5189 86.787 79.557 76.493 V = 1413.03

Space group: P-1
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,-y,-z

Z(prime) = 1
Molecule 01 = C9 H10 N3 O2 S2
Centroid = 0.0106 0.7458 0.4458

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 ---> 1_455_01]		1.06	2.55	3.174	117.1
N11---H10...N12	[1_555_01 ---> 1_455_01]		1.06	1.84	2.896	177.2
N11---H11...O11	[1_555_01 ---> 2_566_01]		1.05	1.76	2.777	161.7

==========

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

91_SLFZ

==========

6.5105 19.1510 17.6624 90.000 98.689 90.000 V = 2176.92

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.2041 0.1962 0.2205

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A

==========

92_SLFZ

==========

8.3346 9.7463 10.5348 101.762 93.929 93.843 V = 832.94

Space group: P-1
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,-y,-z

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.5055 0.6673 0.7648

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01 ---> 1_455_01]		1.03	1.98	2.968	160.1
N11---H11...O11	[1_555_01 ---> 2_677_01]		1.02	2.37	3.111	128.1

==========

93_SLFZ

==========

8.2866 11.5419 15.4143 79.817 88.639 76.525 V = 1410.87

Space group: P-1
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,-y,-z

Z(prime) = 2
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.5343 0.8212 0.3987
Molecule 02 = C9 H9 N3 O2 S2
Centroid = 0.4240 0.6658 0.8358

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H11...O12	[1_555_01 ---> 1_455_01]		1.03	1.96	2.952	162.0
N13---H17...O21	[1_555_01 ---> 1_555_02]		1.04	1.77	2.801	169.3
N21---H20...O21	[1_555_02 ---> 1_455_02]		1.03	2.42	3.297	142.7
N21---H20...N12	[1_555_02 ---> 1_455_01]		1.03	2.62	3.333	126.5
N21---H21...O11	[1_555_02 ---> 2_666_01]		1.03	1.97	2.978	164.3

==========

94_SLFZ

==========

8.4105 31.6737 11.6376 90.000 95.105 90.000 V = 3087.86

Space group: P21/n
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,y+0.50,-z+0.50
[3] -x,-y,-z
[4] x+0.50,-y+0.50,z+0.50

Z(prime) = 2
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.3916 0.3956 0.9306
Molecule 02 = C9 H9 N3 O2 S2
Centroid = 1.0047 0.3005 0.3354

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A

S3. Geometrical parameters of hydrogen bonds between SLFZ molecules

N11---H10...O21 [1_555_01 ---> 1_555_02] 1.03 1.89 2.898 165.4
N11---H11...O12 [1_555_01 ---> 1_655_01] 1.03 1.92 2.918 164.7
N21---H20...O21 [1_555_02 ---> 4_554_02] 1.03 1.97 2.980 166.7
N21---H21...O22 [1_555_02 ---> 1_655_02] 1.03 1.91 2.917 164.8

==========

95_SLFZ

==========

10.6023 8.1642 35.1366 90.000 90.000 90.000 V = 3041.40

Space group: Pbca
Symmetry operators read from CIF:
[1] x,y,z
[2] -x+0.50,-y,z+0.50
[3] -x,y+0.50,-z+0.50
[4] x+0.50,-y+0.50,-z
[5] -x,-y,-z
[6] x+0.50,y,-z+0.50
[7] x,-y+0.50,z+0.50
[8] -x+0.50,y+0.50,z

Z(prime) = 1
Molecule 01 = C9 H9 N3 O2 S2
Centroid = 0.6045 0.4041 0.5889

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H11...O12	[1_555_01	---> 1_545_01]	1.03	1.98	2.962	158.2
N13---H17...O11	[1_555_01	---> 5_666_01]	1.06	2.62	3.324	123.2
N13---H17...N12	[1_555_01	---> 5_666_01]	1.06	1.77	2.822	173.0

==========

96_SLFZ

==========

7.6295 8.7769 11.3046 101.353 92.999 97.446 V = 733.56

Space group: P-1
Symmetry operators read from CIF:
[1] x,y,z
[2] -x,-y,-z

Z(prime) = 1
Molecule 01 = C9 H8 N3 O2 S2
Centroid = 0.7521 0.7747 0.9334

INTERMOLECULAR HYDROGEN BONDS

D---H...A	ARU1	ARU2	D-H	H...A	D...A	D-H...A
N11---H10...O11	[1_555_01	---> 2_767_01]	1.03	2.24	3.158	148.7
N11---H11...N13	[1_555_01	---> 2_777_01]	1.04	1.94	2.974	169.3

S4. Hydrogen-bond connectivity tables for SLFZ molecules

- **Neutral [SLFZ]**: H*n*0, H*n*1, H*n*7 available as donors, O*n*1, O*n*2, N*n*1, N*n*2 available as acceptors.
- **Cation [SLFZ]$^{+}$**: H*n*0, H*n*1, H*n*X, H*n*7 available as donors, O*n*1, O*n*2, N*n*2 available as acceptors.
- **Anion [SLFZ]$^{-}$**: H*n*0, H*n*1 available as donors, O*n*1, O*n*2, N*n*1, N*n*2, N*n*3 available as acceptors.
- Symbols + and – indicate connections between molecules of the same or opposite handedness, respectively.

1p	O11	O12	N11	N12	O21	O22	N21	N22
H10	+							
H11		–						
H17	–			–				
H20			+					
H21					+			
H27								–

2p	O11	O12	N11	N12	O21	O22	N21	N22
H10						–		
H11	+			+				
H17					–			
H20		–						
H21					+			+
H27	–							

3p	O11	O12	N11	N12	O21	O22	N21	N22
H10								–
H11					+			
H17							+	
H20	+							
H21	+							
H27			+					

4p	O11	O12	N11	N12
H10	+			
H11	+			
H17			+	

5p	O11	O12	N11	N12
H10				–
H11	+ –			
H17			+	

1 [SLFZ]	O11	O12	N11	N12	O21	O22	N21	N22
H10					+ –			
H11					–			–
H17	–			–				
H20								
H21			+					
H27		–						

2 [SLFZ]	O11	O12	N11	N12
H10				+
H11		+		
H17				

3 [SLFZ]	O11	O12	N11	N12	O21	O22	N21	N22
H10	+							
H11		–						
H17								+
H20					–			
H21					–	+		
H27				+				

4 [SLFZ]	O11	O12	N11	N12	O21	O22	N21	N22
H10						–		
H11					+			
H17								+
H20		+						
H21	–							
H27				+				

5 [SLFZ]	O11	O12	N11	N12
H10	+			
H11				
H17				–

S4. Hydrogen-bond connectivity tables for SLFZ molecules

- **Neutral [SLFZ]**: H*n*0, H*n*1, H*n*7 available as donors, O*n*1, O*n*2, N*n*1, N*n*2 available as acceptors.
- **Cation [SLFZ]$^{+}$**: H*n*0, H*n*1, H*n*X, H*n*7 available as donors, O*n*1, O*n*2, N*n*2 available as acceptors.
- **Anion [SLFZ]$^{-}$**: H*n*0, H*n*1 available as donors, O*n*1, O*n*2, N*n*1, N*n*2, N*n*3 available as acceptors.
- Symbols + and – indicate connections between molecules of the same or opposite handedness, respectively.

