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Supporting information for article:

Room temperature ferroelasticity and unusual sequence of phase transitions in the crystal of (N2H5)3[CdCl5]

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Table S1 Crystallographic data for $(N_2H_5)_3[CdCl_5]$ crystal (structure solution in the phase I in *Pc* space group). Molecular mass: M = 388.83 gmol^{-1}.

Crystal data	
Crystal system,	Monoclinic,
space group	*Pc*
Phase, temperature (K)	**I**, 280(2) K
***a* (Å)**	22.646(5)
***b* (Å)**	7.4535(18)
***c* (Å)**	28.464(7)
***α* (°)**	
***β* (°)**	90.03(3)
γ (°)	
***V* (Å^3)**	4804(2)
Z	16
***μ* (mm^{-1})**	2.90
***F*(000)**	3040
Crystal size (mm)	1.05 × 0.07 × 0.05
Crystal colour	colourless
Crystal form	needle
Θ range (°)	3.66 – 30.24
h, k, l range	-29 ≤ h ≤ 30 -10 ≤ k ≤ 10 -39 ≤ l ≤ 38
Measured reflections	45255
Independent reflections	23424
Observed refl. (*I*>2*δ*(*I*))	14631
Transmission max/min	0.315/0.875
R_{int}	0.025
Refinement on	F^2
Data/restraints/parameters	23424/22/841
***R*[*F*^{2} > 2σ(*F*^{2})]**	0.057
***wR*(*F*^{2})**	0.151
GooF = *S*	1.08
$\Delta\rho_{max}/\Delta\rho_{min}$ (ēÅ^{-3})	1.06 − 1.96

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S1. Crystal structure description of $(N_2H_5)_3[CdCl_5]$ in Pc space group (phase I).

In the solution in the *Pc* space group the $(N_2H_5)_3[CdCl_5]$ crystal can be described as follows. The studied crystal is composed of $N_2H_5^+$ ions and 1D chains of a zig-zag coordination polymer $([CdCl_5]^{3-})_n$ analogously to the crystal of $(N_2H_5)_3[CdBr_5]$ (Czapla *et al*., 2019). In the structure four kinds of chains extending along the crystallographic *b* axis can be distinguished that are built up from $\{CdCl_5\}^{3-}$ units bridged by Cl atoms forming anionic substructure. In the asymmetric part of the unit cell four dimeric fragments of the formula $\{Cd_2Cl_{10}\}^{6-}$ created by the $\{CdCl_5\}^{3-}$ units with bridging chlorine atoms as well as 24 hydrazinium cations can be observed. Each of the dimeric species is comprised of two $\{CdCl_5\}^{3-}$ units joined each other by a common vertex, *viz*., bridging Cl atoms denoted as Cl6, Cl16, Cl26 and Cl36 (Fig. S1). The coordination sphere of each Cd atom adopts geometry of a slightly distorted octahedron whereby the sixth coordination place is occupied by a bridging Cl atom.

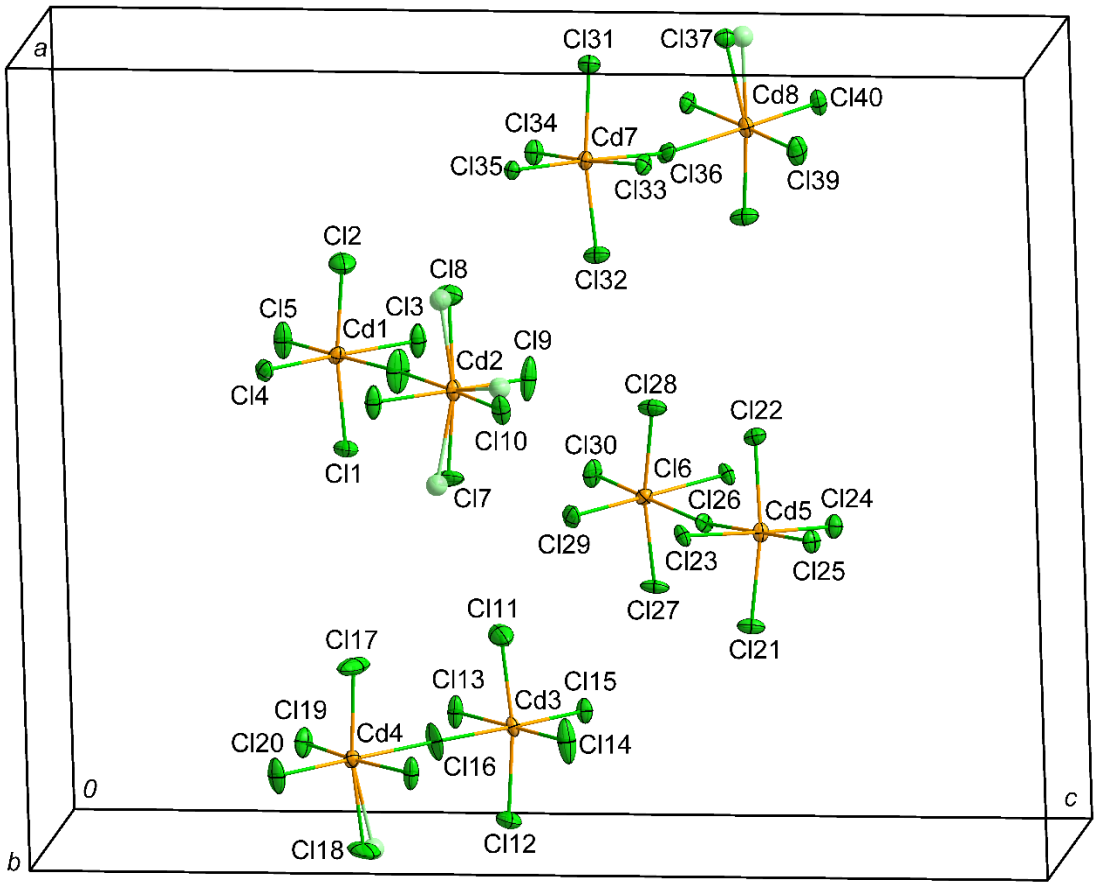


Fig. S1. Crystal structure and the atom-numbering scheme for the dimeric fragments of the formula$\{Cd_2Cl_{10}\}^{6-}$ at room temperature (phase I; *Pc* space group). Hydrazine cations were omitted for clarity. The minor occupancy components of the disordered Cl atoms were marked as balls of arbitrary radii of light green colour.

Values of the geometry parameters, such as Cd–$Cl_{terminal}$, Cd–$Cl_{bridging}$ distances and Cd–Cl–Cd angles are comparable to those in another polymeric cadmium halide structures that are comprised of of a) vertex-sharing octahedral units (see for example: Chapuis *et al*., 1975; Chapuis, 1977; Lu *et al*., 2013; Sun *et al*., 2017; Wei, 1987; Willett, 1977; Yu *et al*., 2009); b) face-sharing octahedral units (see for example: Ma *et al*., 2006; Morosin, 1972; Peral *et al*., 2000). In the studied structure Cd–$Cl_{terminal}$ bond lengths range from 2.519(5) to 2.651(5) Å, Cd–$Cl_{bridging}$ bond lengths equal 2.642(5) – 2.742(4) Å and Cd–Cl–Cd angles range between 168.0(2) and 179.2(2)° (Table 2). Within each $\{Cd_2Cl_{10}\}^{6-}$ unit two Cd atoms and seven Cl atoms are placed in approximately the same plane, namely the nearly planar $\{Cl_3Cd–Cl–CdCl_3\}$ fragments of the chains can be distinguished (Fig. 2). The distinct deviation from the planarity is visible in the case of bridging: Cl26 (0.224(4) Å), Cl36 (0.259(4) Å) and terminal: Cl29 (0.249(3) Å), Cl30 (0.254(3) Å), Cl39 (0.300(4) Å) and Cl40 (0.300(3) Å) atoms. Due to the fact that four dimeric species of the formula $\{Cd_2Cl_{10}\}^{6-}$ are observed in the asymmetric part of the unit cell, four kinds of polymeric chains of the $([CdCl_5]^{3-})_n$ can be considered. In the crystal some terminal Cl atoms (*viz*. Cl7, Cl8, Cl10, Cl18 and Cl37 atoms) as well as some hydrazinium ions are disordered over two positions.

