



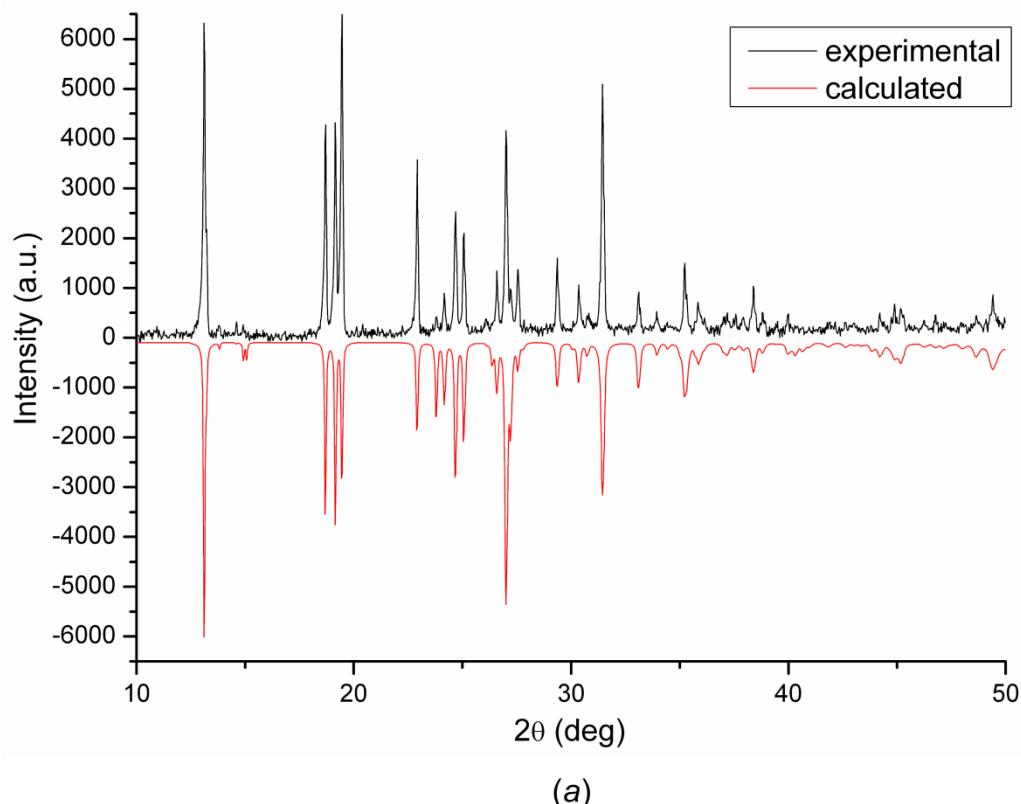
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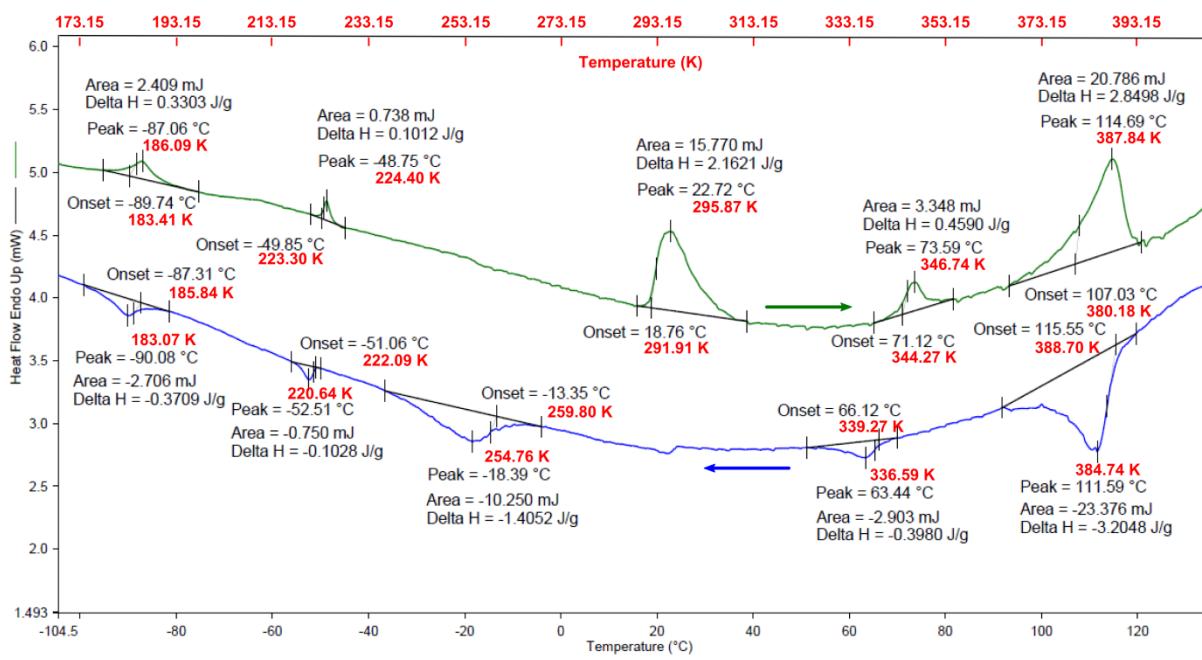
Supporting information for article:

Reversible *chair*↔*skew* conformational interconversion of 1,3,2-dioxaphosphorinane ring in solid state

Katarzyna Anna Ślepokura

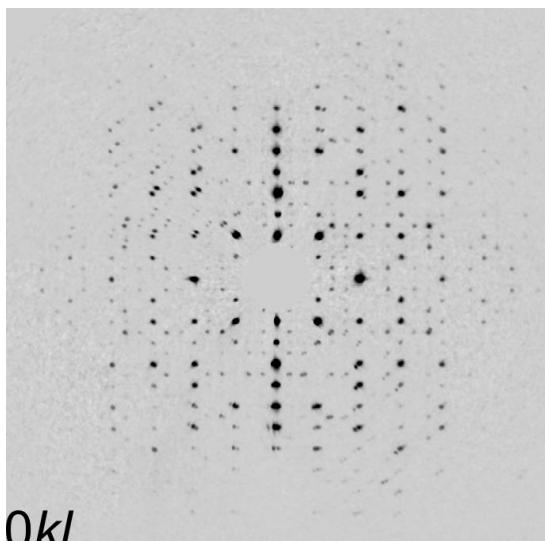


(a)

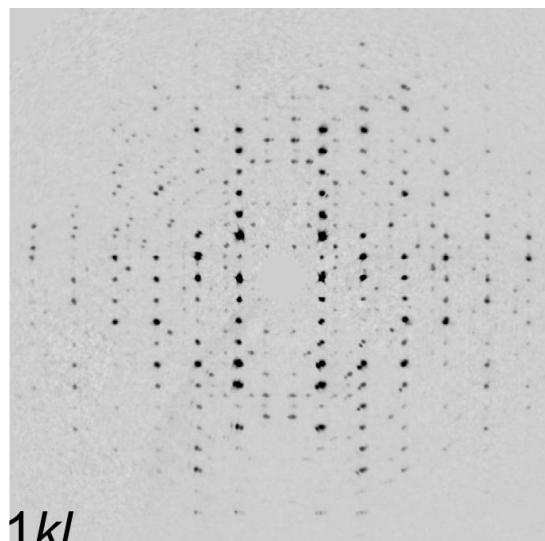


(b)

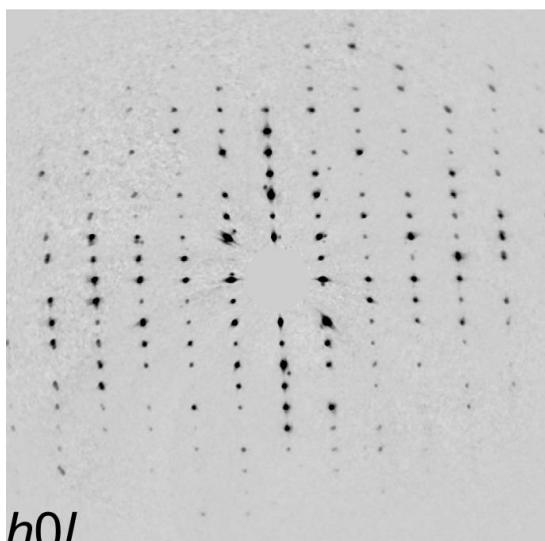
Figure S1 (a) X-ray powder diffraction pattern for the sample of $\beta\text{-NH}_4[(\text{MeO})_2\text{cDHAP}]$ and (b) DSC traces (on cooling and heating) for $\beta\text{-NH}_4[(\text{MeO})_2\text{cDHAP}]$ (sample mass 7.29 mg, ramp rate of 20 K min⁻¹)