6 [SLFZ]	O11	O12	N11	N12
H10		–		
H11	–	+		
H17	–			–

7 [SLFZ]	O11	O12	N11	N12
H10				
H11		+		
H17				–

8 [SLFZ]	O11	O12	N11	N12
H10	–			
H11		+		
H17				–

9 [SLFZ]	O11	O12	N11	N12
H10		+		
H11				
H17				–

10 [SLFZ]	O11	O12	N11	N12
H10	–			–
H11	–	–		
H17		+		

11 [SLFZ]	O11	O12	N11	N12
H10	–			
H11		+		
H17	–			–

12 [SLFZ]	O11	O12	N11	N12
H10	–			
H11		+		
H17	–			–

13 [SLFZ]	O11	O12	N11	N12
H10	–			
H11		+		
H17	–			–

14 [SLFZ]	O11	O12	N11	N12
H10	–			
H11		+		
H17	–			–

15 [SLFZ]	O11	O12	N11	N12
H10	–			
H11		+		
H17				–

16 [SLFZ]	O11	O12	N11	N12
H10		+		
H11	+			
H17				–

17 [SLFZ]	O11	O12	N11	N12
H10		+		
H11	+			
H17				–

18 [SLFZ]	O11	O12	N11	N12
H10	–			
H11		+		
H17	–			–

19 [SLFZ]	O11	O12	N11	N12
H10		+		
H11	+			
H17				–

S4. Hydrogen-bond connectivity tables for SLFZ molecules

- **Neutral [SLFZ]**: H*n*0, H*n*1, H*n*7 available as donors, O*n*1, O*n*2, N*n*1, N*n*2 available as acceptors.
- **Cation [SLFZ]$^{+}$**: H*n*0, H*n*1, H*n*X, H*n*7 available as donors, O*n*1, O*n*2, N*n*2 available as acceptors.
- **Anion [SLFZ]$^{-}$**: H*n*0, H*n*1 available as donors, O*n*1, O*n*2, N*n*1, N*n*2, N*n*3 available as acceptors.
- Symbols + and – indicate connections between molecules of the same or opposite handedness, respectively.

20 [SLFZ]	O11	O12	N11	N12	O21	O22	N21	N22
H10					–			
H11		+						
H17	–			–				
H20			–					
H21						+		
H27	+							

21 [SLFZ]	O11	O12	N11	N12
H10	–			
H11		+		
H17	–			–

22 [SLFZ]	O11	O12	N11	N12
H10	–			
H11		+		
H17	–			–

23 [SLFZ]	O11	O12	N11	N12	O21	O22	N21	N22
H10					–			
H11		+						
H17	–			–				
H20	–							
H21					+			
H27								

24 [SLFZ]	O11	O12	N11	N12
H10				
H11	–			
H17				–

25 [SLFZ]	O11	O12	N11	N12	O21	O22	N21	N22
H10		+						
H11					–			
H17					–			–
H20						+		
H21	–							
H27				–				

26 [SLFZ]	O11	O12	N11	N12
H10				
H11				
H17				+

27 [SLFZ]	O11	O12	N11	N12
H10				
H11				
H17				–

28 [SLFZ]	O11	O12	N11	N12
H10	–			
H11		+		
H17	–			–

29 [SLFZ]	O11	O12	N11	N12
H10	–			
H11		+		
H17	–			–

30 [SLFZ]	O11	O12	N11	N12
H10	–			
H11		+		
H17	–			–

S4. Hydrogen-bond connectivity tables for SLFZ molecules

- **Neutral [SLFZ]**: H*n*0, H*n*1, H*n*7 available as donors, O*n*1, O*n*2, N*n*1, N*n*2 available as acceptors.
- **Cation [SLFZ]$^{+}$**: H*n*0, H*n*1, H*n*X, H*n*7 available as donors, O*n*1, O*n*2, N*n*2 available as acceptors.
- **Anion [SLFZ]$^{-}$**: H*n*0, H*n*1 available as donors, O*n*1, O*n*2, N*n*1, N*n*2, N*n*3 available as acceptors.
- Symbols + and – indicate connections between molecules of the same or opposite handedness, respectively.

31 [SLFZ]	O11	O12	N11	N12
H10	–			
H11		+		
H17	–			–

32 [SLFZ]	O11	O12	N11	N12
H10	–			
H11		+		
H17	–			–

33 [SLFZ]	O11	O12	N11	N12
H10	–			
H11		+		
H17				–

34 [SLFZ]	O11	O12	N11	N12
H10	–			
H11		+		
H17				–

35 [SLFZ]	O11	O12	N11	N12	O21	O22	N21	N22
H10					–			
H11		+						
H17					–			–
H20	–							
H21						+		
H27	–			–				

36 [SLFZ]	O11	O12	N11	N12
H10	+	–		
H11				
H17	–			–

37 [SLFZ]	O11	O12	N11	N12
H10				
H11		+		
H17	–			–

38 [SLFZ]	O11	O12	N11	N12
H10	+			
H11				
H17				–

39 [SLFZ]	O11	O12	N11	N12	O21	O22	N21	N22
H10		+						
H11	–							
H17					+			+
H20					+			
H21						–		
H27	+			+				

40 [SLFZ]	O11	O12	N11	N12	O21	O22	N21	N22
H10		+						
H11	–							
H17								+
H20					+			
H21						–		
H27	+			+				

41 [SLFZ]	O11	O12	N11	N12	O21	O22	N21	N22
H10					–			
H11						+		
H17	–			–				
H20	–							
H21		+						
H27					–			–

S4. Hydrogen-bond connectivity tables for SLFZ molecules

- **Neutral [SLFZ]**: H*n*0, H*n*1, H*n*7 available as donors, O*n*1, O*n*2, N*n*1, N*n*2 available as acceptors.
- **Cation [SLFZ]$^{+}$**: H*n*0, H*n*1, H*n*X, H*n*7 available as donors, O*n*1, O*n*2, N*n*2 available as acceptors.
- **Anion [SLFZ]$^{-}$**: H*n*0, H*n*1 available as donors, O*n*1, O*n*2, N*n*1, N*n*2, N*n*3 available as acceptors.
- Symbols + and – indicate connections between molecules of the same or opposite handedness, respectively.