The crystal exhibits architecture stabilized by the network of numerous N–H···Cl and N–H···N hydrogen bonds. In the structure layers and pseudo-layers approximately parallel to the crystallographic (100) plane can be distinguished (Fig. S2). The anionic chains composed of $\{Cd_2Cl_{10}\}^{6-}$ dimeric species of the Cd1 and Cd2 atoms form a layer-like arrangement along with $N_2H_5^+$ ions that contain nitrogen atoms labelled N25, N26, N33 and N34 as follows. Within the pseudo-layer polymeric chains interact with cations via the N25–H25A···Cl9 hydrogen bonds, while the cations itself are involved in the N26–H26C···N34^{ii} and N33–H33A···N25 hydrogen bonds forming a chain (symmetry codes: (ii) = x, y+1, z).

The chains built up from dimeric units of the Cd3 and Cd4 atoms and $N_2H_5^+$ ions consisting of N atoms denoted as N7, N8, N11 and N12 are also organized in a pseudo-layer approximately parallel to the (100) plane, where the only N7–H7A···Cl20^{vii} hydrogen bond is responsible for the interaction between the polymeric chain and cations ((vii) = x, -y+$^3/_2$, z+$^1/_2$). The hydrazinium ions are also involved in the N7–H7B···N12, N11–H11B···N8^{vi} and N12–H12A···N7 hydrogen bonds ((vi) = x, y–1, z) resulting in the formation a chain, analogously to the layer described before.

The chains comprising of the dimeric species of the Cd5 and Cd6 and hydrazinium ions disordered over two positions (viz., N atoms are labelled N43 – N46 and N51 – N54) are arranged in a layer created by the N43–H43A···Cl24^{v}, N44–H44A···Cl30^{ii} and N53–H53B···Cl25^{v} and N54–H54A···Cl30 ((v) = x, –y+$^1/_2$, z–$^1/_2$) hydrogen bonds.

A mutual arrangement of the dimeric species involving Cd7 and Cd8 atoms and cations of nitrogen atoms labelled N35, N36, N47 – N50 (disordered cation) can be described as a layer-like arrangement stabilized by the interactions: N36–H36B···Cl35, N50–H50A···Cl34, N36–H36C···N48, N36–H36C···N50 and N48–H48B···N36.

Between adjacent layers and pseudo-layers hydrazinium ions can be observed, which interact with layers and pseudo-layers mainly via hydrogen bonds of the N–H···Cl but also N–H···N kind.

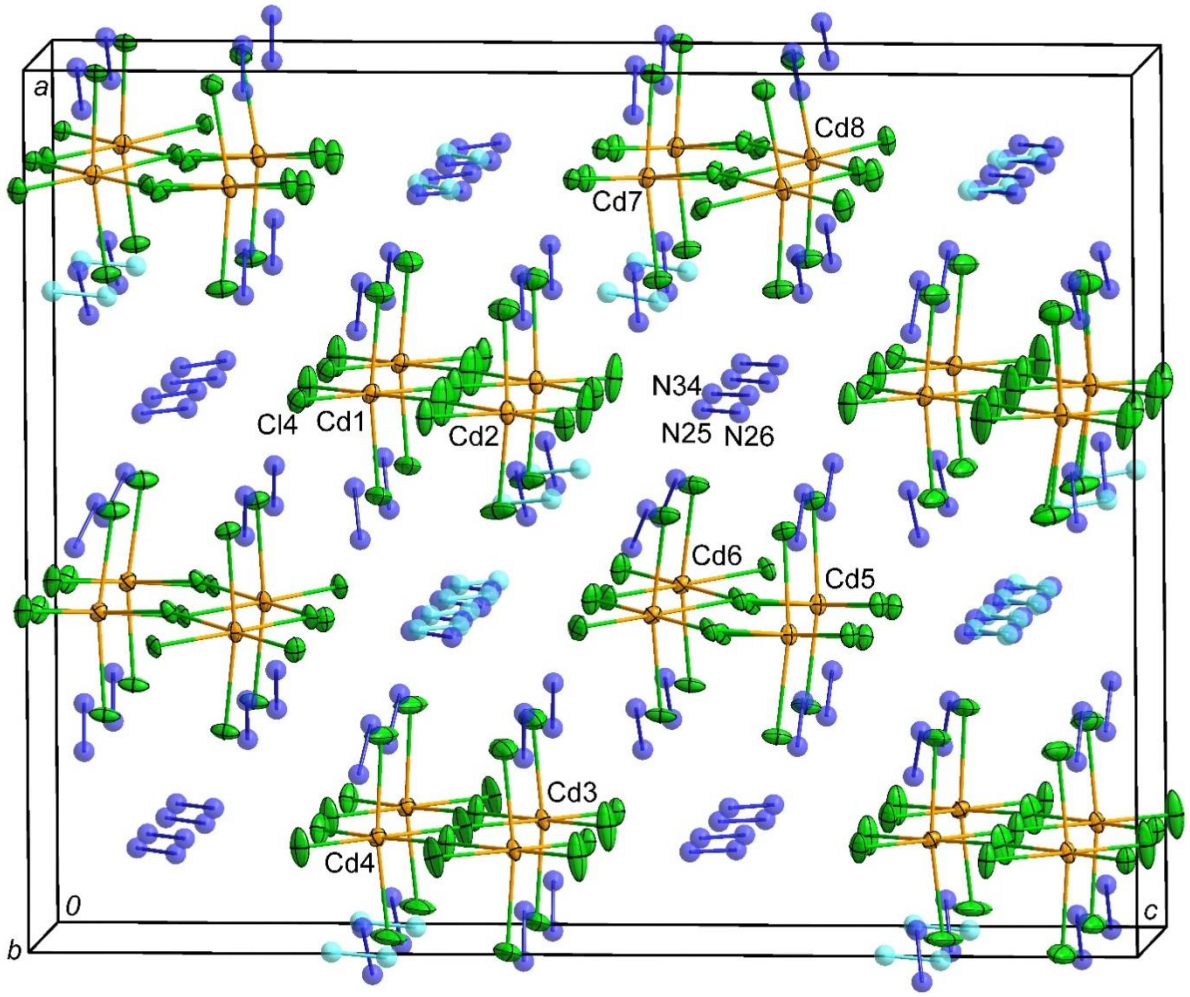


Fig. S2. Packing diagram for the crystal at room temperature (phase I) showing a layered architecture viewed down the *b* axis. Displacement ellipsoids of Cd and Cl atoms are shown at the 50% probability level. Due to the disorder of some hydrazinium cations N atoms are depicted as balls of arbitrary radii. H atoms were omitted for clarity.

S2. *Procedure of selection of the space group for the phase I* ***(model in space group P2₁/c)***

The determined lattice cell parameters do not clearly indicate that the crystal belongs to a monoclinic system (the monoclinic angle is 90.03° close to 90.0°). However, observations of the domain structure under a polarizing microscope as well as X-ray studies at 340 K above the phase transition proved that at room temperature the crystal belongs to a monoclinic system.

The polarized microscopy observations indicate that the crystal exhibits a typical ferroelastic type domain structure at room temperature and thermal studies reveal that it undergoes a phase transition at about 327 K. The crystal structure solution at 340 K was found in the space group *Pnma* (R = 0.035). Since the crystal is a ferroelastic at room temperature and exhibits orthorhombic symmetry at 340 K (above the phase transition), the as-grown crystal can be assigned to a monoclinic system at room temperature.