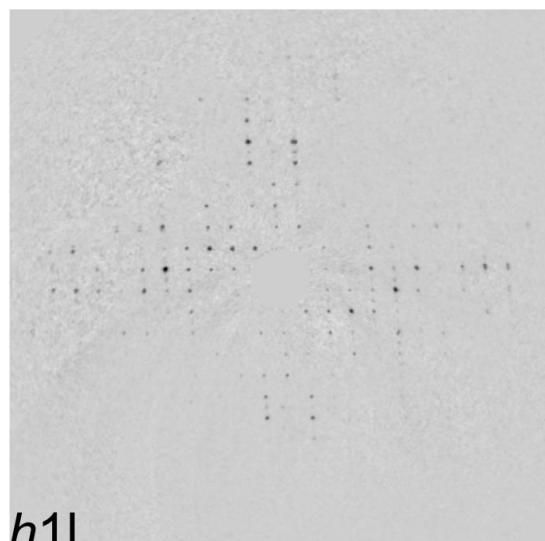
$0kl$



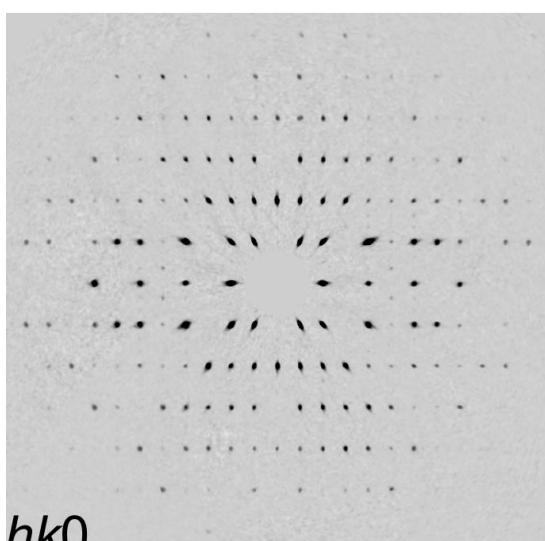
$1kl$



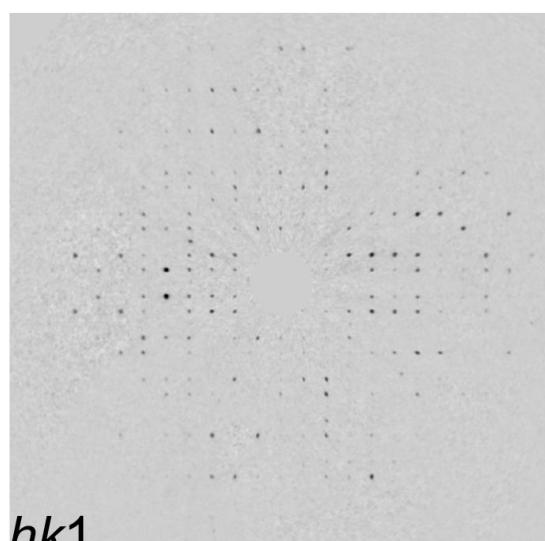
$h0l$



$h1l$

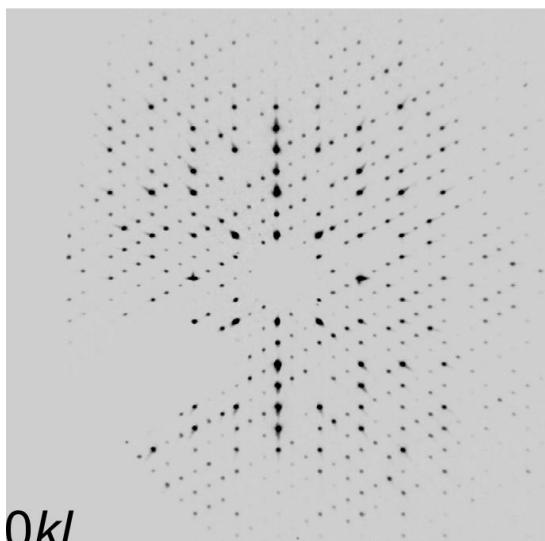


$hk0$

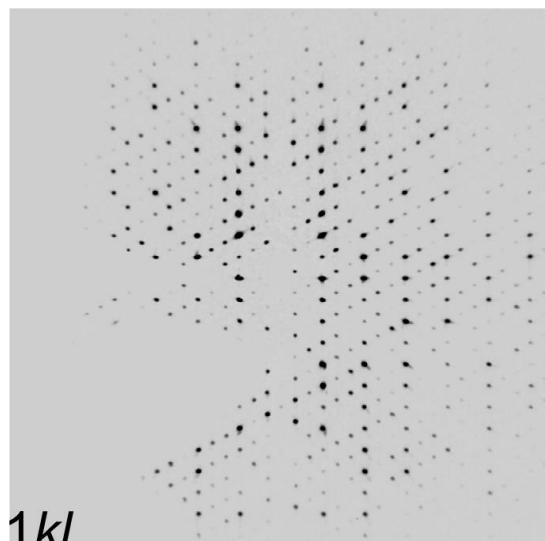


$hk1$

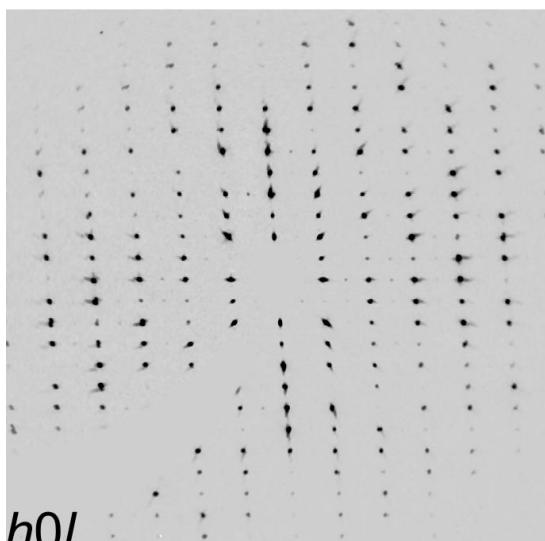
HTP



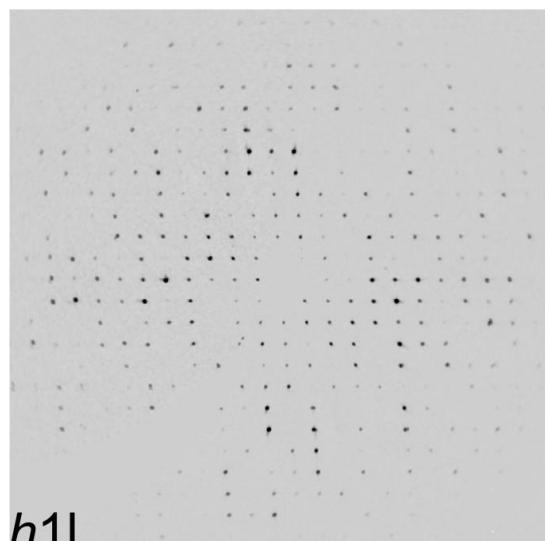
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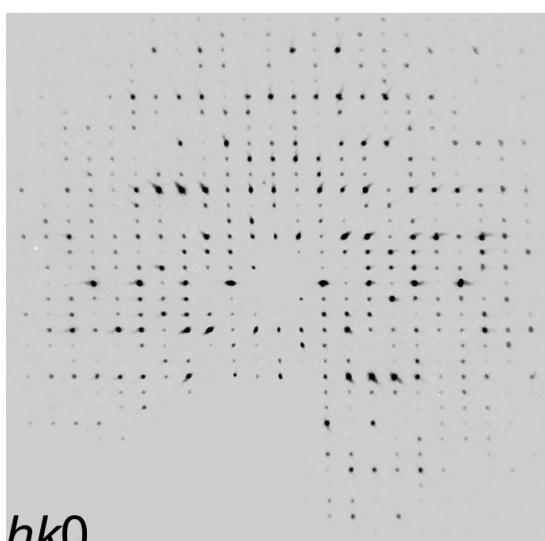
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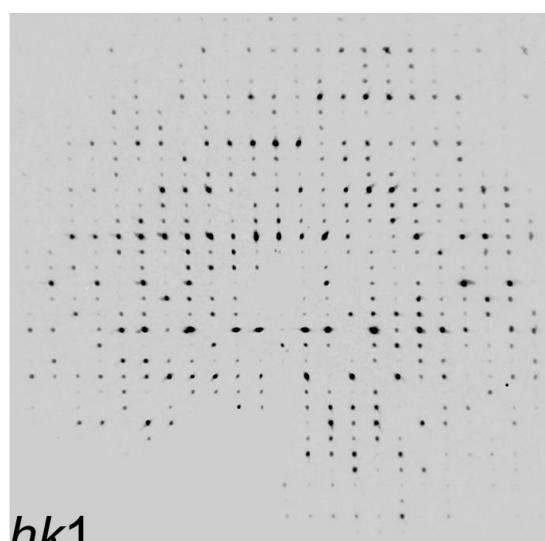
$h0l$



$h1l$

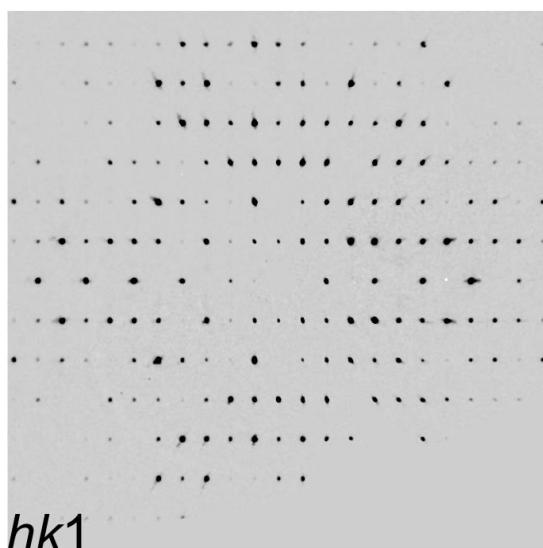
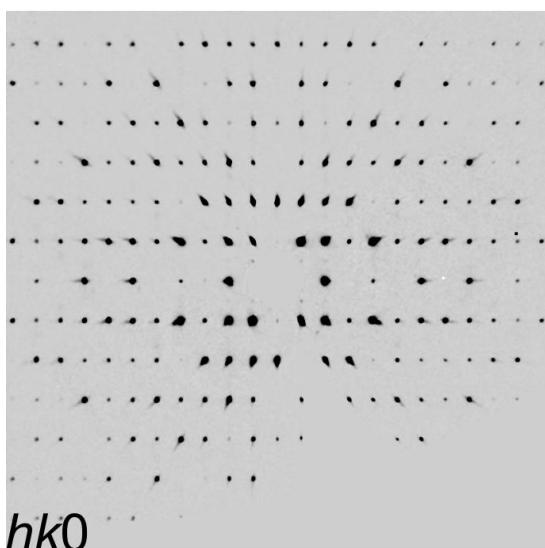
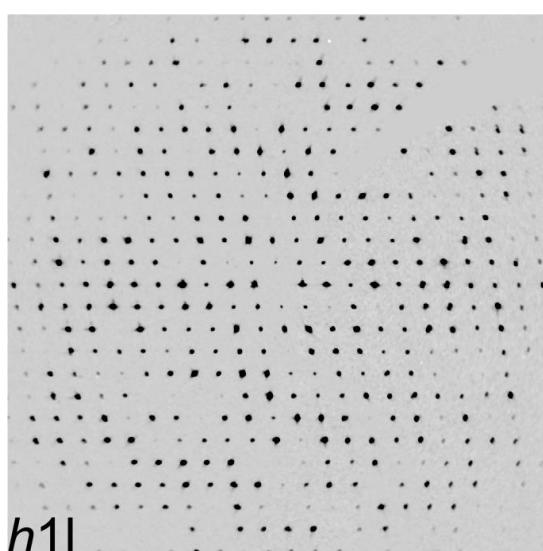
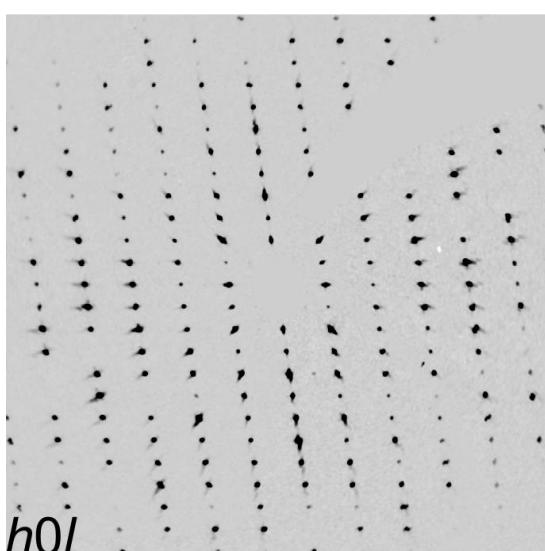
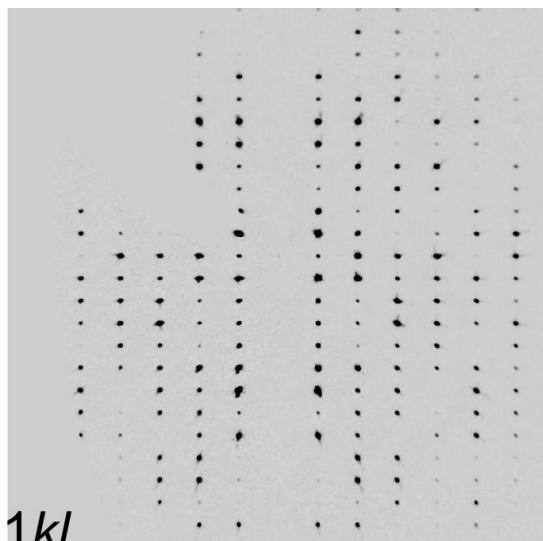
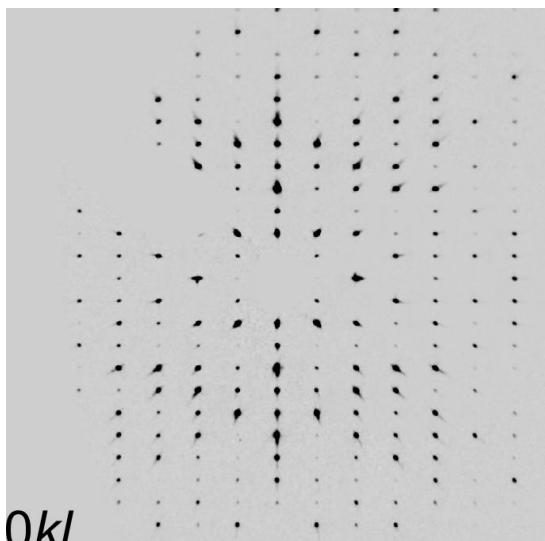