42 [SLFZ]	O11	O12	N11	N12
H10	+			
H11	+			
H17				

43 [SLFZ]	O11	O12	N11	N12
H10	+			
H11		+		
H17				

44 [SLFZ]	O11	O12	N11	N12
H10		+		
H11		–		
H17	–			–

45 [SLFZ]	O11	O12	N11	N12	O21	O22	N21	N22
H10								
H11								
H17								+
H20								
H21								
H27	+			+				

46 [SLFZ]	O11	O12	N11	N12
H10		+		
H11	+			
H17				–

47 [SLFZ]	O11	O12	N11	N12
H10		+		
H11	–			
H17				–

48 [SLFZ]	O11	O12	N11	N12
H10	+			+
H11	–			
H17				

49 [SLFZ]	O11	O12	N11	N12
H10		–		
H11		+		
H17				

50 [SLFZ]	O11	O12	N11	N12
H10	+			
H11		+		
H17				–

51 [SLFZ]	O11	O12	N11	N12
H10				
H11	+			
H17				

52 [SLFZ]	O11	O12	N11	N12
H10	+			
H11				
H17				–

53 [SLFZ]	O11	O12	N11	N12
H10				
H11				
H17				–

54 [SLFZ]	O11	O12	N11	N12
H10				
H11				
H17				–

S4. Hydrogen-bond connectivity tables for SLFZ molecules

- **Neutral [SLFZ]**: H*n*0, H*n*1, H*n*7 available as donors, O*n*1, O*n*2, N*n*1, N*n*2 available as acceptors.
- **Cation [SLFZ]$^{+}$**: H*n*0, H*n*1, H*n*X, H*n*7 available as donors, O*n*1, O*n*2, N*n*2 available as acceptors.
- **Anion [SLFZ]$^{-}$**: H*n*0, H*n*1 available as donors, O*n*1, O*n*2, N*n*1, N*n*2, N*n*3 available as acceptors.
- Symbols + and – indicate connections between molecules of the same or opposite handedness, respectively.

55 [SLFZ]	O11	O12	N11	N12
H10				
H11				
H17				

56 [SLFZ]	O11	O12	N11	N12
H10	+			
H11		–		
H17				

57 [SLFZ]	O11	O12	N11	N12
H10	+			
H11		–		
H17				

58 [SLFZ]	O11	O12	N11	N12
H10	+			
H11		–		
H17				

59 [SLFZ]	O11	O12	N11	N12
H10	+			
H11		–		
H17				

60 [SLFZ]$^{-}$	O11	O12	N11	N12	N13
H10		–			
H11	+			+	

61 [SLFZ]$^{-}$	O11	O12	N11	N12	N13
H10				+	
H11	–				

62 [SLFZ]$^{-}$	O11	O12	N11	N12	N13
H10		+			
H11	+			+	

63 [SLFZ]$^{-}$	O11	O12	N11	N12	N13
H10		+			
H11	+			+	

64 [SLFZ]$^{-}$	O11	O12	N11	N12	N13
H10	+				
H11	–				

65 [SLFZ]$^{-}$	O11	O12	N11	N12	N13	O21	O22	N21	N22	N23
H10		+								
H11						+				
H20							+			
H21	+									

66 [SLFZ]$^{-}$	O11	O12	N11	N12	N13
H10	–				
H11					+

67 [SLFZ]$^{-}$	O11	O12	N11	N12	N13	O21	O22	N21	N22	N23
H10	+									
H11							–			
H20						+				
H21	+									

68 [SLFZ]$^{-}$	O11	O12	N11	N12	N13
H10	–				
H11					–

S4. Hydrogen-bond connectivity tables for SLFZ molecules

- **Neutral [SLFZ]**: H*n*0, H*n*1, H*n*7 available as donors, O*n*1, O*n*2, N*n*1, N*n*2 available as acceptors.
- **Cation [SLFZ]$^{+}$**: H*n*0, H*n*1, H*n*X, H*n*7 available as donors, O*n*1, O*n*2, N*n*2 available as acceptors.
- **Anion [SLFZ]$^{-}$**: H*n*0, H*n*1 available as donors, O*n*1, O*n*2, N*n*1, N*n*2, N*n*3 available as acceptors.
- Symbols + and – indicate connections between molecules of the same or opposite handedness, respectively.

69 [SLFZ]$^{-}$	O11	O12	N11	N12	N13
H10	+				
H11		+			

70 [SLFZ]$^{-}$	O11	O12	N11	N12	N13
H10			–		
H11		+			

71 [SLFZ]$^{+}$	O11	O12	N12
H10			
H11			–
H1X			
H17			

72 [SLFZ]$^{-}$	O11	O12	N11	N12	N13
H10		+			
H11	+				

73 [SLFZ]$^{-}$	O11	O12	N11	N12	N13
H10	+				
H11	+	+			

74 [SLFZ]$^{-}$	O11	O12	N11	N12	N13
H10					
H11					

75 [SLFZ]$^{+}$	O11	O12	N12
H1X			
H10			+
H11	–		
H17			

76 [SLFZ]$^{+}$	O11	O12	N12
H1X			
H10			
H11			
H17		–	

77 [SLFZ]$^{-}$	O11	O12	N11	N12	N13
H10					
H11					–

78 [SLFZ]$^{-}$	O11	O12	N11	N12	N13
H10	+				
H11				–	

79 [SLFZ]$^{-}$	O11	O12	N11	N12	N13
H10					
H11					–

80 [SLFZ]$^{-}$	O11	O12	N11	N12	N13	O21	O22	N21	N22	N23
H10										
H11							+			
H20	–	–								
H21		+								

81 [SLFZ]$^{+}$	O11	O12	N12
H1X			
H10			
H11	–		–
H17			

82 [SLFZ]$^{-}$	O11	O12	N11	N12	N13
H10	+				
H11	–				

S4. Hydrogen-bond connectivity tables for SLFZ molecules

- **Neutral [SLFZ]**: H*n*0, H*n*1, H*n*7 available as donors, O*n*1, O*n*2, N*n*1, N*n*2 available as acceptors.
- **Cation [SLFZ]$^{+}$**: H*n*0, H*n*1, H*n*X, H*n*7 available as donors, O*n*1, O*n*2, N*n*2 available as acceptors.
- **Anion [SLFZ]$^{-}$**: H*n*0, H*n*1 available as donors, O*n*1, O*n*2, N*n*1, N*n*2, N*n*3 available as acceptors.
- Symbols + and – indicate connections between molecules of the same or opposite handedness, respectively.