The analysis of the Ewald sphere suggests the primitive cell *P*. The symmetry of the diffraction pattern on the zero and first layers along the three crystallographic directions, i.e. on the layers: *0kl,1kl, h0l, h1l, hk0* and *hk1* was analyzed. The diffraction pattern reveals the symmetry *mm* on the layers: *0kl, 1kl, h0l, h1l, hk0* and *hk1*.

Subsequently, the systematic absences were analyzed, which could indicate the existence of screw axes and glide planes.The following reflection conditions were observed:

h0l: *h* = 2*n*, *h00*: *h* = 2*n*, *00l* = 2*n* and *0k0*: *k* = 2*n*. These observations allowed the crystal to be assigned to the group *P*2₁/*c*.

S3. ***Refinement***

Phase I (model in space group *P*2₁/*c*)

After the refinement on the difference Fourier map the additional maxima close to N atoms were observed, which were interpreted as an effect of partially disordered hydrazinium cations and introduced mainly with restraint for the N—N distance of 1.43 Å by means of DFIX command. The disorder of $(N_2H_5)^+$ ions was modelled over two or three positions using PART commands. The disorder of cations modelled over three positions was also handled using SUMP instructions in order to restrain the sum of occupation factors to unity. Moreover, the additional maxima located in the difference Fourier map appeared; these peaks were observed close to Cl1, Cl2, Cl12 and Cl18 atoms and introduced as Cl01, Cl02, Cl21 and Cl81. The disorder of all Cl atoms was modelled over two positions with occupancies of: 0.85(2) (Cl1) and 0.15(2) (Cl01); 0.85(2) (Cl2) and 0.15(2) (Cl02); 0.80(5) (Cl12) and 0.20(5) (Cl21); 0.69(5) (Cl18) and 0.31(5) (Cl81). The minor-occupancy components were refined isotropically.

Phase I (model in space group *Pc*)

The preliminary atomic coordinates of Cd and Cl atoms were taken from the structure solution of the phase I in the *P*2₁/*c*. In the solution the instructions LATT -1 and 'MOVE 1 1 1 -1' and L.S. egualed 0

(0 cycles full-matrix least-squares) were introduced. After the refinement new atomic coordinates were obtained and the symmetry operation of –x, ½+y, ½–z was replaced by symmetry operation: x, ½–y, ½+z. Afterwards, the coordinates for Cd and Cl atoms from the solution in the $P2_1/c$ were also introduced to the new solution. Upon refinement, the Fourier differential map revealed high maxima close to Cl atoms at a distance of about 3.0 – 3.4 Å, which were interpreted as nitrogen atoms and introduced to the structure solution. After this procedure on Fourier differential map additional maxima close to N atoms appeared that indicated partially disordered hydrazinium cations and were introduced mainly with restraint for the N—N distance of 1.45 Å using DFIX command. The disorder of $N_2H_5^+$ ions was modelled over two positions using PART commands. Afterwards, the additional maxima located in the difference Fourier map appeared, which were close to Cl7, Cl8, Cl10, Cl18 and Cl37 atoms and introduced as Cl70, Cl80, Cl01, Cl81 and Cl73. The disorder of all Cl atoms was modelled over two positions with occupancies of: 0.67(2) (Cl7 and Cl8) and 0.33(2) (Cl70 and Cl80); 0.88(5) (Cl10) and 0.12(5) (Cl01); 0.68(5) (Cl18) and 0.32(5) (Cl81); 0.76(6) (Cl37) and 0.24(6) (Cl73). The minor-occupancy components were refined isotropically.

Phase II

In the phase II after the refinement of the positions of all atoms derived from anionic chain and cations, on the difference Fourier map the additional maxima appeared. These peaks were located close to nitrogen atoms and were interpreted as a disorder of hydrazinium cations as follows. The disorder of one kind of $(N_2H_5)^+$ ions was modelled over two positions, with occupancies of 0.614(12) (N1, N2) and 0.386(12) (N3, N4) using PART commands. The disorder of second kind of cations was modelled over three positions using PART and SUMP instructions as well as restraint for the N—N distance of 1.43 Å, using DFIX command and refined with s.o.f. equalled 0.420(11) (N5, N6), 0.404(11) (N7, N8) and 0.176(14) (N9, N10).

Phase III

The studied crystal in the phase III (structures at 321 and 324 K) is isomorphous with this in the phase II. Therefore the preliminary atomic coordinates of Cd, Cl and N atoms in the phases III (at 321 and 324 K) were taken from the structure solution of the phase II. The disorder of hydrazinium cations is observed in the III phase, which is the same and handled in analogous way as in the phase II. Additionally, in the phase III (at 321 K) a disorder of terminal Cl1 and Cl5 atoms is observed, while in the structure at 324 K Cl1 atom is disordered over two positions.

Phase IV

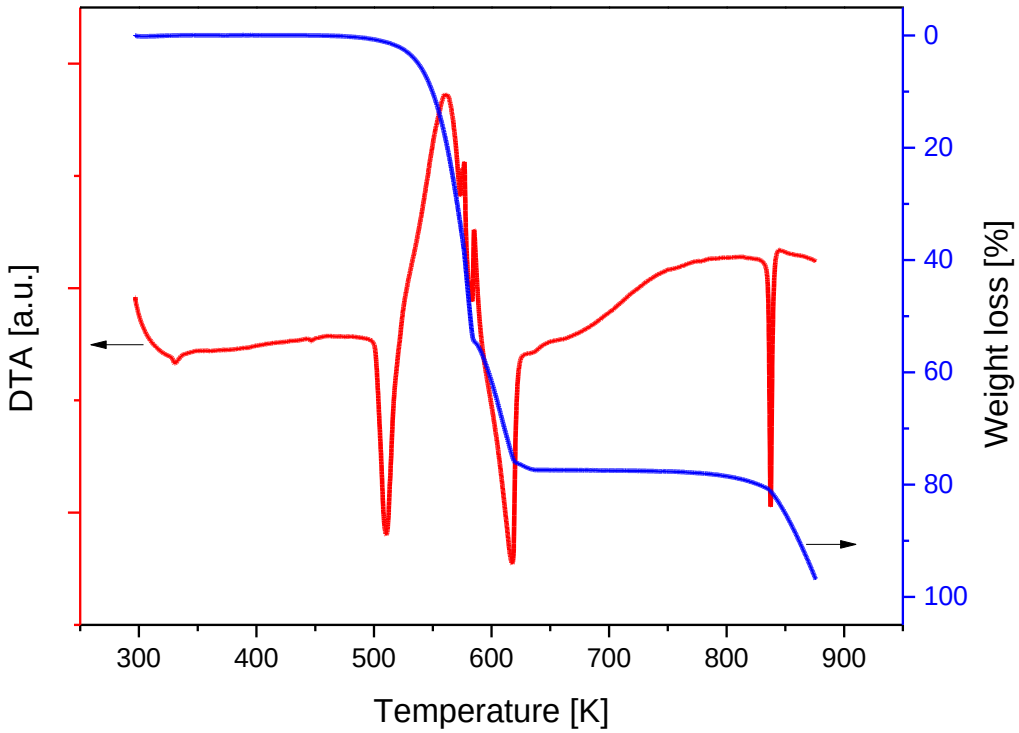
After the refinement on the difference Fourier map additional maxima close to Cd1 and Cd3 atoms as well as some N atoms were found that indicated the disorder. The disorder of Cd1 and Cd3 atoms was modelled over three positions, with occupancies of 0.980(7), 0.010(3) and 0.010(3). The minor-

occupancy components were refined isotropically. The peaks close to N atoms were introduced using DFIX distance restraint (viz. N—N bonds were restrained to 1.43 Å) and modelled over two positions using PART instructions.

Phase V

In structure solution of the phase V the disorder of hydrazinium cations was observed, analogously to the solutions in the phases 1 – IV. The final difference Fourier map revealed additional maxima close to N atoms, which were introduced as N3, N4, N7 and N8. The disorder was modelled using PART -1 command to exclude bonds to symmetry generated nitrogen atoms. Finally, the created model showed that the cations are disordered over two positions. Moreover, the restraint for the N—N distance of 1.430(5) Å was applied by means of DFIX command.