$hk0$

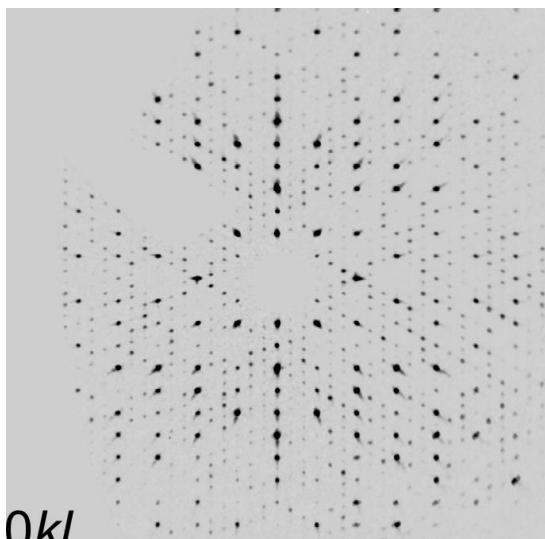


$hk1$

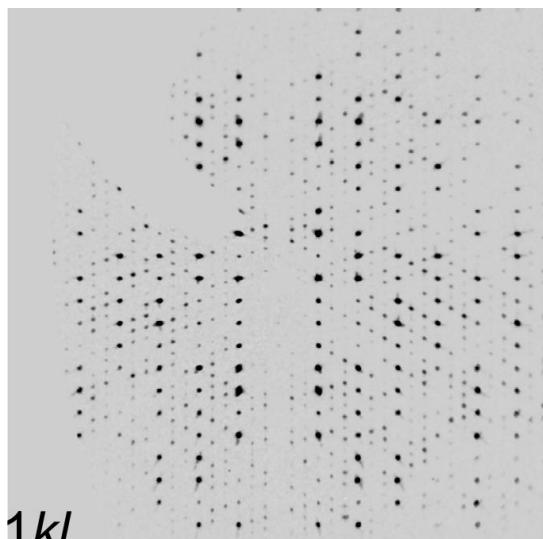
RTP



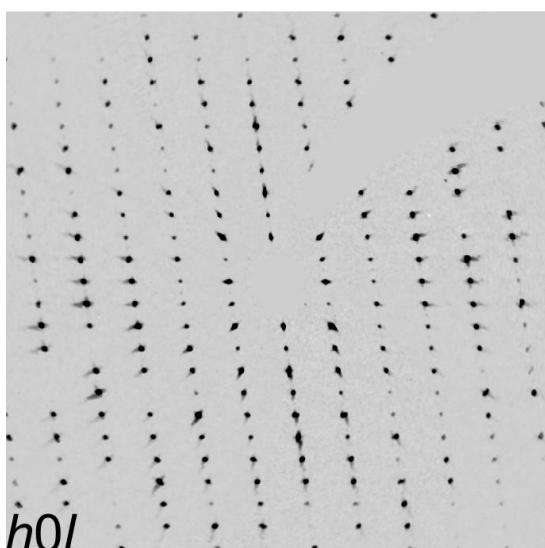
MTP



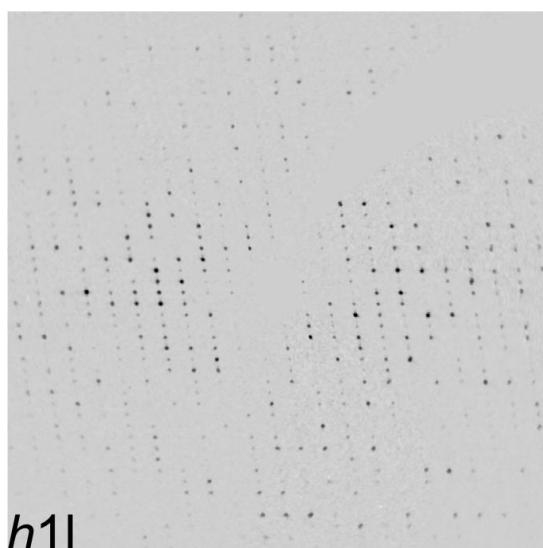
$0kl$



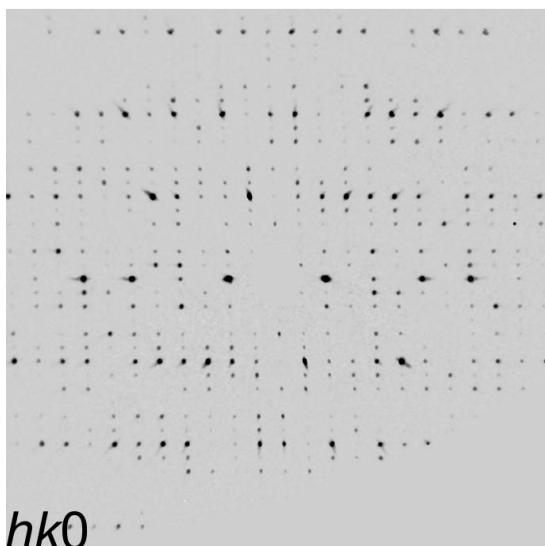
$1kl$



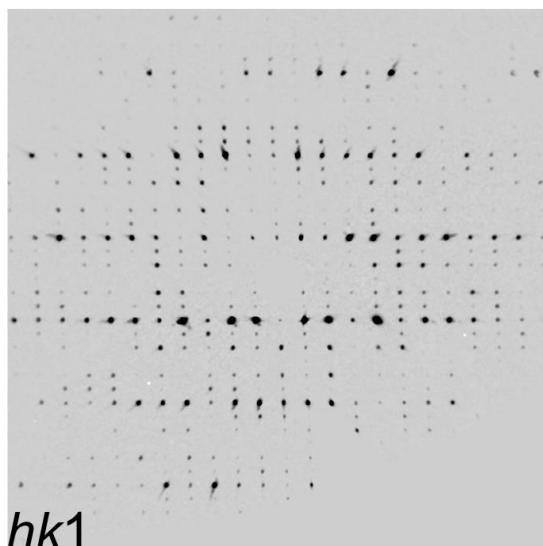
$h0l$



$h1l$



$hk0$



$hk1$

LTP

Figure S2 Reconstruction of reciprocal layers for $\beta\text{-NH}_4[(\text{MeO})_2\text{cDHAP}]$ measured at different temperatures. Two layer vectors define the layer: L1 – to the right, L2 – positive right-handed from L1. For $0kl$ and $1kl$ vectors L1 and L2 are: [010], [001] (for monoclinic **HTP** and **MTP**), and [03-1], [001] (for triclinic **RTP** and **LTP**). For $h0l$ and $h1l$, L1 and L2 are: [-100], [001] (for all). For $hk0$ and $hk1$, L1 and L2 are: [-100], L2: [010] (for all).

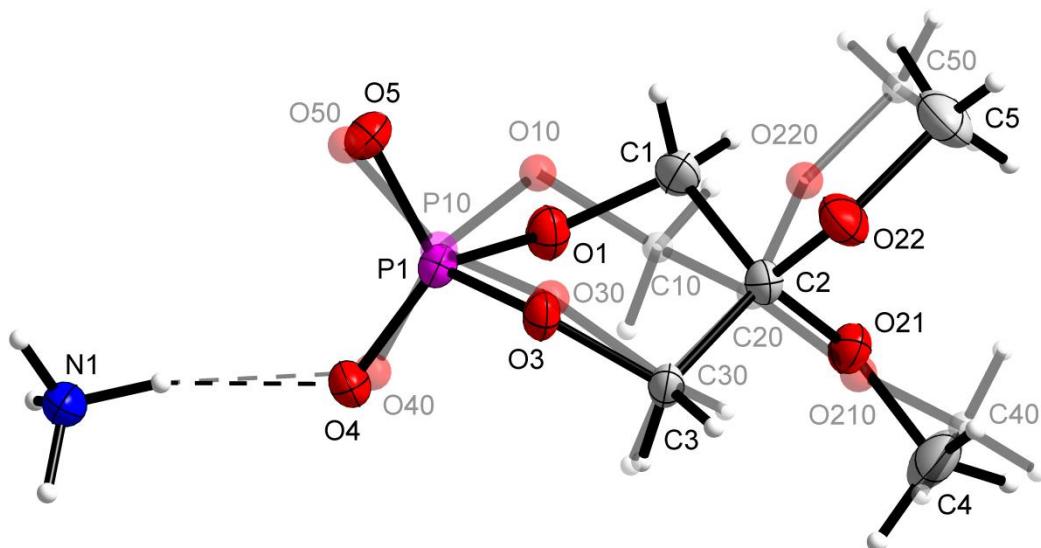


Figure S3 Asymmetric unit in **MTP**, showing the atom-numbering scheme and symmetry-independent hydrogen bonds (dashed lines). Two positions of the disordered $(\text{MeO})_2\text{cDHAP}^-$ anion are shown: *skew*, with site occupation factor amounting 0.7821(19) – black bonds and labels, and *chair*, with s.o.f. = 0.2179(19) – transparent bonds and atoms (shown as spheres) and grey labels. Displacement ellipsoids are shown at the 40% probability level.