83 [SLFZ]$^{+}$	O11	O12	N12	O21	O22	N22
H1X						
H10	+		+	+		
H11						
H17						
H2X						
H20				+		+
H21						
H27						

84 [SLFZ]$^{+}$	O11	O12	N12
H10	+		+
H11		+	
H1X			
H17			

85 [SLFZ]$^{+}$	O11	O12	N12	O21	O22	N22
H1X						
H10						
H11				–		–
H17						
H2X						
H20						
H21	–		–			
H27						

86 [SLFZ]$^{+}$	O11	O12	N12	O22	O21	N22
H1X						
H10	+		+			
H11						
H17						
H2X						
H20					+	+
H21						
H27						

87 [SLFZ]$^{+}$	O11	O12	N12
H10			
H11			–
H1X			
H17			

88 [SLFZ]$^{-}$	O11	O12	N11	N12	N13
H10	+				
H11		+			

89 [SLFZ] / [SLFZ]$^{-}$	O11	O12	N11	N12	O21	O22	N21	N22	O31	O32	N31	N32	N33	O41	O42	N41	N42	N43
H10	+			+														
H11					+													
H17																		+
H20					+			+										
H21	+																	
H27													+					
H30									+									
H31															+			
H40														+				
H41										+								

90 [SLFZ]$^{+}$	O11	O12	N12
H1X			
H10	+		+
H11	–		
H17			

S4. Hydrogen-bond connectivity tables for SLFZ molecules

- **Neutral [SLFZ]**: H*n*0, H*n*1, H*n*7 available as donors, O*n*1, O*n*2, N*n*1, N*n*2 available as acceptors.
- **Cation [SLFZ]$^{+}$**: H*n*0, H*n*1, H*n*X, H*n*7 available as donors, O*n*1, O*n*2, N*n*2 available as acceptors.
- **Anion [SLFZ]$^{-}$**: H*n*0, H*n*1 available as donors, O*n*1, O*n*2, N*n*1, N*n*2, N*n*3 available as acceptors.
- Symbols + and – indicate connections between molecules of the same or opposite handedness, respectively.

91 [SLFZ]	O11	O12	N11	N12	N13
H10					
H11					
H17					

92 [SLFZ]	O11	O12	N11	N12
H10	+			
H11	–			
H17				

93 [SLFZ]	O11	O12	N11	N12	O21	O22	N21	N22
H10								
H11		+						
H17					+			
H20				+	+			
H21	–							
H27								

94 [SLFZ]	O11	O12	N11	N12	O21	O22	N21	N22
H10					+			
H11		+						
H17								
H20					–			
H21						+		
H27								

95 [SLFZ]	O11	O12	N11	N12
H10				
H11		+		
H17	–			–

96 [SLFZ]$^{-}$	O11	O12	N11	N12	N13
H10	–				
H11					–

S5. Summary of SLFZ molecule connectivity and networks

- Centroids of SLFZ molecules are geometric (not mass-weighted), based on all atoms, including H.
- H-bond definition: (1) d(D···A) < (vdw(D) + vdw(A) + 0.50) Å; (2) d(H···A) < (vdw(H) + vdw(A)) Å; (3) D—H···A > 100°.
- **Net dimensions, point symbols and net symbols refer to connections between SFLZ molecules only**
- [+P] indicates that SLFZ also forms a hydrogen bond to/from a partner molecule

Polymorphs (Total: 5)

	Space group	Mol Index 1555_XX		Centroid X	Centroid Y	Centroid Z	Connected SLFZ molecules	Vertex Coord No.	Net Dim.	Point Symbol	Net Symbol
1p	P21/c	01	R	0.7561	0.7992	0.3688	[1555.02] [4564.01] [4565.01] [2645.01] [2655.01] [3776.01]	6	3D	$(4^4.5^3.6^7.7)$	[unknown]
		02	R	0.8066	0.2131	0.0481	[1555.01] [2745.02] [2755.02] [3755.02]	4		$(5^2.6^3.7)$	
2p	P21/n	01	R	0.7461	0.4793	0.6110	[1555.02] [2646.01] [2646.02] [1655.02] [2656.01] [2656.02]	6	2D	$(3^6.4^6.5^3)$ [one node type]	**hxl**
		02	S	0.2234	0.4496	0.8943	[1555.01] [1455.01] [2546.02] [2556.02] [2646.01] [2656.01]	6			
3p	P21/c	01	R	0.7272	0.2737	0.9869	[1555.02] [1545.02] [2646.02] [3767.02]	4	2D	$(4^4.6^2)$ [one node type]	**sql**
		02	R	0.7807	0.7848	0.7766	[1555.01] [1565.01] [2656.01] [3767.01]	4			
4p	P21/c	01	R	0.0515	0.7261	0.3686	[2555.01] [1455.01] [2545.01] [1655.01]	4	2D	$(4^4.6^2)$	**sql**
5p	P21/n	01	R	0.3948	0.7109	0.8431	[4465.01] [2546.01] [2556.01] [4564.01]	4	2D	$(4^4.6^2)$	**sql**

Polymorph 1, molecule 01 only (deleting molecule 02 from the structure)

1p	P21/c	01	R	0.7561	0.7992	0.3688	[4564.01] [4565.01] [2645.01] [2655.01] [3776.01]	5	3D	$(4^4.6^6)$	**nov**

Polymorph 01, molecule 02 only (deleting molecule 01 from the structure)

1p	P21/c	02	R	0.8066	0.2131	0.0481	[2745.02] [2755.02] [3755.02]	3	2D	(6^3)	**hcb**

S5. Summary of SLFZ molecule connectivity and networks

- Centroids of SLFZ molecules are geometric (not mass-weighted), based on all atoms, including H.
- H-bond definition: (1) d(D···A) < (vdw(D) + vdw(A) + 0.50) Å; (2) d(H···A) < (vdw(H) + vdw(A)) Å; (3) D—H···A > 100°.
- **Net dimensions, point symbols and net symbols refer to connections between SFLZ molecules only**
- [+P] indicates that SLFZ also forms a hydrogen bond to/from a partner molecule

Co-crystals (Total: 63)