S4. DTA and DTG analysis



The DTG curve proves chemical and thermal stability of the studied crystal up to about 470 K. Above this temperature apparent decomposition is observed. The DTA scan reveals peak of the phase transition at about 325 K that corresponds to the first heating anomaly observed in the DSC experiment.

S5. ***Geometry of hydrogen bonds in phases I – V.***

Geometry of hydrogen bonds in phase I (model for $P2_1/c$ space group)

Symmetry codes: \$1 x, -y+1/2, z+1/2; \$2 -x, -y+1, -z+1; \$3 x, -y+3/2, z+1/2; \$4 x, y-1, z; \$5 -x+1, y-1/2, -z+3/2; \$6 -x, -y+2, -z+1; \$7 x, y+1, z; \$8 -x+1, y+1/2, -z+3/2; \$9 -x+1, -y+1, -z+1; \$10 -x+1, -y+2, -z+1; \$11 -x, -y, -z+1; \$12 -x, y-1/2, -z+1/2; \$13 -x, y+1/2, -z+1/2.

D-H	H···A	D···A	<(DHA)	
0.89	2.68	3.455(6)	146.1	N1-H1A...Cl8
0.89	2.69	3.279(6)	124.2	N1-H1A...Cl10
0.89	3.09	3.648(7)	122.8	N1-H1B...Cl16_\$1
0.89	2.67	3.485(6)	152.9	N1-H1B...Cl17_\$1
0.89	2.71	3.362(8)	131.3	N2-H2A...Cl16_\$2
0.89	2.75	3.341(8)	124.6	N2-H2A...Cl16_\$1
0.89	2.95	3.640(17)	135.3	N2-H2A...Cl18_\$2
0.89	2.76	3.432(15)	133.6	N2-H2A...Cl81_\$2
0.89	2.53	3.334(7)	151.4	N2-H2B...Cl19_\$1
0.89	2.78	3.296(7)	118.6	N2-H2B...Cl20_\$3
0.89	2.36	3.195(7)	157.1	N2-H2C...Cl17_\$3
0.89	2.35	3.205(7)	160.3	N3-H3A...Cl11
0.89	2.55	3.344(7)	148.5	N3-H3B...Cl14_\$4
0.89	2.76	3.302(7)	120.9	N3-H3B...Cl15
0.89	2.94	3.610(15)	133.3	N3-H3C...Cl12_\$5
0.89	2.76	3.408(17)	131.1	N3-H3C...Cl21_\$5
0.89	2.72	3.358(7)	129.8	N3-H3C...Cl13
0.89	2.71	3.326(7)	127.6	N3-H3C...Cl13_\$5
0.89	2.66	3.469(6)	150.9	N4-H4A...Cl11_\$4
0.89	3.07	3.641(6)	123.3	N4-H4A...Cl13_\$5
0.89	2.66	3.441(6)	146.5	N4-H4B...Cl7
0.89	2.71	3.284(6)	123.4	N4-H4B...Cl10
0.89	2.46	3.305(6)	159.3	N5-H5A...Cl17_\$3
0.89	2.47	3.317(6)	158.7	N5-H5B...Cl11
0.89	2.32	3.135(9)	151.6	N6-H6A...N17_e
0.89	2.34	3.16(3)	154.9	N6-H6A...N19_f
0.89	2.00	2.880(7)	171.8	N6-H6B...N7
0.89	2.30	3.123(9)	154.4	N6-H6C...N10_a
0.89	2.29	3.11(3)	152.7	N6-H6C...N12_b
0.89	2.11	2.974(8)	164.2	N7-H7A...N1
0.89	2.11	2.978(8)	163.9	N7-H7B...N4
0.89	2.59	3.424(6)	155.7	N8-H8A...Cl12_\$5
0.89	2.68	3.47(2)	148.4	N8-H8A...Cl21_\$5
0.89	2.10	2.985(7)	175.7	N8-H8B...N5_\$4
0.89	2.58	3.419(7)	157.2	N8-H8C...Cl18_\$2
0.89	2.65	3.447(17)	149.9	N8-H8C...Cl81_\$2
0.89	2.40	3.278(11)	167.6	N9_a-H9A_a...Cl18_\$2
0.89	2.18	3.04(3)	162.7	N9_a-H9A_a...Cl81_\$2
0.89	2.80	3.430(13)	129.2	N9_a-H9B_a...Cl16_\$2
0.89	2.68	3.406(12)	139.4	N9_a-H9B_a...Cl16_\$3
0.89	2.72	3.242(10)	118.6	N9_a-H9C_a...Cl19_\$2

0.89	2.57	3.307(9)	141.2	N9_a-H9C_a...Cl20_$6
0.89	2.99	3.705(10)	138.9	N10_a-H10A_a...Cl2_$3
0.89	2.61	3.307(9)	136.1	N10_a-H10A_a...Cl4_$3
0.89	2.75	3.482(11)	140.7	N10_a-H10B_a...Cl18_$6
0.89	2.99	3.75(4)	145.3	N10_a-H10B_a...Cl81_$6
0.89	2.81	3.46(4)	130.5	N11_b-H11A_b...Cl5_$3
0.89	2.77	3.43(4)	132.5	N11_b-H11A_b...Cl18_$2
0.89	2.65	3.26(5)	126.9	N11_b-H11A_b...Cl81_$2
0.89	2.66	3.38(4)	138.4	N11_b-H11B_b...Cl19_$2
0.89	2.65	3.31(4)	131.7	N11_b-H11B_b...Cl20_$6
0.89	2.96	3.77(4)	152.1	N11_b-H11C_b...Cl4_$3
0.89	2.63	3.37(3)	141.7	N12_b-H12B_b...Cl16_$3
0.89	2.38	3.268(14)	172.6	N13_c-H13A_c...Cl7_$7
0.89	2.83	3.36(2)	119.6	N13_c-H13B_c...Cl01
0.89	2.77	3.485(13)	138.8	N13_c-H13C_c...Cl11
0.89	2.59	3.165(12)	123.1	N13_c-H13C_c...Cl14
0.89	2.73	3.498(17)	145.5	N14_c-H14A_c...Cl7
0.89	2.76	3.192(14)	111.0	N14_c-H14A_c...Cl9
0.89	2.48	3.350(16)	166.0	N14_c-H14B_c...Cl10_$7
0.89	2.39	3.196(15)	150.0	N15_d-H15A_d...Cl7
0.89	2.76	3.489(13)	140.1	N15_d-H15B_d...Cl11
0.89	2.68	3.348(13)	132.4	N15_d-H15B_d...Cl15
0.89	2.78	3.54(2)	144.6	N16_d-H16A_d...Cl9
0.89	2.65	3.157(16)	117.5	N16_d-H16A_d...Cl10_$7
0.89	3.02	3.551(18)	120.3	N16_d-H16A_d...Cl11
0.89	3.06	3.649(18)	125.2	N16_d-H16B_d...Cl1
0.89	2.82	3.37(3)	121.2	N16_d-H16B_d...Cl01
0.89	2.68	3.307(16)	128.2	N16_d-H16B_d...Cl3
0.89	2.74	3.462(19)	139.0	N16_d-H16B_d...Cl6
0.89	2.69	3.56(2)	166.5	N16_d-H16C_d...Cl7_$7
0.89	3.01	3.708(10)	137.0	N17_e-H17A_e...Cl1_$3
0.89	2.60	3.298(10)	136.2	N17_e-H17A_e...Cl4_$3
0.89	2.80	3.508(12)	137.6	N17_e-H17B_e...Cl12_$8
0.89	3.08	3.82(5)	142.2	N17_e-H17B_e...Cl21_$8
0.89	2.76	3.434(12)	133.2	N18_e-H18A_e...Cl13
0.89	2.76	3.433(12)	133.6	N18_e-H18A_e...Cl13_$8
0.89	2.40	3.249(11)	160.6	N18_e-H18B_e...Cl12_$5
0.89	2.15	2.98(4)	154.6	N18_e-H18B_e...Cl21_$5
0.89	2.74	3.237(9)	116.5	N18_e-H18C_e...Cl14_$5
0.89	2.53	3.305(9)	146.2	N18_e-H18C_e...Cl15_$8
0.89	2.70	3.12(3)	110.0	N19_f-H19B_f...Cl11
0.89	2.97	3.58(3)	127.1	N19_f-H19B_f...Cl12_$5
0.89	2.63	3.27(6)	128.9	N19_f-H19B_f...Cl21_$5
0.89	2.68	3.16(3)	115.6	N19_f-H19B_f...N6
0.89	2.52	3.36(3)	159.2	N19_f-H19C_f...Cl13_$8
0.89	2.45	3.30(4)	159.9	N20_f-H20A_f...Cl15_$8
0.89	2.76	3.44(4)	134.4	N20_f-H20B_f...Cl12_$5
0.89	2.60	3.23(6)	129.1	N20_f-H20B_f...Cl21_$5
0.89	2.70	3.40(4)	135.7	N20_f-H20B_f...Cl14_$5