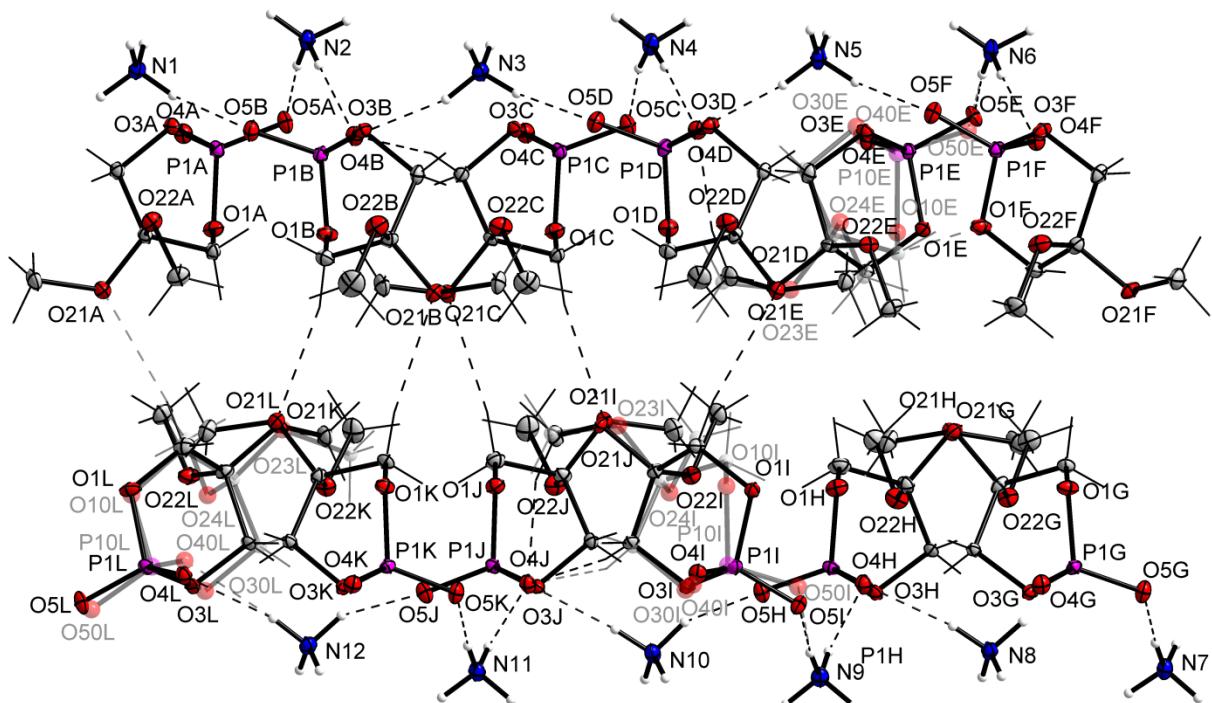


Figure S4 Asymmetric unit in LTP, showing the atom-numbering scheme (for P, O, N atoms) and symmetry-independent hydrogen bonds (dashed lines). Two positions of the disordered (MeO)₂cDHAP⁻ anions **E**, **I** and **L** are shown: with higher occupancy factors – black bonds and labels; with lower s.o.f.s – transparent bonds and atoms (shown as spheres) and grey labels. Displacement ellipsoids are shown at the 40% probability level.

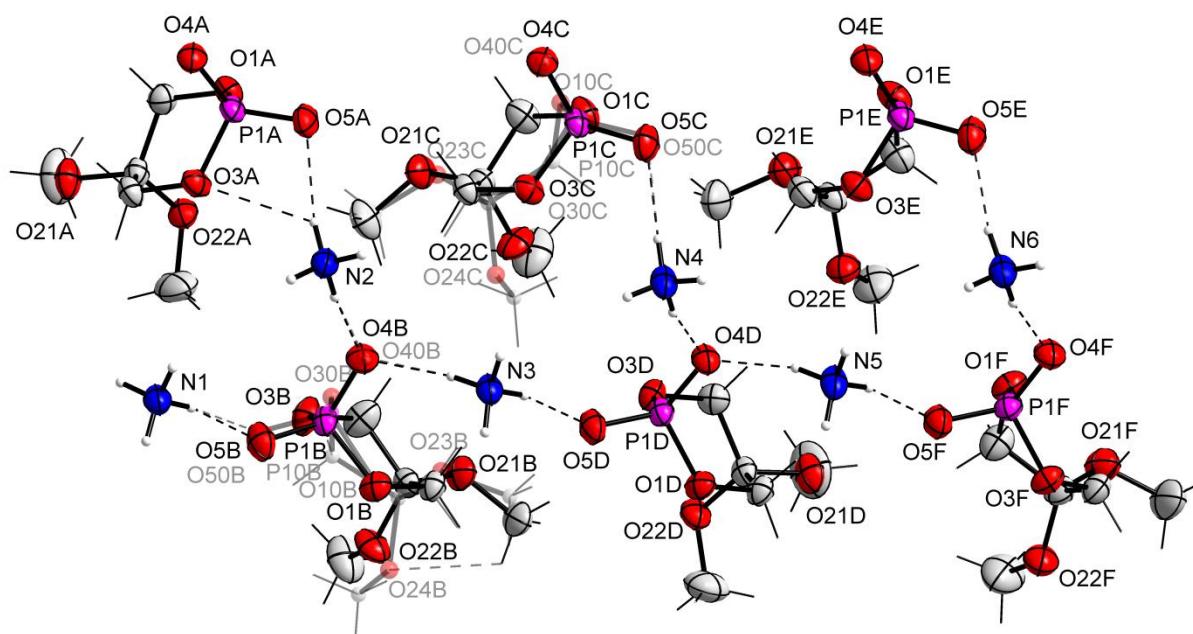


Figure S5 Asymmetric unit in RTP, showing the atom-numbering scheme (for P, O, N atoms) and symmetry-independent hydrogen bonds (dashed lines). Two positions of the disordered $(\text{MeO})_2\text{cDHAP}^-$ anions **B** and **C** are shown: with higher occupancy factors – black bonds and labels; with lower s.o.f.s – transparent bonds and atoms (shown as spheres) and grey labels. Displacement ellipsoids are shown at the 40% probability level.

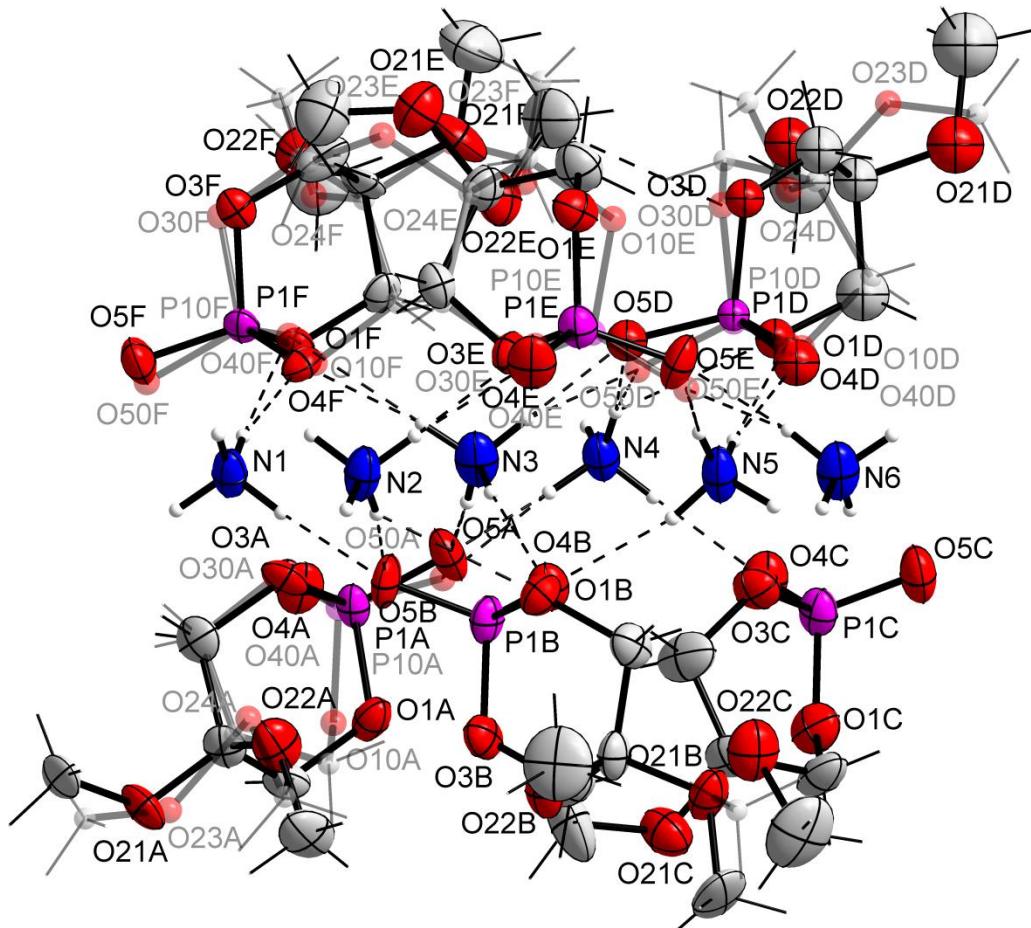


Figure S6 Asymmetric unit in HTP, showing the atom-numbering scheme (for P, O, N atoms) and symmetry-independent hydrogen bonds (dashed lines). Two positions of the disordered $(\text{MeO})_2\text{cDHAP}^-$ anions **A**, **D**, **E** and **F** are shown: with higher occupancy factors – black bonds and labels; with lower s.o.f.s – transparent bonds and atoms (shown as spheres) and grey labels. Disorder of Me group in **B** is also shown. Displacement ellipsoids are shown at the 30% probability level.