	Space group	Mol Index 1555_XX		Centroid X	Centroid Y	Centroid Z	Connected SLFZ molecules	Vertex Coord No.	Net Dim.	Point Symbol	Net Symbol
1	P-1	01	R	0.4052	0.2079	0.8001	[1555.02] [1455.02] [2566.02] [2657.01] [2666.02]	5	2D	$(4^6{\cdot}6^4)$	[unknown]
		02	R	0.4312	0.7538	0.5957	[1555.01] [2566.01] [1655.01] [2666.01] [+P]	4 [+1]		(4^6)	
2	P21	01	R	0.6852	0.1458	0.6981	[1455.01] [2646.01] [1655.01] [2656.01] [+P] [+P]	4 [+2]	2D	$(4^4{\cdot}6^2)$	**sql**
3	Pc	01	R	0.5346	0.3843	0.4393	[1555.02] [1455.01] [2464.01] [1655.01] [2665.01] [+P]	5 [+1]	3D	$(4^6{\cdot}6^4)$ [one node type]	**bnn**
		02	R	0.4795	0.1493	0.8057	[1555.01] [2454.02] [1455.02] [1655.02] [2655.02]	5			
4	Cc	01	R	0.6061	0.8578	0.7320	[1555.02] [3455.02] [4465.02] [3556.02] [4565.02]	5	3D	$(4^4{\cdot}6^6)$ [one node type]	[unknown]
		02	R	0.6024	0.6359	0.2832	[1555.01] [3444.01] [4464.01] [3545.01] [4564.01]	5			
5	P21/c	01	R	0.2042	0.6423	0.0863	[1455.01] [1655.01] [3665.01] [+P]	3 [+1]	1D	$(4^2{\cdot}6)$	[ladder]
6	P21/c	01	R	0.1854	0.3984	0.2771	[4454.01] [1455.01] [3565.01] [1655.01] [4655.01]	5	3D	$(4^6{\cdot}6^4)$	**bnn**
7	P21/c	01	R	0.8685	0.8273	0.4721	[1455.01] [1655.01] [3776.01] [+P]	3 [+1]	1D	$(4^2{\cdot}6)$	[ladder]
8	P21/n	01	R	0.3361	0.1604	0.5456	[1455.01] [4455.01] [4554.01] [1655.01] [3656.01]	5	3D	$(4^6{\cdot}6^4)$	**bnn**
9	P21/n	01	R	0.6526	0.6524	0.8792	[2646.01] [2656.01] [3667.01] [+P]	3 [+1]	2D	(6^3)	**hcb**
10	P21/n	01	R	0.1213	0.3553	0.1873	[4555.01] [4454.01] [1455.01] [4455.01] [4554.01] [1655.01]	6	2D	$(3^6{\cdot}4^6{\cdot}5^3)$	**hxl**
11	P21/n	01	R	0.3702	0.1571	0.5487	[1455.01] [4455.01] [4554.01] [1655.01] [3656.01]	5	3D	$(4^6{\cdot}6^4)$	**bnn**
12	P21/n	01	R	0.3876	0.1590	0.5641	[1455.01] [4455.01] [4554.01] [1655.01] [3656.01]	5	3D	$(4^6{\cdot}6^4)$	**bnn**
13	P21/n	01	R	0.3634	0.1550	0.5687	[1455.01] [4455.01] [4554.01] [1655.01] [3656.01]	5	3D	$(4^6{\cdot}6^4)$	**bnn**
14	P21/n	01	R	0.3255	0.1523	0.5762	[1455.01] [4455.01] [4554.01] [1655.01] [3656.01]	5	3D	$(4^6{\cdot}6^4)$	**bnn**
15	P21/n	01	R	0.3184	0.8438	0.4569	[1455.01] [4464.01] [4565.01] [1655.01] [3676.01]	5	3D	$(4^6{\cdot}6^4)$	**bnn**
16	P21/n	01	R	0.3855	0.6541	0.1344	[2555.01] [2545.01] [2645.01] [2655.01] [3665.01]	5	3D	$(4^4{\cdot}6^6)$	**sqp**
17	P21/n	01	R	0.3876	0.6550	0.1362	[2555.01] [2545.01] [2645.01] [2655.01] [3665.01]	5	3D	$(4^4{\cdot}6^6)$	**sqp**

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Co-crystals (Total: 63)

	Space group	Mol Index 1555_XX		Centroid X	Centroid Y	Centroid Z	Connected SLFZ molecules	Vertex Coord No.	Net Dim.	Point Symbol	Net Symbol
18	P21/n	01	R	0.3874	0.1587	0.5516	[1455.01] [4455.01] [4554.01] [1655.01] [3656.01]	5	3D	$(4^6{\cdot}6^4)$	**bnn**
19	P21/n	01	R	0.3867	0.6251	0.1453	[2555.01] [2545.01] [2645.01] [2655.01] [3665.01]	5	3D	$(4^4{\cdot}6^6)$	**sqp**
20	P21/n	01	R	0.1197	0.6038	0.8759	[1555.02] [1455.01] [4465.02] [3567.01] [1655.01] [2656.02]	6	3D	$(4^9{\cdot}6^6)$	[unknown]
		02	S	0.5747	0.5141	0.6190	[1555.01] [1455.02] [4564.01] [2646.01] [1655.02]	5		$(4^7{\cdot}6^3)$	
21	P21/n	01	R	0.3882	0.1596	0.5423	[1455.01] [4455.01] [4554.01] [1655.01] [3656.01]	5	3D	$(4^6{\cdot}6^4)$	**bnn**
22	P21/n	01	R	0.3537	0.1597	0.5549	[1455.01] [4455.01] [4554.01] [1655.01] [3656.01]	5	3D	$(4^6{\cdot}6^4)$	**bnn**
23	P21/n	01	R	0.7981	0.1697	0.8802	[1555.02] [2646.01] [1655.02] [2656.01] [3757.01]	5	3D	$(4^4{\cdot}6^6)$	[unknown]
		02	S	0.3898	0.3029	0.8938	[1555.01] [1455.01] [2546.02] [2556.02] [+P]	4 [+1]		$(4^4{\cdot}6^2)$	
24	C2/c	01	R	0.6072	0.7331	0.4223	[4564.01] [4565.01] [3676.01] [+P] [+P]	3 [+2]	2D	(6^3)	**hcb**
25	P212121	01	R	0.4842	0.3850	0.3467	[1555.02] [3556.02] [3566.02] [4645.01] [4655.01]	5	3D	$(4^4{\cdot}6^6)$ [one node type]	**noz**
		02	S	0.5047	0.6287	0.6388	[1555.01] [3456.01] [3466.01] [4646.02] [4656.02]	5			
26	Aba2	01	R	0.1441	0.8820	0.2637	[2575.01] [+P] [+P]	1 [+2]	0D	—	—
27	Pbca	01	R	0.3756	0.7021	0.4303	[5666.01] [+P] [+P] [+P]	1 [+3]	0D	—	—
28	P21/n	01	R	0.4128	0.1558	0.5665	[1455.01] [4455.01] [4554.01] [1655.01] [3656.01]	5	3D	$(4^6{\cdot}6^4)$	**bnn**
29	P21/n	01	R	0.3707	0.1535	0.5756	[1455.01] [4455.01] [4554.01] [1655.01] [3656.01]	5	3D	$(4^6{\cdot}6^4)$	**bnn**
30	P21/n	01	R	0.3704	0.1594	0.5702	[1455.01] [4455.01] [4554.01] [1655.01] [3656.01]	5	3D	$(4^6{\cdot}6^4)$	**bnn**
31	P21/n	01	R	0.3966	0.1554	0.5637	[1455.01] [4455.01] [4554.01] [1655.01] [3656.01]	5	3D	$(4^6{\cdot}6^4)$	**bnn**
32	P21/n	01	R	0.3469	0.1567	0.5811	[1455.01] [4455.01] [4554.01] [1655.01] [3656.01]	5	3D	$(4^6{\cdot}6^4)$	**bnn**
33	P21/n	01	R	0.3531	0.1654	0.5476	[1455.01] [4455.01] [4554.01] [1655.01] [3656.01]	5	3D	$(4^6{\cdot}6^4)$	**bnn**
34	P21/n	01	R	0.3637	0.1746	0.5251	[1455.01] [4455.01] [4554.01] [1655.01] [3656.01]	5	3D	$(4^6{\cdot}6^4)$	**bnn**