0.89	3.07	3.74(4)	133.9	N20_f-H20C_f...Cl4_$3
0.89	2.73	3.48(4)	143.6	N20_f-H20C_f...Cl5_$3
0.89	2.92	3.637(16)	138.5	N21_g-H21A_g...Cl2
0.89	2.79	3.47(3)	134.1	N21_g-H21A_g...Cl02
0.89	2.90	3.457(16)	121.9	N21_g-H21A_g...Cl3
0.89	2.48	3.123(19)	129.4	N21_g-H21A_g...Cl6
0.89	2.82	3.236(17)	110.4	N21_g-H21B_g...Cl9
0.89	2.49	3.340(16)	161.1	N21_g-H21B_g...Cl10_$7
0.89	2.66	3.49(2)	155.0	N21_g-H21C_g...Cl8
0.89	2.84	3.517(13)	133.8	N22_g-H22A_g...Cl17_$3
0.89	2.65	3.197(13)	121.1	N22_g-H22A_g...Cl19_$3
0.89	2.40	3.286(14)	170.9	N22_g-H22B_g...Cl8_$7
0.89	2.33	3.157(17)	153.5	N23_h-H23A_h...Cl8
0.89	2.73	3.487(15)	144.1	N23_h-H23B_h...Cl17_$3
0.89	2.74	3.368(15)	128.8	N23_h-H23B_h...Cl20_$3
0.89	2.81	3.59(3)	146.3	N24_h-H24A_h...Cl8_$7
0.89	2.87	3.61(3)	141.1	N24_h-H24B_h...Cl2
0.89	2.62	3.37(4)	141.9	N24_h-H24B_h...Cl02
0.89	2.58	3.25(3)	132.5	N24_h-H24B_h...Cl3
0.89	2.99	3.45(3)	114.2	N24_h-H24B_h...Cl6
0.89	2.72	3.59(3)	164.8	N24_h-H24C_h...Cl9
0.89	2.85	3.61(2)	144.7	N25_i-H25A_i...Cl12
0.89	3.13	3.90(3)	146.2	N25_i-H25A_i...Cl21
0.89	2.58	3.044(18)	113.5	N25_i-H25A_i...Cl15
0.89	2.37	3.25(2)	168.4	N25_i-H25B_i...Cl1_$9
0.89	2.89	3.76(3)	163.9	N25_i-H25B_i...Cl01_$9
0.89	2.75	3.56(2)	151.2	N26_i-H26A_i...Cl1_$10
0.89	2.36	3.11(3)	142.2	N26_i-H26A_i...Cl01_$10
0.89	2.73	3.179(18)	112.9	N26_i-H26A_i...Cl5_$10
0.89	2.49	3.068(18)	123.3	N26_i-H26B_i...Cl3_$10
0.89	2.95	3.43(2)	115.8	N26_i-H26B_i...Cl6_$9
0.89	2.89	3.67(2)	147.9	N26_i-H26B_i...Cl7_$9
0.89	2.45	3.29(2)	158.9	N26_i-H26C_i...Cl4_$9
0.89	2.70	3.38(2)	133.7	N27_j-H27A_j...Cl14
0.89	3.00	3.72(2)	139.1	N27_j-H27A_j...Cl15
0.89	2.94	3.66(2)	138.8	N27_j-H27B_j...Cl7_$9
0.89	2.31	3.18(2)	168.4	N27_j-H27C_j...Cl1_$10
0.89	1.86	2.73(3)	162.0	N27_j-H27C_j...Cl01_$10
0.89	2.62	3.49(3)	164.8	N28_j-H28A_j...Cl5_$10
0.89	2.55	3.33(3)	147.0	N28_j-H28B_j...Cl6_$9
0.89	2.44	3.25(3)	151.6	N29_k-H29A_k...Cl5_$10
0.89	2.44	2.89(3)	111.2	N29_k-H29B_k...Cl12
0.89	3.06	3.60(4)	120.3	N29_k-H29B_k...Cl15
0.89	2.85	3.30(4)	112.4	N29_k-H29C_k...Cl01_$10
0.89	2.94	3.75(4)	152.9	N29_k-H29C_k...Cl14
0.89	2.71	3.57(4)	164.6	N30_k-H30A_k...Cl1_$9
0.89	2.87	3.71(4)	156.8	N30_k-H30B_k...Cl3_$10
0.89	2.58	3.11(3)	118.9	N30_k-H30B_k...Cl7_$9
0.89	2.78	3.53(5)	142.9	N31_l-H31A_l...N31_$2l