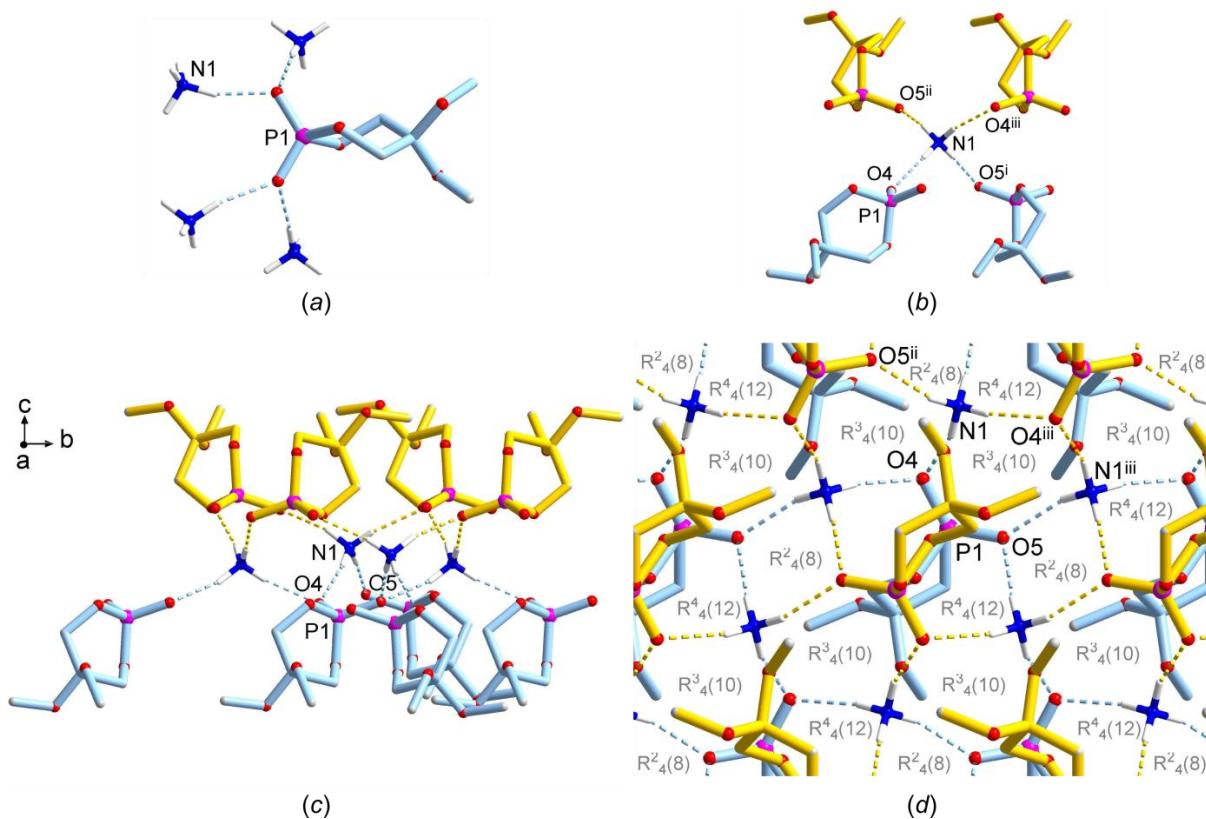


Figure S7 Skew-puckered $(\text{MeO})_2\text{cDHAP}^-$ anions and ammonium cations in **MTP** interacting via $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds (dashed lines) to form double-layer. Different layers and related hydrogen bonds are shown in pale blue and yellow. (a) Four NH_4^+ surrounding one organic anion, (b) four adjacent phosphate anions from different layers (pale blue and yellow) hydrogen-bonded to one NH_4^+ , (c) side view of double-layer; (d) top view of double-layer with graph-set notation ascribed to ring motifs formed by inter-double-layer hydrogen bonds. For clarity C-bonded H atoms are omitted, and only skew-puckered positions [s.o.f. = 0.7821(19)] of disordered anions are shown. Symmetry codes are given in Tables S3.

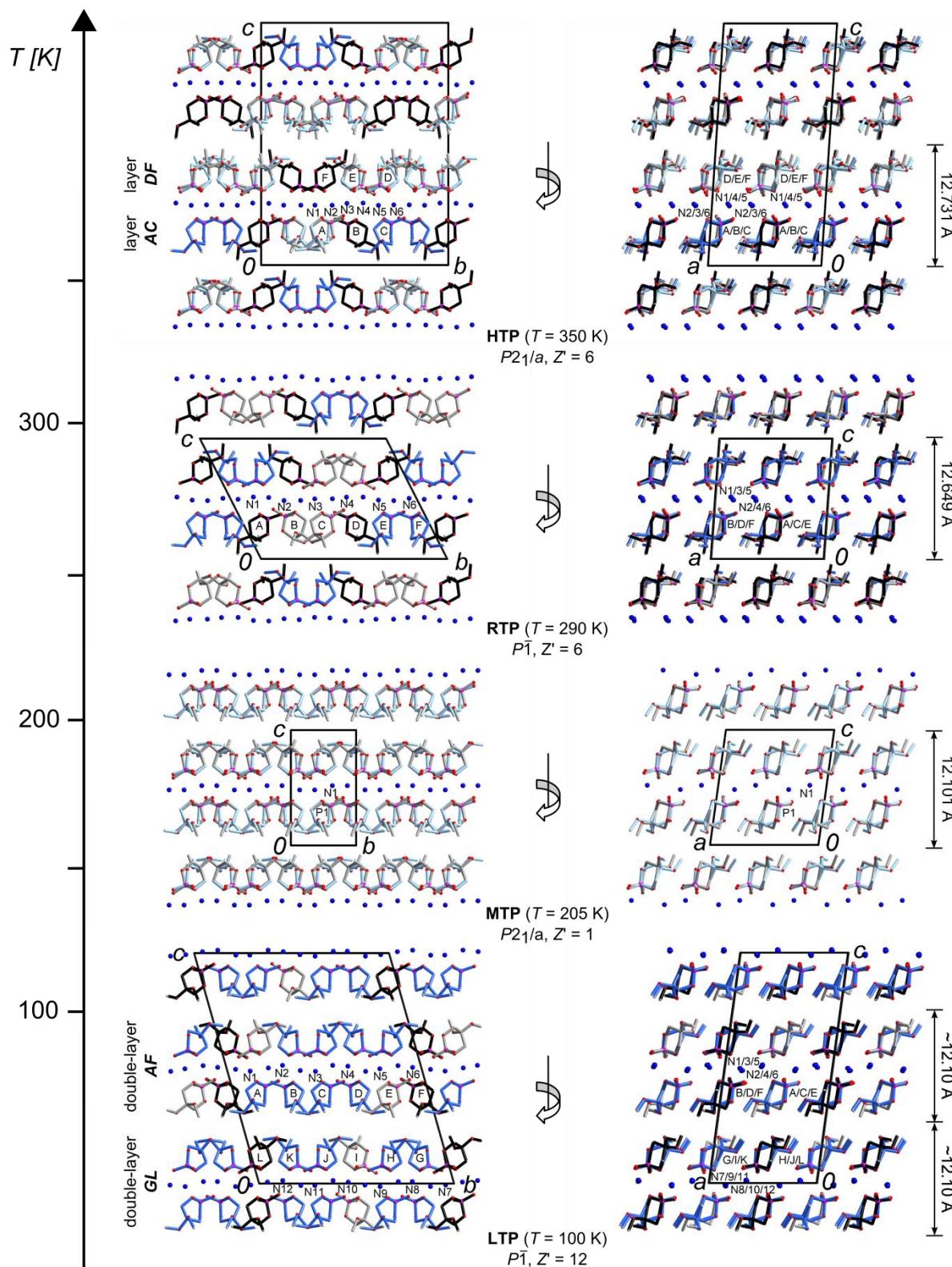


Figure S8 The composition and mutual orientation of double-layers in **HTP**, **RTP**, **MTP** and **LTP** of $\beta\text{-NH}_4[(\text{MeO})_2\text{cDHAP}]$, shown in two side views. Conformationally homogeneous positions are shown in blue (*skew* conformers) and black (*chair* conformers). Conformationally disordered positions: *skew*-puckered – pale blue, *chair*-puckered – grey. For **RTP** and **LTP** only positions with higher occupancy factors are shown. H atoms are omitted.

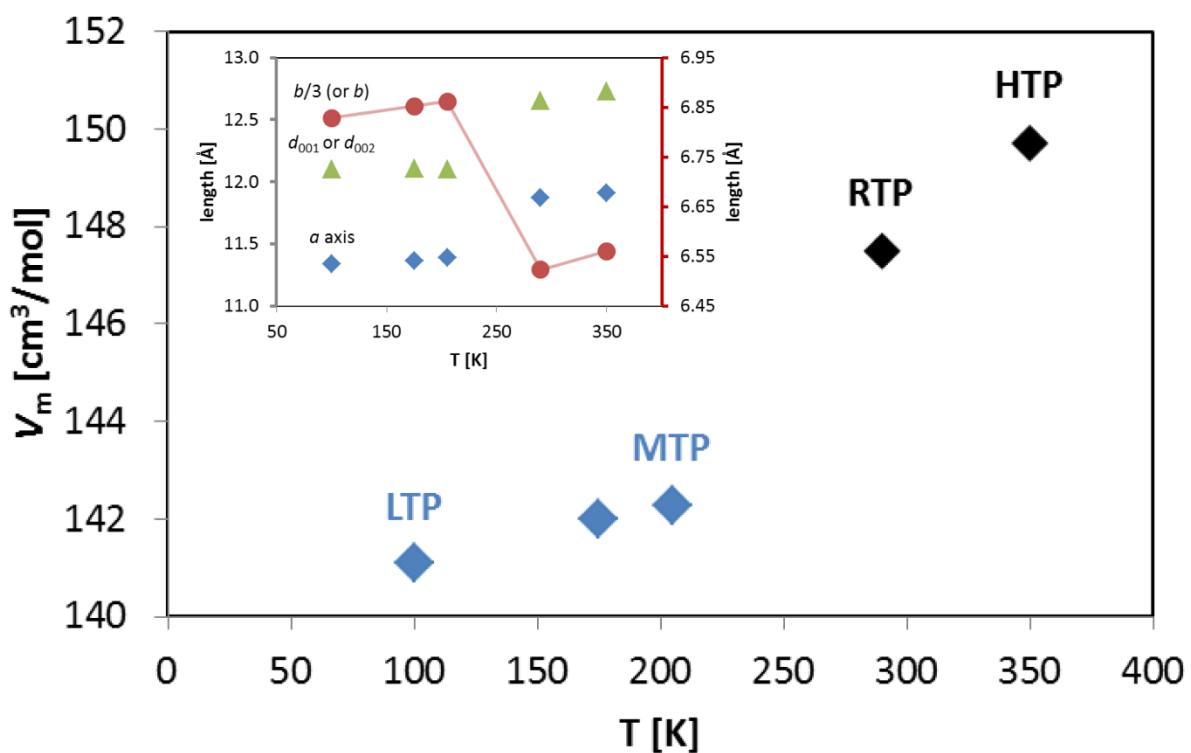


Figure S9 Molar volume (V_m) (and cell parameters – inset) in the crystal of β - $\text{NH}_4[(\text{MeO})_2\text{cDHAP}]$ at different temperatures.