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Co-crystals (Total: 63)

	Space group	Mol Index 1555_XX		Centroid X	Centroid Y	Centroid Z	Connected SLFZ molecules	Vertex Coord No.	Net Dim.	Point Symbol	Net Symbol
35	P21 SLFZ only = P21/n	01	R	0.3655	0.1559	0.5717	[1555.02] [1455.01] [2556.02] [1655.01] [2655.02]	5	3D	$(4^6{\cdot}6^4)$ [one node type]	**bnn**
		02	S	0.6447	-0.1547	0.4314	[1555.01] [1455.02] [2546.01] [2645.01] [1655.02]	5			
36	P21/c	01	R	0.6925	0.6284	0.4158	[1455.01] [4464.01] [4665.01] [1655.01] [3766.01] [+P]	5 [+1]	3D	$(4^6{\cdot}6^4)$	**bnn**
37	P21/c	01	R	0.8280	0.8256	0.4327	[1455.01] [1655.01] [3776.01] [+P]	3 [+1]	1D	$(4^2{\cdot}6)$	[ladder]
38	P21/c	01	R	0.2645	0.4202	0.1526	[1455.01] [1655.01] [3665.01] [+P]	3 [+1]	1D	$(4^2{\cdot}6)$	[ladder]
39	Pbca	01	R	0.5601	0.7022	0.8035	[7555.01] [1555.02] [7545.01] [4646.01] [4656.01]	5	3D	$(4^4{\cdot}6^6)$	[unknown]
		02	R	0.5580	0.6687	0.9519	[1555.01] [3467.02] [3567.02] [7645.02] [7655.02]	5		$(4^4{\cdot}6^5{\cdot}8)$	
40	Pbca	01	R	0.5556	0.7023	0.8025	[7555.01] [1555.02] [7545.01] [4646.01] [4656.01]	5	3D	$(4^4{\cdot}6^6)$	[unknown]
		02	R	0.5708	0.6715	0.9516	[1555.01] [3467.02] [3567.02] [7645.02] [7655.02]	5		$(4^4{\cdot}6^5{\cdot}8)$	
41	P21/c SLFZ only = P21/n in smaller cell	01	R	0.9055	0.1596	0.9527	[1555.02] [4555.02] [4655.02] [1656.02] [3757.01]	5	3D	$(4^6{\cdot}6^4)$ [one node type]	**bnn**
		02	R	0.4295	0.1585	0.4659	[1555.01] [1454.01] [4454.01] [4554.01] [3656.02]	5			
42	P21/c	01	R	0.5137	0.3011	0.3895	[1455.01] [2645.01] [1655.01] [2655.01] [+P]	4 [+1]	2D	$(4^4{\cdot}6^2)$	**sql**
43	P43 Inverted wrt ADEDIX02 (P41)	01	R	0.2244	0.8556	0.1884	[1545.01] [1565.01] [4565.01] [2654.01] [+P]	4 [+1]	3D	$(6^5{\cdot}8)$	**cds**
44	P21/c	01	R	0.8035	0.5458	0.6326	[4564.01] [4565.01] [3666.01] [2746.01] [2756.01]	5	3D	$(4^4{\cdot}6^6)$	**nov**
45	P-1	01	R	0.7707	0.6571	0.2511	[1555.02] [+P] [+P]	1 [+2]	0D	—	—
		02	R	0.2871	0.7528	0.3388	[1555.01] [+P] [+P]	1 [+2]			
46	P21/n	01	R	0.1344	0.2002	0.3872	[2555.01] [2445.01] [2455.01] [2545.01] [3556.01]	5	3D	$(4^4{\cdot}6^6)$	**sqp**
47	Pbca	01	R	0.4932	0.3827	0.3521	[4645.01] [7645.01] [4655.01] [7655.01] [5666.01]	5	3D	$(4^4{\cdot}6^6)$	**noz**
48	P21/n	01	R	0.0524	0.8231	0.4178	[1455.01] [4465.01] [4564.01] [1655.01] [+P]	4 [+1]	2D	$(4^4{\cdot}6^2)$	**sql**

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Co-crystals (Total: 63)