0.89	2.51	3.217(13)	137.1	N31_l-H31B_l...Cl8
0.89	2.82	3.42(2)	125.8	N31_l-H31B_l...Cl19_$1
0.89	2.38	3.258(14)	169.2	N31_l-H31C_l...Cl2_$2
0.89	2.37	3.23(2)	164.4	N31_l-H31C_l...Cl02_$2
0.89	2.75	3.54(5)	148.0	N32_l-H32A_l...N32_$11l
0.89	2.87	3.50(2)	129.3	N32_l-H32B_l...Cl20_$12
0.89	1.82	2.45(5)	126.3	N33_m-H33A_m...N33_$2m
0.89	2.86	3.42(3)	121.9	N33_m-H33B_m...Cl20_$12
0.89	2.77	3.41(3)	129.7	N34_m-H34A_m...Cl8
0.89	1.92	2.52(5)	123.1	N34_m-H34B_m...N34_$11m
0.89	2.92	3.46(3)	121.0	N34_m-H34C_m...Cl2_$2
0.89	2.77	3.27(3)	117.1	N34_m-H34C_m...Cl02_$2
0.89	2.57	3.29(3)	138.9	N34_m-H34C_m...Cl19_$1
0.89	2.52	3.09(2)	122.7	N35_n-H35A_n...Cl3_$4
0.89	2.79	3.50(2)	137.9	N35_n-H35A_n...Cl6
0.89	2.49	3.28(2)	147.0	N35_n-H35B_n...Cl4
0.89	2.61	3.11(2)	116.2	N35_n-H35B_n...Cl5_$4
0.89	2.69	3.57(3)	170.0	N35_n-H35C_n...Cl2_$4
0.89	2.25	3.11(3)	162.5	N35_n-H35C_n...Cl02_$4
0.89	2.97	3.58(3)	127.2	N36_n-H36B_n...Cl18_$12
0.89	2.58	3.026(18)	111.8	N36_n-H36B_n...Cl20_$12
0.89	2.41	3.23(2)	153.2	N36_n-H36C_n...Cl2
0.89	2.95	3.75(3)	150.3	N36_n-H36C_n...Cl02
0.89	2.47	3.22(2)	143.3	N37_o-H37A_o...Cl2_$4
0.89	1.95	2.74(3)	147.9	N37_o-H37A_o...Cl02_$4
0.89	3.04	3.71(2)	133.7	N37_o-H37B_o...Cl18_$12
0.89	2.62	3.374(18)	142.8	N37_o-H37B_o...Cl19_$12
0.89	2.55	3.37(3)	152.5	N38_o-H38A_o...Cl6
0.89	2.83	3.45(3)	127.4	N38_o-H38B_o...Cl2
0.89	2.61	3.46(3)	162.1	N38_o-H38C_o...Cl5_$4
0.89	2.98	3.45(5)	115.3	N39_p-H39A_p...Cl02_$4
0.89	2.93	3.74(4)	152.7	N39_p-H39A_p...Cl3_$4
0.89	2.63	3.14(3)	117.8	N39_p-H39A_p...Cl8
0.89	2.71	3.54(4)	154.4	N39_p-H39B_p...Cl2
0.89	3.05	3.65(3)	126.7	N39_p-H39B_p...Cl6
0.89	2.76	3.34(3)	123.8	N40_p-H40A_p...Cl4
0.89	2.88	3.75(3)	165.6	N40_p-H40B_p...Cl19_$12
0.89	2.38	3.22(3)	157.4	N40_p-H40C_p...Cl5_$4
0.89	2.55	3.270(17)	138.3	N41_q-H41A_q...Cl7_$9
0.89	2.75	3.265(17)	118.2	N41_q-H41A_q...Cl14_$10
0.89	2.35	3.154(17)	150.6	N41_q-H41B_q...Cl1
0.89	2.26	3.11(2)	159.5	N41_q-H41B_q...Cl01
0.89	2.65	3.251(15)	125.5	N41_q-H41C_q...Cl15_$9
0.89	2.95	3.410(16)	114.2	N42_q-H42A_q...Cl15
0.89	2.78	3.382(15)	125.9	N42_q-H42B_q...Cl14
0.89	2.83	3.27(3)	112.4	N43_r-H43C_r...Cl15
0.89	2.70	3.33(3)	129.0	N44_r-H44A_r...Cl14
0.89	3.04	3.90(3)	164.3	N44_r-H44B_r...Cl14_$10
0.89	2.95	3.38(3)	111.4	N45_s-H45A_s...Cl1

0.89	2.66	3.19(3)	119.7	N45_s-H45A_s...Cl01
0.89	2.32	3.20(3)	175.1	N45_s-H45B_s...Cl14_$10
0.89	2.73	3.41(3)	134.2	N46_s-H46A_s...Cl7_$9
0.89	2.74	3.22(3)	115.7	N46_s-H46A_s...Cl15_$9
0.89	2.67	3.38(3)	137.3	N46_s-H46B_s...Cl1
0.89	2.79	3.41(3)	127.3	N46_s-H46B_s...Cl01
0.89	1.96	2.44(5)	111.7	N46_s-H46C_s...N46_$9s

Geometry of hydrogen bonds in phase II

Symmetry codes: $1 x+1/2, -y+3/2, z+1/2; $2 -x+1, -y+3/2, z+1/2; $3 -x+3/2, y-1/2, -z+3/2; $4 -x+3/2, y+1/2, -z+3/2; $5 x, y-1, z; $6 x, y-1/2, -z+1/2; $7 -x+3/2, y-1/2, -z+1/2; $8 -x+1, -y+1, -z+1; $9 -x+3/2, y, z; $10 -x+3/2, y+1/2, -z+1/2.

D-H	H···A	D···A	<(DHA)	
0.91	2.62	3.434(5)	149.1	N1_a-H1A_a...Cl1_$1
0.91	2.55	3.434(5)	163.1	N1_a-H1B_a...Cl1_$2
0.91	2.05	2.819(13)	141.2	N1_a-H1C_a...N2_$3a
0.91	1.99	2.819(13)	150.3	N2_a-H2A_a...N1_$4a
0.91	3.06	3.545(8)	115.4	N2_a-H2B_a...Cl4
0.91	2.08	2.876(16)	146.1	N3_b-H3A_b...N4_$4b
0.91	2.40	3.289(4)	164.8	N3_b-H3B_b...Cl1_$2
0.91	2.63	3.289(4)	129.7	N3_b-H3C_b...Cl1_$1
0.91	2.75	3.427(11)	132.5	N3_b-H3C_b...Cl5_$3
0.91	2.15	2.876(16)	136.1	N4_b-H4A_b...N3_$3b
0.91	2.62	3.442(10)	151.4	N5_c-H5A_c...Cl4
0.91	2.66	3.167(10)	116.1	N5_c-H5A_c...Cl5_$5
0.91	2.70	3.594(9)	169.1	N5_c-H5B_c...Cl1_$5
0.91	2.95	3.633(11)	132.8	N5_c-H5C_c...Cl1_$6
0.91	2.69	3.398(10)	135.4	N5_c-H5C_c...Cl6
0.91	2.66	3.226(8)	121.1	N5_c-H5C_c...Cl6_$7
0.91	2.37	3.279(11)	175.5	N6_c-H6A_c...Cl1
0.91	2.73	3.509(9)	143.8	N6_c-H6B_c...Cl1_$8
0.91	2.72	3.258(9)	119.2	N6_c-H6B_c...Cl4_$8
0.91	2.75	3.483(16)	138.2	N7_d-H7A_d...Cl5_$5
0.91	3.03	3.71(2)	132.9	N7_d-H7A_d...Cl6_$7
0.91	2.83	3.440(12)	125.4	N7_d-H7B_d...Cl1
0.91	2.65	3.287(19)	127.4	N7_d-H7B_d...Cl6
0.91	2.80	3.52(2)	137.5	N7_d-H7C_d...Cl1_$8
0.91	2.69	3.143(14)	112.1	N7_d-H7C_d...Cl4
0.91	2.93	3.622(11)	134.0	N8_d-H8A_d...Cl1_$8
0.91	2.56	3.301(11)	139.3	N8_d-H8A_d...Cl5_$8
0.91	2.49	3.268(10)	143.9	N8_d-H8B_d...Cl1_$5
0.91	2.71	3.41(3)	134.7	N9_e-H9A_e...Cl4
0.91	2.55	3.15(3)	123.4	N9_e-H9A_e...Cl5_$5
0.91	2.35	2.91(3)	119.8	N9_e-H9B_e...Cl1_$8
0.91	2.91	3.64(3)	138.7	N9_e-H9C_e...Cl1_$5
0.91	2.50	2.96(2)	112.2	N10_e-H10A_e...Cl1_$6
0.91	2.74	3.60(3)	159.8	N10_e-H10A_e...Cl6_$7
0.91	2.97	3.81(3)	154.1	N10_e-H10C_e...Cl1

Geometry of hydrogen bonds in phase III (321 K)

Symmetry codes: $1 x+1/2, -y+3/2, z+1/2; $2 x, y-1/2, -z+3/2; $3 -x+1, -y+3/2, z+1/2; $4 -x+3/2, y-1/2, - $5 -x+3/2, y+1/2, -z+3/2; $6 -x+3/2, y, z; $7 x, y-1, z; $8 x, y-1/2, -z+1/2; $9 -x+3/2, y-1/2, -z+1/2; $10 -x+1, -y+1, -z+1; $11 x-1/2, -y+1, -z+1; $12 -x+3/2, y-1, z; $13 -x+3/2, y+1/2, -z+1/2.