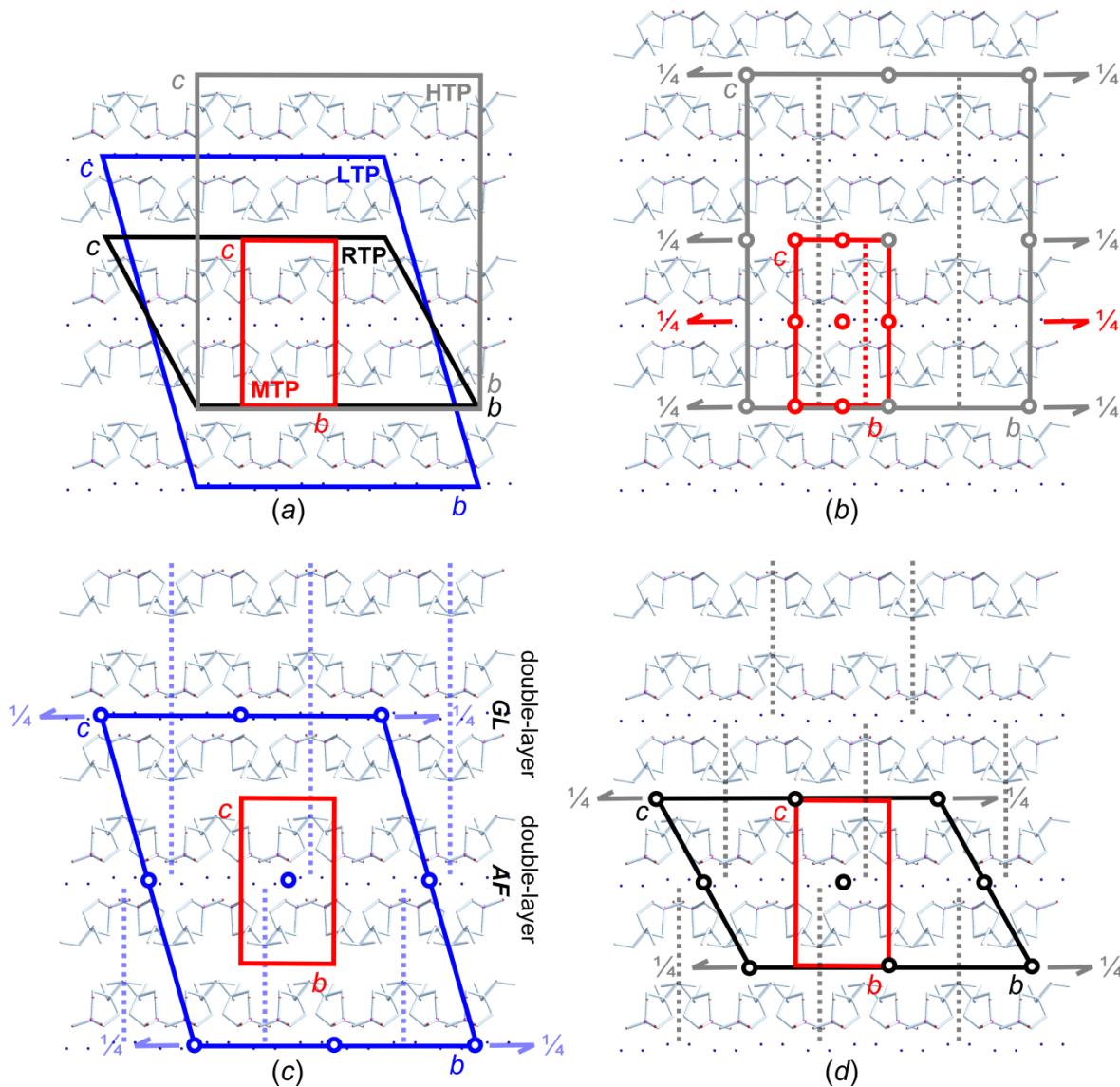


Figure S10 (a) View of the unit cells of $\beta\text{-NH}_4[(\text{MeO})_2\text{cDHAP}]$ at different temperatures, projected along the a axis. (b) Symmetry elements in monoclinic phases: **HTP** (shown in grey) and **MTP** (grey and red). (c), (d) Triclinic phases: (pseudo)symmetry elements present in **LTP** and **RTP** are shown in blue and black, respectively. Local non-crystallographic pseudosymmetry is shown with transparent lines.

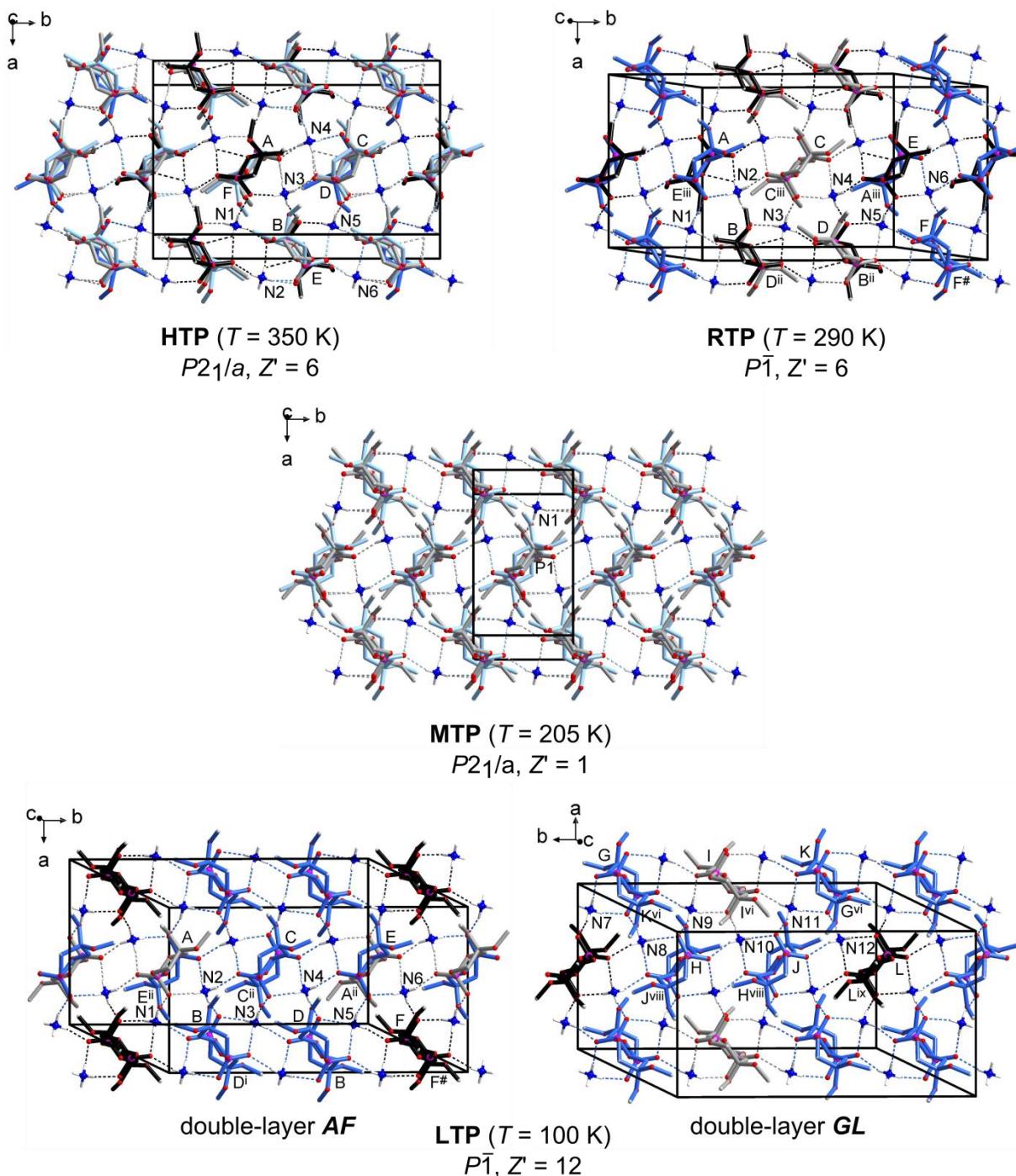


Figure S11 Double-layers in **HTP**, **RTP**, **MTP** and **LTP** of $\beta\text{-NH}_4[(\text{MeO})_2\text{cDHAP}]$ viewed down the \mathbf{c}^* axis. Colour scheme and convention the same as in Fig. 2. H atoms are omitted. Symmetry codes are as in Tables S1-S4, and (#) $-x+2, -y+2, -z+1$.

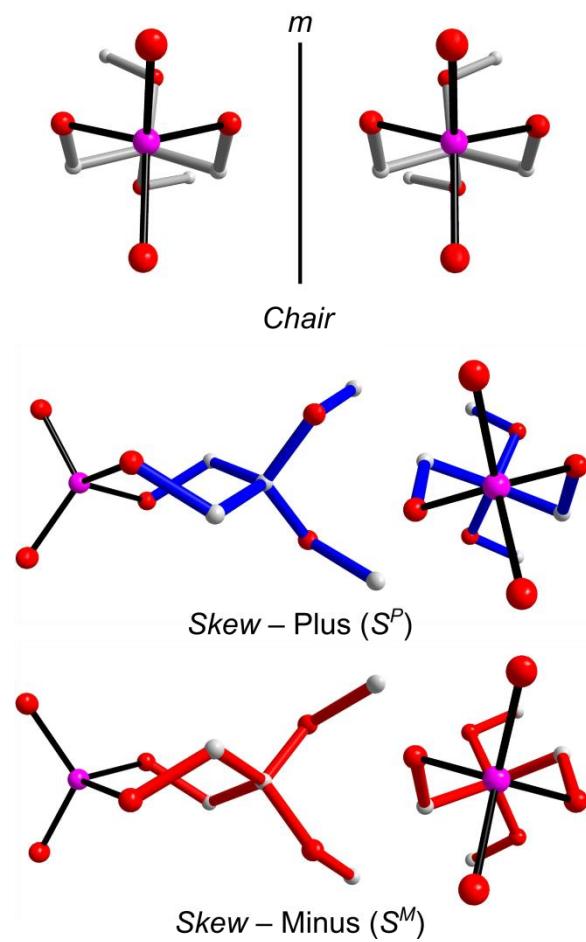


Figure S12 Various types of $(\text{MeO})_2\text{cDHAP}^-$ anions: *chair* conformers related by the mirror plane (viewed down the P–C2 line), and two forms of *skew* conformers: revealing Plus and Minus helicity. H atoms are omitted.