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49	P21/c	01	R	0.7426	0.1862	0.1835	[4555.01] [4554.01] [2645.01] [2655.01] [+P] [+P] [+P]	4 [+3]	2D	$(4^4{\cdot}6^2)$	**sql**
50	P21/n	01	R	0.2737	0.9065	0.1164	[2555.01] [1455.01] [2545.01] [1655.01] [3675.01] [+P]	5 [+1]	3D	$(4^6{\cdot}6^4)$	**bnn**
51	P21/n	01	R	0.9268	0.6037	0.7431	[2746.01] [2756.01] [+P] [+P]	2 [+2]	1D	—	[zig-zag]
52	P21/c	01	R	0.2590	0.4039	0.6327	[1455.01] [1655.01] [3666.01] [+P]	3 [+1]	1D	$(4^2{\cdot}6)$	[ladder]
53	P21/c	01	R	0.1959	0.1322	0.4407	[3656.01] [+P] [+P]	1 [+2]	0D	—	—
54	P21/c	01	R	0.2188	0.4017	0.1777	[3565.01] [+P] [+P]	1 [+2]	0D	—	—
55	P-1	01	R	0.2252	0.1192	1.0460	[+P] [+P]	0 [+2]	—	—	—
56	P21/n	01	R	0.5898	0.3682	0.6642	[1455.01] [4455.01] [4554.01] [1655.01] [+P] [+P] [+P]	4 [+3]	2D	$(4^4{\cdot}6^2)$	**sql**
57	P21/n	01	R	0.6026	0.3693	0.6602	[1455.01] [4455.01] [4554.01] [1655.01] [+P] [+P]	4 [+2]	2D	$(4^4{\cdot}6^2)$	**sql**
58	P21/n	01	R	0.6003	0.3683	0.6603	[1455.01] [4455.01] [4554.01] [1655.01] [+P] [+P]	4 [+2]	2D	$(4^4{\cdot}6^2)$	**sql**
59	P21/n	01	R	0.5986	0.3691	0.6506	[1455.01] [4455.01] [4554.01] [1655.01] [+P] [+P]	4 [+2]	2D	$(4^4{\cdot}6^2)$	**sql**
92	P-1	01	R	0.5055	0.6673	0.7648	[1455.01] [1655.01] [2677.01] [+P] [+P]	3 [+2]	1D	$(4^2{\cdot}6)$	[ladder]
93	P-1	01	R	0.5343	0.8212	0.3987	[1555.02] [1455.01] [1655.01] [1655.02] [2666.02] [+P]	5 [+1]	1D	$(3^3{\cdot}4^6{\cdot}5)$ [one node type]	[tube]
		02	R	0.4240	0.6658	0.8358	[1555.01] [1455.01] [1455.02] [1655.02] [2666.01] [+P] [+P]	5 [+2]			
94	P21/n	01	R	0.3916	0.3956	0.9306	[1555.02] [1455.01] [1655.01] [+P]	3 [+1]	2D	$(4^2{\cdot}6)$	[unknown]
		02	R	1.0047	0.3005	0.3354	[1555.01] [1455.02] [4455.02] [4554.02] [1655.02] [+P]	5 [+1]		$(4^6{\cdot}6^4)$	
95	Pbca	01	R	0.6045	0.4041	0.5889	[1545.01] [1565.01] [5666.01] [+P] [+P]	3 [+2]	1D	$(4^2{\cdot}6)$	[ladder]

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Salts (Total: 30)

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60	Pna21	01	R	0.6445	0.8381	0.5772	[3644.01] [3655.01] [2674.01] [2675.01] [+P]	4 [+1]	3D	$(6^5{\cdot}8)$	**dmp**
61	Pna21	01	R	0.3997	0.3469	0.3684	[3545.01] [3554.01] [2664.01] [2665.01] [+P]	4 [+1]	3D	$(6^5{\cdot}8)$	**dmp**
62	P212121	01	R	0.2044	0.2572	0.3162	[4555.01] [4545.01] [4645.01] [4655.01] [+P] [+P]	4 [+2]	2D	$(4^4{\cdot}6^2)$	**sql**
63	P212121	01	R	0.2001	0.2691	0.3180	[4555.01] [4545.01] [4645.01] [4655.01] [+P] [+P]	4 [+2]	2D	$(4^4{\cdot}6^2)$	**sql**
64	Fdd2	01	R	0.3074	0.4368	0.5624	[12555.01] [4454.01] [1554.01] [1556.01] [+P] [+P]	4 [+2]	2D	$(4^4{\cdot}6^2)$	**sql**
65	P21	01	R	0.6668	0.8420	0.4395	[1555.02] [1565.02] [2646.01] [2656.01] [+P] [+P]	4 [+2]	2D	$(4^4{\cdot}6^2)$ [one node type]	**sql**
		02	R	0.3113	0.3231	0.0805	[1555.01] [1545.01] [2645.02] [2655.02] [+P] [+P]	4 [+2]			
66	P21/c	01	R	0.1193	0.8625	0.7004	[4565.01] [4564.01] [2546.01] [2556.01] [+P] [+P] [+P]	4 [+3]	2D	$(4^4{\cdot}6^2)$	**sql**
67	P21/c	01	R	0.0914	0.4719	0.6692	[1555.02] [1545.01] [1565.01] [4565.02] [+P] [+P]	4 [+2]	2D	$(4^4{\cdot}6^2)$ [one node type]	**sql**
		02	S	0.4023	0.9766	0.5681	[1555.01] [1545.02] [1565.02] [4564.01] [+P] [+P]	4 [+2]			
68	C2/c	01	R	0.5389	0.7346	0.5353	[7666.01] [3676.01] [+P] [+P] [+P]	2 [+3]	1D	—	[zig-zag]
69	P212121	01	R	0.5452	0.5642	0.3903	[1455.01] [4645.01] [1655.01] [4655.01] [+P] [+P]	4 [+2]	2D	$(4^4{\cdot}6^2)$	**sql**
70	P21/c	01	R	0.8360	0.5287	0.5691	[1545.01] [1565.01] [3776.01] [+P] [+P] [+P]	3 [+3]	1D	$(4^2{\cdot}6)$	[ladder]
71	C2/c	01	R	0.3837	0.4982	0.5869	[3666.01] [+ N—H···F]	1 [+ N—H···F]	0D	—	—
72	P212121	01	R	0.1911	0.2876	0.3449	[4555.01] [4545.01] [4645.01] [4655.01] [+P]	4 [+1]	2D	$(4^4{\cdot}6^2)$	**sql**
73	P212121	01	R	0.5234	0.5544	0.3960	[1455.01] [4645.01] [1655.01] [4655.01] [+P]	4 [+1]	2D	$(4^4{\cdot}6^2)$	**sql**
74	P-1	01	R	0.3129	0.3338	0.1730	[+P] [+P] [+P] [+P] [+P]	0 [+5]	—	—	—
75	P21/c	01	R	–0.1295	0.6115	0.1502	[1455.01] [4464.01] [1655.01] [4665.01] [+P] [+P] [+P]	4 [+3]	2D	$(4^4{\cdot}6^2)$	**sql**
76	P21/c	01	R	0.0511	0.7303	0.1311	[4564.01] [4565.01] [+P] [+P] [+P]	2 [+3]	1D	—	[linear]
77	P21/c	01	R	0.7578	0.5305	0.6129	[3666.01] [+P] [+P] [+P]	1 [+3]	0D	—	—