D-H	H···A	D···A	<(DHA)	
0.91	2.61	3.420(5)	149.3	N1_a-H1A_a...Cl1_$1
0.91	2.59	3.384(9)	146.2	N1_a-H1A_a...Cl11_$1
0.91	2.87	3.33(3)	113.1	N1_a-H1A_a...Cl51_$2
0.91	2.55	3.420(5)	159.9	N1_a-H1B_a...Cl1_$3
0.91	2.49	3.384(9)	169.5	N1_a-H1B_a...Cl11_$3
0.91	2.08	2.842(16)	141.2	N1_a-H1C_a...N2_$4a
0.91	2.02	2.842(16)	150.6	N2_a-H2A_a...N1_$5a
0.91	3.03	3.517(8)	115.5	N2_a-H2B_a...Cl4
0.91	2.82	3.254(17)	110.4	N2_a-H2B_a...Cl51_$6
0.91	2.03	2.815(16)	142.9	N3_b-H3A_b...N4_$5b
0.91	2.35	3.238(5)	164.5	N3_b-H3B_b...Cl1_$3
0.91	2.48	3.321(9)	154.2	N3_b-H3B_b...Cl11_$3
0.91	2.63	3.238(5)	124.9	N3_b-H3C_b...Cl1_$1
0.91	2.67	3.321(9)	129.7	N3_b-H3C_b...Cl11_$1
0.91	2.69	3.396(12)	134.7	N3_b-H3C_b...Cl5_$4
0.91	2.96	3.56(4)	125.0	N3_b-H3C_b...Cl51_$4
0.91	2.78	3.56(4)	144.4	N3_b-H3C_b...Cl51_$2
0.91	2.86	3.291(14)	110.3	N4_b-H4A_b...Cl4
0.91	1.91	2.815(16)	172.2	N4_b-H4A_b...N3_$4b
0.91	2.59	3.419(16)	151.6	N5_c-H5A_c...Cl4
0.91	2.66	3.148(15)	114.7	N5_c-H5A_c...Cl5_$7
0.91	3.07	3.56(3)	116.0	N5_c-H5A_c...Cl51_$7
0.91	2.80	3.691(18)	166.9	N5_c-H5B_c...Cl1_$7
0.91	2.35	3.242(18)	166.4	N5_c-H5B_c...Cl11_$7
0.91	2.98	3.63(2)	130.5	N5_c-H5C_c...Cl1_$8
0.91	3.01	3.68(2)	132.2	N5_c-H5C_c...Cl11_$8
0.91	2.71	3.418(17)	134.9	N5_c-H5C_c...Cl6
0.91	2.62	3.220(14)	124.1	N5_c-H5C_c...Cl6_$9
0.91	2.22	3.132(15)	176.6	N6_c-H6A_c...Cl1
0.91	2.67	3.581(16)	175.8	N6_c-H6A_c...Cl11
0.91	2.85	3.570(14)	137.5	N6_c-H6B_c...Cl1_$10
0.91	2.89	3.631(16)	139.2	N6_c-H6B_c...Cl11_$10
0.91	2.71	3.284(13)	122.0	N6_c-H6B_c...Cl4_$10
0.91	2.72	3.42(3)	134.9	N6_c-H6B_c...Cl51_$11
0.91	2.79	3.50(4)	136.5	N7_d-H7A_d...Cl5_$7
0.91	2.66	3.29(4)	127.8	N7_d-H7A_d...Cl51_$12
0.91	2.97	3.64(4)	131.8	N7_d-H7A_d...Cl6_$9
0.91	2.77	3.33(3)	121.2	N7_d-H7B_d...Cl1
0.91	3.06	3.68(4)	127.0	N7_d-H7B_d...Cl11_$8
0.91	2.64	3.25(3)	124.9	N7_d-H7B_d...Cl6
0.91	2.86	3.59(4)	138.5	N7_d-H7C_d...Cl1_$10
0.91	2.99	3.64(4)	130.0	N7_d-H7C_d...Cl11_$10
0.91	2.70	3.17(3)	113.3	N7_d-H7C_d...Cl4

0.91	2.88	3.56(2)	132.7	N8_d-H8A_d...Cl1_$10
0.91	2.76	3.49(2)	137.2	N8_d-H8A_d...Cl11_$10
0.91	2.48	3.196(15)	136.2	N8_d-H8A_d...Cl5_$10
0.91	2.88	3.58(3)	135.2	N8_d-H8A_d...Cl51_$10
0.91	1.99	2.76(3)	141.1	N8_d-H8A_d...Cl51_$11
0.91	2.57	3.40(2)	151.6	N8_d-H8B_d...Cl1_$7
0.91	2.13	2.96(2)	152.1	N8_d-H8B_d...Cl11_$7
0.91	2.56	3.27(4)	134.7	N9_e-H9A_e...Cl4
0.91	2.84	3.41(6)	121.4	N9_e-H9A_e...Cl5_$7
0.91	2.69	3.12(7)	110.5	N9_e-H9A_e...Cl51_$12
0.91	3.02	3.57(7)	120.7	N9_e-H9B_e...Cl1
0.91	3.01	3.72(6)	136.8	N9_e-H9B_e...Cl4_$10
0.91	3.08	3.64(6)	121.7	N9_e-H9C_e...Cl11_$7
0.91	2.42	2.92(3)	114.6	N9_e-H9C_e...Cl11_$10
0.91	2.67	3.35(5)	132.7	N9_e-H9C_e...Cl51_$11
0.91	2.69	3.56(3)	161.5	N10_e-H10A_e...Cl6_$9

Geometry of hydrogen bonds in phase IV

Symmetry codes: $1 x, y+1, z; $2 -x+1, y, z; $3 x, y+1, z+1; $4 x-1/2, y+1/2, -z+2; $5 -x+3/2, y+1/2, -z+2; $6 x, y-1, z; $7 x-1/2, y-1/2, -z+2; $8 -x+3/2, y-1/2, -z+2; $9 -x+3/2, y+1/2, -z+1; $10 -x+3/2, y-1/2, -z+1; $11 x+1/2, y-1/2, -z+1; $12 -x+1, y-1, z; $13 x+1/2, y+1/2, -z+1.

D-H	**H···A**	**D···A**	**<(DHA)**	
0.89	2.85	3.289(14)	112.3	N1-H1A...Cl10
0.89	2.33	3.157(15)	154.1	N1-H1A...N9_c
0.89	2.51	3.25(3)	140.4	N1-H1A...N12_d
0.89	2.09	2.92(2)	154.4	N1-H1B...N3_$1
0.89	2.46	3.157(15)	135.8	N1-H1C...N9_$2c
0.89	2.44	3.25(3)	151.7	N1-H1C...N12_$2d
0.89	2.82	3.413(13)	125.5	N2-H2A...Cl5_$3
0.89	2.59	3.327(5)	140.2	N2-H2A...Cl12_$4
0.89	2.47	3.327(5)	160.8	N2-H2B...Cl12_$5
0.89	2.06	2.92(2)	162.8	N3-H3A...N1_$6
0.89	2.15	2.995(10)	158.3	N3-H3B...N22_$7
0.89	2.16	2.995(10)	156.8	N3-H3C...N22_$8
0.89	2.62	3.415(7)	149.9	N4-H4A...Cl11
0.89	2.07	2.93(2)	162.9	N4-H4B...N2
0.89	2.59	3.38(3)	148.3	N5_a-H5A_a...Cl4
0.89	2.67	3.20(3)	118.7	N5_a-H5A_a...Cl5_$1
0.89	2.61	3.50(3)	172.5	N5_a-H5B_a...Cl2_$1
0.89	2.53	3.10(2)	122.0	N5_a-H5C_a...Cl3_$1
0.89	2.69	3.39(3)	136.0	N5_a-H5C_a...Cl6
0.89	2.93	3.56(3)	128.5	N5_a-H5C_a...Cl7_$2
0.89	2.44	3.32(3)	172.6	N6_a-H6A_a...Cl2
0.89	2.82	3.50(2)	134.3	N6_a-H6C_a...Cl12_$9
0.89	2.65	3.19(2)	119.3	N6_a-H6C_a...Cl15_$9
0.89	2.97	3.64(3)	133.7	N7_b-H7A_b...Cl3_$1
0.89	2.80	3.55(4)	142.4	N7_b-H7A_b...Cl5_$1
0.89	2.97	3.54(3)	123.4	N7_b-H7B_b...Cl2
0.89	2.69	3.36(3)	133.7	N7_b-H7B_b...Cl6
0.89	2.72	3.16(3)	111.5	N7_b-H7C_b...Cl4