Table S1 Hydrogen-bond geometry (\AA , $^\circ$) for HTP

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|---------------------------|--------------|--------------------|-------------|----------------------|
| N1—H1N…O5B | 0.90 | 1.93 | 2.801(5) | 163 |
| N1—H2N…O4A ⁱ | 0.90 | 2.02 | 2.908(8) | 169 |
| N1—H2N…O40A ⁱ | 0.90 | 1.79 | 2.685(18) | 173 |
| N1—H3N…O4F | 0.90 | 1.90 | 2.786(7) | 167 |
| N1—H3N…O40F | 0.90 | 1.96 | 2.846(9) | 167 |
| N1—H4N…O1F ⁱ | 0.90 | 2.59 | 3.211(8) | 126 |
| N1—H4N…O5F ⁱ | 0.90 | 2.07 | 2.961(11) | 169 |
| N1—H4N…O50F ⁱ | 0.90 | 1.84 | 2.725(13) | 166 |
| N2—H5N…O4A ⁱⁱ | 0.90 | 1.95 | 2.845(7) | 175 |
| N2—H5N…O40A ⁱⁱ | 0.90 | 1.74 | 2.622(15) | 167 |
| N2—H6N…O5F ⁱ | 0.90 | 1.88 | 2.767(7) | 168 |
| N2—H6N…O50F ⁱ | 0.90 | 1.89 | 2.756(9) | 161 |
| N2—H7N…O4E | 0.90 | 1.91 | 2.805(10) | 173 |
| N2—H7N…O40E | 0.90 | 2.02 | 2.909(14) | 168 |
| N2—H8N…O1B | 0.90 | 2.55 | 3.191(6) | 129 |
| N2—H8N…O5B | 0.90 | 2.04 | 2.923(6) | 166 |
| N3—H9N…O4F | 0.90 | 1.83 | 2.717(9) | 168 |
| N3—H9N…O40F | 0.90 | 2.17 | 3.065(12) | 174 |
| N3—H10N…O4B | 0.90 | 1.94 | 2.812(5) | 162 |
| N3—H11N…O5D | 0.90 | 1.92 | 2.801(7) | 168 |
| N3—H11N…O50D | 0.90 | 1.93 | 2.786(7) | 157 |
| N3—H12N…O5A | 0.90 | 1.87 | 2.741(10) | 162 |
| N3—H12N…O50A | 0.90 | 2.24 | 3.12(2) | 167 |
| N4—H13N…O5A | 0.90 | 1.86 | 2.748(7) | 167 |

| | | | | |
|---------------------------------|------|------|-----------|-----|
| N4—H13N···O50A | 0.90 | 1.99 | 2.885(14) | 175 |
| N4—H14N···O4C | 0.90 | 1.92 | 2.822(6) | 177 |
| N4—H15N···O4E ⁱⁱⁱ | 0.90 | 1.80 | 2.682(8) | 168 |
| N4—H15N···O40E ⁱⁱⁱ | 0.90 | 2.06 | 2.954(12) | 170 |
| N4—H16N···O1D | 0.90 | 2.45 | 3.082(7) | 128 |
| N4—H16N···O5D | 0.90 | 2.15 | 3.011(9) | 161 |
| N4—H16N···O50D | 0.90 | 1.84 | 2.677(10) | 154 |
| N5—H17N···O4B | 0.90 | 1.92 | 2.797(6) | 164 |
| N5—H18N···O4D | 0.90 | 1.96 | 2.839(8) | 165 |
| N5—H18N···O40D | 0.90 | 1.89 | 2.760(8) | 161 |
| N5—H19N···O5E | 0.90 | 2.03 | 2.900(10) | 164 |
| N5—H19N···O50E | 0.90 | 1.80 | 2.640(15) | 155 |
| N5—H20N···O5C ^{iv} | 0.90 | 1.89 | 2.786(6) | 172 |
| N6—H21N···O4D ^{iv} | 0.90 | 1.77 | 2.667(9) | 172 |
| N6—H21N···O40D ^{iv} | 0.90 | 2.05 | 2.947(10) | 175 |
| N6—H22N···O4C ⁱⁱ | 0.90 | 1.90 | 2.784(5) | 169 |
| N6—H23N···O5E | 0.90 | 1.97 | 2.842(8) | 164 |
| N6—H23N···O50E | 0.90 | 1.80 | 2.638(11) | 154 |
| N6—H24N···O5C ^{iv} | 0.90 | 1.92 | 2.815(6) | 171 |
| C50D—H50D···O10E ⁱⁱⁱ | 0.96 | 2.61 | 3.424(15) | 143 |
| C5F—H5F1···O3F ^v | 0.96 | 2.61 | 3.391(13) | 139 |

Symmetry codes: (i) $x+1/2, -y+1/2, z$; (ii) $x+1, y, z$; (iii) $x-1, y, z$; (iv) $x+1/2, -y+3/2, z$; (v) $x-1/2, -y+1/2, z$.

Table S2 Hydrogen-bond geometry (\AA , $^\circ$) for RTP

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|-----------------------------|--------------|--------------------|-------------|----------------------|
| N1—H1N…O5B | 0.90 | 1.84 | 2.728(2) | 168 |
| N1—H1N…O50B | 0.90 | 2.00 | 2.899(7) | 173 |
| N1—H2N…O4F ⁱ | 0.90 | 1.90 | 2.804(2) | 176 |
| N1—H3N…O5F ⁱⁱ | 0.90 | 1.94 | 2.826(2) | 167 |
| N1—H4N…O4E ⁱⁱⁱ | 0.90 | 1.88 | 2.771(2) | 173 |
| N2—H5N…O4B | 0.90 | 1.94 | 2.832(3) | 172 |
| N2—H5N…O40B | 0.90 | 1.73 | 2.627(8) | 173 |
| N2—H6N…O3A | 0.90 | 2.51 | 3.123(2) | 126 |
| N2—H6N…O5A | 0.90 | 2.01 | 2.890(2) | 164 |
| N2—H7N…O4E ⁱⁱⁱ | 0.90 | 1.91 | 2.8045(18) | 175 |
| N2—H8N…O5C ⁱⁱⁱ | 0.90 | 1.85 | 2.740(2) | 170 |
| N2—H8N…O50C ⁱⁱⁱ | 0.90 | 2.01 | 2.900(11) | 173 |
| N3—H9N…O4B | 0.90 | 2.00 | 2.898(3) | 173 |
| N3—H9N…O40B | 0.90 | 1.85 | 2.740(10) | 169 |
| N3—H10N…O5D | 0.90 | 1.89 | 2.7747(17) | 168 |
| N3—H11N…O1D ⁱⁱ | 0.90 | 2.60 | 3.1736(19) | 122 |
| N3—H11N…O5D ⁱⁱ | 0.90 | 2.02 | 2.908(2) | 171 |
| N3—H12N…O4C ⁱⁱⁱ | 0.90 | 1.94 | 2.821(3) | 164 |
| N3—H12N…O40C ⁱⁱⁱ | 0.90 | 1.75 | 2.633(12) | 166 |
| N4—H13N…O4D | 0.90 | 1.92 | 2.8027(19) | 167 |
| N4—H14N…O5C | 0.90 | 1.91 | 2.805(3) | 170 |
| N4—H14N…O50C | 0.90 | 2.13 | 3.035(18) | 178 |
| N4—H15N…O5A ⁱⁱⁱ | 0.90 | 1.92 | 2.789(2) | 162 |
| N4—H16N…O4C ⁱⁱⁱ | 0.90 | 2.01 | 2.885(3) | 165 |

| | | | | |
|---|------|------|------------|-----|
| N4—H16 <i>N</i> ···O40 <i>C</i> ⁱⁱⁱ | 0.90 | 1.89 | 2.763(17) | 163 |
| N5—H17 <i>N</i> ···O5 <i>F</i> | 0.90 | 1.90 | 2.7818(18) | 166 |
| N5—H18 <i>N</i> ···O4 <i>D</i> | 0.90 | 1.93 | 2.810(2) | 165 |
| N5—H19 <i>N</i> ···O5 <i>B</i> ⁱⁱ | 0.90 | 1.85 | 2.745(3) | 170 |
| N5—H19 <i>N</i> ···O50 <i>B</i> ⁱⁱ | 0.90 | 2.13 | 3.029(10) | 177 |
| N5—H20 <i>N</i> ···O4 <i>A</i> ⁱⁱⁱ | 0.90 | 1.95 | 2.815(2) | 162 |
| N6—H21 <i>N</i> ···O4 <i>F</i> | 0.90 | 1.89 | 2.7745(19) | 168 |
| N6—H22 <i>N</i> ···O5 <i>E</i> | 0.90 | 1.92 | 2.811(2) | 168 |
| N6—H23 <i>N</i> ···O4 <i>A</i> ⁱⁱⁱ | 0.90 | 1.90 | 2.7972(18) | 171 |
| N6—H24 <i>N</i> ···O5 <i>E</i> ^{iv} | 0.90 | 1.89 | 2.777(2) | 168 |
| C4 <i>B</i> —H4 <i>B</i> 3···O4 <i>C</i> ^v | 0.96 | 2.51 | 3.303(5) | 140 |

Symmetry codes: (i) $x, y-1, z$; (ii) $-x+2, -y+1, -z+1$; (iii) $-x+1, -y+1, -z+1$; (iv) $-x+1, -y+2, -z+1$; (v) $x+1, y, z$.