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78	P21/c	01	R	0.2107	0.6386	0.3662	[2555.01] [2545.01] [4564.01] [4565.01] [+P]	4 [+1]	2D	$(4^4{\cdot}6^2)$	**sql**
79	P21/c	01	R	0.7460	0.5316	0.6074	[3666.01] [+P] [+P] [+P] [+P]	1 [+4]	0D	—	—
80	P21/c	01	R	0.2218	0.2435	0.5565	[1555.02] [1545.01] [3666.02] [+P] [+P] [+P]	3 [+3]	1D	$(4^2{\cdot}6)$ [one node type]	[ladder]
		02	R	0.2934	0.7196	0.7023	[1555.01] [1565.01] [3666.01] [+P] [+P]	3 [+2]			
81	P21/c	01	R	0.7962	0.2607	0.4827	[4555.01] [4554.01] [+P] [+P] [+P] [+P]	2 [+4]	1D	—	[linear]
82	P21/n	01	R	0.3678	0.3201	0.5715	[4555.01] [4454.01] [2546.01] [2556.01] [+P] [+P]	4 [+2]	2D	$(4^4{\cdot}6^2)$	**sql**
83	P21/n	01	R	0.8503	0.4097	0.5663	[1545.01] [1565.01] [1555.02] [+P] [+P] [+P] [+P]	3 [+4]	1D	$(4^2{\cdot}6)$ [one node type]	[ladder]
		02	R	0.5779	0.5844	0.3003	[1545.02] [1565.02] [1555.01] [+P] [+P] [+P] [+P]	3 [+4]			
84	P21/c	01	R	0.4597	0.3989	0.1873	[1455.01] [2645.01] [1655.01] [2655.01] [+ N—H···F]	4 [+ N—H···F]	2D	$(4^4{\cdot}6^2)$	**sql**
85	Cc [from C2/c, Z' = 1]	01	R	0.3828	0.4878	0.5856	[1555.02] [+P] [+P] [+P] [+P]	1 [+4]	0D	—	—
		02	S	0.6165	0.5066	0.4159	[1555.01] [+P] [+P] [+P] [+P]	1 [+4]			
86	Pna21 [from Pbcn, Z' = 1]	01	R	0.5558	0.7324	0.3473	[1545.01] [1565.01] [+P] [+P] [+P]	2 [+3]	1D	—	[linear]
		02	R	0.9459	0.7372	0.6523	[1545.02] [1565.02] [+P] [+P] [+P]	2 [+3]	1D	—	[linear]
87	P21/n	01	R	0.0975	0.8760	0.4234	[3576.01] [+P] [+P] [+P] [+P]	1 [+4]	0D	—	—
88	P21/c	01	R	0.2056	0.8747	0.7195	[2646.01] [2656.01] [+P] [+P] [+P]	2 [+3]	1D	—	[zig-zag]
96	P-1	01	R	0.7521	0.7747	0.9334	[2767.01] [2777.01] [+P] [+P] [+P] [+P] [+P]	2 [+5]	1D	—	[zig-zag]

S5. Summary of SLFZ molecule connectivity and networks

- Centroids of SLFZ molecules are geometric (not mass-weighted), based on all atoms, including H.
- H-bond definition: (1) d(D···A) < (vdw(D) + vdw(A) + 0.50) Å; (2) d(H···A) < (vdw(H) + vdw(A)) Å; (3) D—H···A > 100°.
- **Net dimensions, point symbols and net symbols refer to connections between SFLZ molecules only**
- [+P] indicates that SLFZ also forms a hydrogen bond to/from a partner molecule

Other (Total: 3)

	Space group	Mol Index 1555_XX		Centroid X	Centroid Y	Centroid Z	Connected molecules	Vertex Coord No.	Net Dim.	Point Symbol	Net Symbol
89	P21 [SLFZ approximates P21/a, Z′ = 2]	01	R	0.5547	0.4991	0.5301	[1555.02] [1555.04] [2646.01] [1655.02] [2656.01]	5	3D	$(4^6 \cdot 6^4)$ [one node type]	**bnn**
		02	S	0.0632	0.2789	0.5285	[1555.01] [1555.03] [1455.01] [2546.02] [2556.02]	5			
		03	R	0.4160	0.4781	0.9631	[1555.02] [1555.04] [1455.04] [2647.03] [2657.03]	5			
		04	S	0.9187	0.2890	0.9658	[1555.01] [1555.03] [1655.03] [2747.04] [2757.04]	5			
90	P-1	01	R	0.0106	0.7458	0.4458	[1455.01] [2566.01] [1655.01] [+P] [+P] [+P]	3 [+3]	1D	$(4^2 \cdot 6)$	[ladder]
91	P21/n	01	R	0.2041	0.1962	0.2205	[+P] [+P] [+ N—H···Cl]	0 [+2] [+ N—H···Cl]	—	—	—

S6. Node shape comparisons

The node shape comparisons are based on nets formed between SLFZ molecules only. The points in the node shape comprise the geometrical centroids of the SLFZ molecule, with connections as listed in S5. For crystal structures containing more than one independent SLFZ molecule, a separate node is extracted for each molecule. These are appended with "_01", "_02", etc. Comparisons are limited to nodes comprising a minimum of 4 points (*i.e.* 3-coordinate SLFZ) and the maximum number of points is 7 (i.e. 6-coordinate SLFZ). The full results set is a 103 vs 103 array of "Continuous Shape Measure" (CShM) values, provided as a separate Excel worksheet. Sub-matrices are also provided for specific comparison of all nodes having the same coordination number (3–6). The full matrix also contains comparisons of nodes with different coordination numbers, as described in the main text.

Comparison of two node shapes is made as described in the main text. For each node shape, the points are converted to Cartesian axes and moved so that the centroid of the entire shape (not necessarily coinciding with the central point of the node shape) is at the origin of the coordinate system. The total RMS distance of all points from the origin is calculated, and the shape is scaled by dividing each origin-point distance by that value. Hence, each node shape is scaled so that the RMS distance of all of its points from the origin is unity. Scaled node shapes are then overlaid using the Kabsch algorithm (best rigid-body overlay), and the CShM value is calculated as described in the main text. Since the Kabsch algorithm requires the points in the two shapes to be mapped, it is necessary to consider all possible mappings to identify the best overlay of two node shapes. Since the number of points in the node shapes is small, all permutations were systematically tested and the best one was kept.

The core calculation method (including the specified scaling procedure) was validated by comparing to the following webpage:

Tuvi-Arad, G. Alon and D. Avnir, CoSyM, http://csm.ouproj.org.il.

This page provides a facility to compare to standard shapes such as the regular tetrahedron, trigonal bipyramid, octahedron, etc. Dummy node shapes with regular geometry were constructed for testing, and it was confirmed that comparison of the scaled node shapes to the standard models produced CShM values matching those produced by the webpage.