0.89	2.76	3.43(4)	132.6	N7_b-H7C_b...Cl12_$9
0.89	2.36	3.25(3)	174.6	N8_b-H8A_b...Cl2_$1
0.89	2.60	3.32(2)	137.7	N8_b-H8B_b...Cl14_$9
0.89	2.49	3.219(14)	139.3	N9_c-H9A_c...Cl9
0.89	2.34	3.157(15)	153.5	N9_c-H9B_c...N1
0.89	2.68	3.516(14)	156.5	N9_c-H9B_c...N2
0.89	2.67	3.527(15)	162.8	N9_c-H9C_c...Cl11
0.89	2.48	3.315(18)	156.6	N10_c-H10A_c...Cl14
0.89	2.80	3.227(15)	110.8	N10_c-H10A_c...Cl15_$1
0.89	2.86	3.42(2)	123.0	N10_c-H10B_c...Cl16
0.89	2.67	3.398(16)	139.5	N10_c-H10B_c...Cl16_$5
0.89	2.50	2.94(3)	111.4	N11_d-H11A_d...Cl7_$2
0.89	2.75	3.22(4)	114.8	N11_d-H11A_d...Cl14
0.89	2.51	3.38(4)	166.6	N11_d-H11B_d...Cl15_$1
0.89	2.73	3.60(4)	165.7	N11_d-H11C_d...Cl10
0.89	2.46	3.33(3)	163.7	N12_d-H12A_d...Cl16
0.89	2.85	3.46(4)	127.5	N12_d-H12C_d...Cl11_$1
0.89	2.65	3.16(3)	117.4	N12_d-H12C_d...Cl12_$5
0.89	2.03	2.77(3)	139.6	N13_e-H13A_e...N14_$10e
0.89	2.52	3.36(2)	157.0	N13_e-H13B_e...Cl7_$11
0.89	2.80	3.22(2)	110.4	N13_e-H13B_e...Cl14_$10
0.89	2.55	3.41(2)	163.9	N13_e-H13C_e...Cl2
0.89	2.00	2.77(3)	143.9	N14_e-H14B_e...N13_$9e
0.89	2.31	3.14(3)	154.9	N15_f-H15A_f...Cl7_$11
0.89	2.19	3.07(6)	174.9	N15_f-H15B_f...N16_$9f
0.89	2.44	3.21(3)	145.3	N15_f-H15C_f...Cl2
0.89	2.27	3.07(6)	149.6	N16_f-H16A_f...N15_$10f
0.89	2.93	3.69(3)	143.5	N17_g-H17A_g...Cl2
0.89	2.69	3.28(3)	124.7	N17_g-H17A_g...Cl3
0.89	2.68	3.24(3)	121.8	N17_g-H17A_g...Cl6
0.89	2.96	3.75(4)	149.3	N17_g-H17B_g...Cl7_$2
0.89	2.60	3.16(3)	122.2	N17_g-H17B_g...Cl9
0.89	2.44	3.33(3)	175.0	N17_g-H17C_g...Cl10_$6
0.89	2.65	3.24(4)	124.7	N18_g-H18A_g...Cl7_$12
0.89	2.83	3.31(2)	115.3	N18_g-H18A_g...Cl15
0.89	2.67	3.55(3)	171.9	N18_g-H18B_g...Cl14
0.89	2.56	3.35(4)	149.0	N19_h-H19A_h...Cl9
0.89	2.54	3.04(3)	116.2	N19_h-H19A_h...Cl10_$6
0.89	2.25	2.97(3)	136.9	N19_h-H19B_h...Cl11
0.89	2.66	3.53(4)	165.6	N19_h-H19C_h...Cl7_$12
0.89	2.86	3.36(4)	117.0	N20_h-H20A_h...Cl7_$2
0.89	2.60	3.42(4)	152.7	N20_h-H20A_h...Cl14
0.89	2.73	3.61(4)	175.8	N20_h-H20B_h...Cl6
0.89	2.78	3.283(11)	117.5	N21-H21A...Cl14
0.89	2.52	3.324(12)	151.2	N21-H21A...Cl15_$1
0.89	2.95	3.602(10)	132.0	N21-H21B...Cl11_$5
0.89	2.68	3.383(12)	136.1	N21-H21B...Cl16
0.89	2.76	3.331(14)	123.0	N21-H21B...Cl16_$5
0.89	2.38	3.202(14)	153.5	N21-H21C...Cl12

0.89	2.67	3.455(11)	147.1	N22-H22A...Cl12_$1
0.89	2.98	3.580(11)	126.3	N22-H22A...Cl16_$5
0.89	2.72	3.465(11)	142.6	N22-H22B...Cl2_$9
0.89	2.69	3.304(11)	127.6	N22-H22B...Cl4_$13

Geometry of hydrogen bonds in phase V

Symmetry codes: $1 x, y, -z+1/2; $2 -x+1/2, -y+1/2, -z+1; $3 -x+1/2, y-1/2, -z+1/2; $4 x-1/2, y-1/2, z; $5 -x+1/2, -y+1/2, z+1/2; $6 -x+1/2, -y+1/2, -z; $7 x+1/2, y-1/2, z; $8 -x+1, -y, z+1/2; $9 -x+1, -y, -z; $10 -x+1, -y+1, -z; $11 -x+1, y, -z+1/2; $12 -x+1, -y+1, z+1/2.

D-H	**H···A**	**D···A**	**<(DHA)**	
0.89	2.87	3.49(2)	128.6	N1-H1A...Cl1
0.89	2.76	3.220(11)	113.5	N1-H1A...Cl4
0.89	2.96	3.76(2)	149.7	N1-H1C...Cl4_$1
0.89	2.68	3.558(13)	171.3	N2-H2A...Cl1_$2
0.89	2.93	3.601(18)	134.1	N2-H2B...Cl1_$3
0.89	2.73	3.422(16)	135.7	N2-H2B...Cl6_$4
0.89	2.63	3.160(12)	119.2	N2-H2B...Cl6_$5
0.89	2.64	3.450(13)	151.1	N2-H2C...Cl4_$6
0.89	2.67	3.191(14)	118.0	N2-H2C...Cl4_$5
0.89	2.62	3.23(4)	125.8	N3-H3A...Cl1_$3
0.89	2.65	3.52(4)	166.6	N3-H3B...Cl6_$5
0.89	2.64	3.09(3)	112.1	N4-H4A...Cl4_$6
0.89	2.69	3.54(3)	158.9	N4-H4A...Cl4_$5
0.89	2.64	3.41(3)	145.9	N4-H4B...Cl1_$6
0.89	3.02	3.70(6)	134.5	N4-H4B...Cl6_$4
0.89	2.43	3.08(5)	129.8	N4-H4C...Cl1
0.89	3.02	3.78(5)	143.8	N4-H4C...Cl4
0.89	2.95	3.57(4)	127.9	N5-H5A...Cl1_$7
0.89	2.60	3.200(17)	125.1	N5-H5A...Cl4_$8
0.89	2.57	3.29(4)	138.9	N5-H5B...Cl1_$3
0.89	2.84	3.329(19)	115.7	N6-H6A...Cl4
0.89	2.50	3.13(3)	128.7	N7-H7A...Cl4_$8
0.89	2.55	3.38(7)	156.9	N7-H7B...Cl1_$7
0.89	2.48	3.18(7)	135.4	N7-H7C...Cl1_$3
0.89	2.92	3.37(3)	113.3	N7-H7C...Cl4_$9
0.89	2.59	3.182(19)	124.6	N8-H8A...Cl4_$1
0.89	3.03	3.44(2)	110.4	N8-H8B...Cl4