Table S3 Hydrogen-bond geometry (\AA , $^\circ$) for **MTP**

| $D\text{---H}\cdots A$ | $D\text{---H}$ | $H\cdots A$ | $D\cdots A$ | $D\text{---H}\cdots A$ |
|----------------------------|----------------|-------------|-------------|------------------------|
| N1—H1N…O4 | 0.94 (2) | 1.82 (2) | 2.739(2) | 163 (2) |
| N1—H1N…O40 | 0.94 (2) | 2.06 (2) | 2.974(5) | 164 (2) |
| N1—H2N…O5 ⁱ | 0.90 (2) | 1.95 (2) | 2.845(2) | 176 (2) |
| N1—H2N…O50 ⁱ | 0.90 (2) | 1.77 (2) | 2.652(5) | 169 (2) |
| N1—H3N…O5 ⁱⁱ | 0.93 (2) | 1.96 (2) | 2.8428(17) | 157 (2) |
| N1—H3N…O50 ⁱⁱ | 0.93 (2) | 1.89 (2) | 2.718(4) | 148 (2) |
| N1—H4N…O4 ⁱⁱⁱ | 0.90 (2) | 1.97 (2) | 2.845(2) | 167 (2) |
| N1—H4N…O40 ⁱⁱⁱ | 0.90 (2) | 2.09 (2) | 2.963(6) | 166 (2) |
| C40—H40C…O40 ^{iv} | 0.97 | 2.47 | 3.146(9) | 127 |

Symmetry codes: (i) $x-1/2, -y+3/2, z$; (ii) $-x+1/2, y-1/2, -z+1$; (iii) $-x+1/2, y+1/2, -z+1$; (iv) $x+1/2, -y+1/2, z$.

Table S4 Hydrogen-bond geometry (\AA , $^\circ$) for **LTP**

| $D\text{---H}\cdots A$ | $D\text{---H}$ | $H\cdots A$ | $D\cdots A$ | $D\text{---H}\cdots A$ |
|---------------------------|----------------|-------------|-------------|------------------------|
| N1—H1N…O5F ⁱ | 0.90 | 1.88 | 2.779(3) | 176 |
| N1—H2N…O4E ⁱⁱ | 0.90 | 2.01 | 2.873(3) | 161 |
| N1—H2N…O40E ⁱⁱ | 0.90 | 1.87 | 2.711(18) | 154 |
| N1—H3N…O5B | 0.90 | 1.99 | 2.831(2) | 156 |
| N1—H4N…O4F ⁱⁱⁱ | 0.90 | 1.99 | 2.875(3) | 168 |
| N2—H5N…O5C ⁱⁱ | 0.90 | 1.94 | 2.815(3) | 165 |
| N2—H6N…O5A | 0.90 | 1.90 | 2.801(3) | 174 |
| N2—H7N…O4B | 0.90 | 1.90 | 2.772(3) | 161 |
| N2—H8N…O4E ⁱⁱ | 0.90 | 1.96 | 2.851(3) | 169 |
| N2—H8N…O40E ⁱⁱ | 0.90 | 1.84 | 2.73(2) | 171 |
| N3—H9N…O4B | 0.90 | 1.99 | 2.859(3) | 162 |

| | | | | |
|-------------------------------|------|------|-----------|-----|
| N3—H10N···O5D | 0.90 | 1.96 | 2.828(2) | 160 |
| N3—H11N···O5D ⁱ | 0.90 | 1.90 | 2.799(3) | 174 |
| N3—H12N···O4C ⁱⁱ | 0.90 | 1.88 | 2.756(3) | 165 |
| N4—H13N···O4C ⁱⁱ | 0.90 | 1.97 | 2.855(3) | 166 |
| N4—H14N···O5A ⁱⁱ | 0.90 | 1.95 | 2.821(3) | 164 |
| N4—H15N···O5C | 0.90 | 1.92 | 2.812(3) | 171 |
| N4—H16N···O4D | 0.90 | 1.89 | 2.774(3) | 166 |
| N5—H17N···O5B ⁱ | 0.90 | 1.91 | 2.801(3) | 172 |
| N5—H18N···O5F | 0.90 | 1.91 | 2.763(2) | 158 |
| N5—H19N···O4A ⁱⁱ | 0.90 | 1.88 | 2.758(3) | 164 |
| N5—H20N···O4D | 0.90 | 1.95 | 2.845(3) | 170 |
| N6—H21N···O5E ^{iv} | 0.90 | 1.90 | 2.765(3) | 161 |
| N6—H21N···O50E ^{iv} | 0.90 | 2.02 | 2.908(12) | 169 |
| N6—H22N···O4F | 0.90 | 1.93 | 2.812(3) | 165 |
| N6—H23N···O5E | 0.90 | 1.86 | 2.757(3) | 173 |
| N6—H23N···O50E | 0.90 | 2.16 | 3.061(19) | 176 |
| N6—H24N···O4A ⁱⁱ | 0.90 | 1.97 | 2.861(3) | 172 |
| N7—H25N···O5G ^v | 0.90 | 1.96 | 2.824(3) | 160 |
| N7—H26N···O5G | 0.90 | 1.89 | 2.785(3) | 175 |
| N7—H27N···O4K ^{vi} | 0.90 | 1.98 | 2.865(3) | 167 |
| N7—H28N···O4L ^{vii} | 0.90 | 1.93 | 2.803(3) | 164 |
| N7—H28N···O40L ^{vii} | 0.90 | 2.24 | 3.110(19) | 162 |
| N8—H29N···O4H | 0.90 | 1.97 | 2.867(3) | 171 |
| N8—H30N···O4K ^{vi} | 0.90 | 1.88 | 2.765(3) | 165 |
| N8—H31N···O5J ^{viii} | 0.90 | 1.91 | 2.806(3) | 178 |
| N8—H32N···O5L ^{vii} | 0.90 | 1.95 | 2.761(3) | 150 |

| | | | | |
|-------------------------------|------|------|-----------|-----|
| N8—H32N···O50L ^{vii} | 0.90 | 2.19 | 2.974(15) | 145 |
| N9—H33N···O4I ^v | 0.90 | 2.02 | 2.892(3) | 162 |
| N9—H33N···O40I ^{vi} | 0.90 | 1.84 | 2.713(16) | 162 |
| N9—H34N···O5I | 0.90 | 1.85 | 2.753(3) | 175 |
| N9—H34N···O50I | 0.90 | 2.19 | 3.088(14) | 173 |
| N9—H35N···O5K ^v | 0.90 | 1.95 | 2.810(2) | 159 |
| N9—H36N···O4H | 0.90 | 1.91 | 2.781(3) | 163 |
| N10—H37N···O4J | 0.90 | 1.97 | 2.871(3) | 176 |
| N10—H38N···O5H ⁱⁱⁱ | 0.90 | 1.89 | 2.787(3) | 178 |
| N10—H39N···O4I ^v | 0.90 | 1.95 | 2.834(3) | 165 |
| N10—H39N···O40I ^{vi} | 0.90 | 1.73 | 2.601(13) | 163 |
| N10—H40N···O5H | 0.90 | 2.02 | 2.825(3) | 148 |
| N11—H41N···O5I ^v | 0.90 | 1.93 | 2.769(3) | 155 |
| N11—H41N···O50I ^{vi} | 0.90 | 1.97 | 2.852(10) | 167 |
| N11—H42N···O4G ^{vi} | 0.90 | 1.98 | 2.862(3) | 166 |
| N11—H43N···O4J | 0.90 | 1.90 | 2.773(3) | 163 |
| N11—H44N···O5K | 0.90 | 1.91 | 2.809(3) | 175 |
| N12—H45N···O4L | 0.90 | 1.98 | 2.869(3) | 168 |
| N12—H45N···O40L | 0.90 | 2.12 | 3.01(3) | 170 |
| N12—H46N···O5L ^{ix} | 0.90 | 1.89 | 2.790(3) | 176 |
| N12—H46N···O50L ^{ix} | 0.90 | 1.72 | 2.62(2) | 176 |
| N12—H47N···O4G ^{vi} | 0.90 | 1.90 | 2.780(3) | 164 |
| N12—H48N···O5J | 0.90 | 2.02 | 2.813(3) | 147 |
| C1B—H1B1···O21K | 0.99 | 2.43 | 3.402(3) | 166 |
| C1C—H1C2···O21J | 0.99 | 2.46 | 3.434(3) | 170 |
| C3C—H3C2···O4B | 0.99 | 2.58 | 3.532(3) | 162 |

| | | | | |
|---------------------------------|------|------|-----------|-----|
| C3D—H3D1···O40E ^x | 0.99 | 2.42 | 3.359(16) | 159 |
| C4D—H4D3···O4E ^x | 0.98 | 2.60 | 3.513(3) | 156 |
| C4D—H4D3···O40E ^x | 0.98 | 2.56 | 3.451(19) | 151 |
| C4E—H4E2···O4D | 0.98 | 2.50 | 3.295(3) | 139 |
| C5E—H5E1···O1F | 0.98 | 2.61 | 3.507(3) | 152 |
| C4F—H4F1···O4A ^{xi} | 0.98 | 2.59 | 3.288(3) | 128 |
| C5F—H5F2···O1E ^x | 0.98 | 2.54 | 3.433(3) | 151 |
| C5H—H5H2···O1F ^{xii} | 0.98 | 2.54 | 3.135(3) | 119 |
| C1I—H1I1···O21D | 0.99 | 2.57 | 3.553(3) | 170 |
| C3I—H3I2···O4J | 0.99 | 2.58 | 3.564(3) | 171 |
| C4I—H4I2···O4J | 0.98 | 2.53 | 3.311(3) | 136 |
| C10I—H10D···O21D | 0.99 | 2.61 | 3.574(9) | 164 |
| C30I—H30D···O4J | 0.99 | 2.59 | 3.534(9) | 160 |
| C1J—H1J1···O21C | 0.99 | 2.50 | 3.477(3) | 171 |
| C3J—H3J1···O40F ^{xii} | 0.99 | 2.58 | 3.547(13) | 164 |
| C1K—H1K2···O21B | 0.99 | 2.53 | 3.508(3) | 171 |
| C1L—H1L2···O21A | 0.99 | 2.60 | 3.582(3) | 171 |
| C3L—H3L1···O4K ^{xii} | 0.99 | 2.60 | 3.578(3) | 169 |
| C30L—H30E···O4K ^{xii} | 0.99 | 2.44 | 3.389(17) | 161 |
| C4L—H4L3···O4K ^{xii} | 0.98 | 2.55 | 3.313(3) | 135 |
| C50L—H50G···O1G ^{xiii} | 0.98 | 2.49 | 3.41(3) | 155 |

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $-x+1, -y+1, -z+1$; (iii) $x, y-1, z$; (iv) $-x+1, -y+2, -z+1$; (v) $-x+2, -y+2, -z$; (vi) $-x+2, -y+1, -z$; (vii) $x, y+1, z$; (viii) $-x+1, -y+1, -z$; (ix) $-x+1, -y, -z$; (x) $x+1, y, z$; (xi) $x+1, y+1, z$; (xii) $x-1, y, z$; (xiii) $x-1, y-1, z$.