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Supporting information for article:

Crystal structure of a new polyoxometalate (POM) compound with a high level of crystallographic disorder

Eliska Skorepova, Ali Harchani, Mohamed Mongi Ftini, Michal Dušek and Amor Haddad

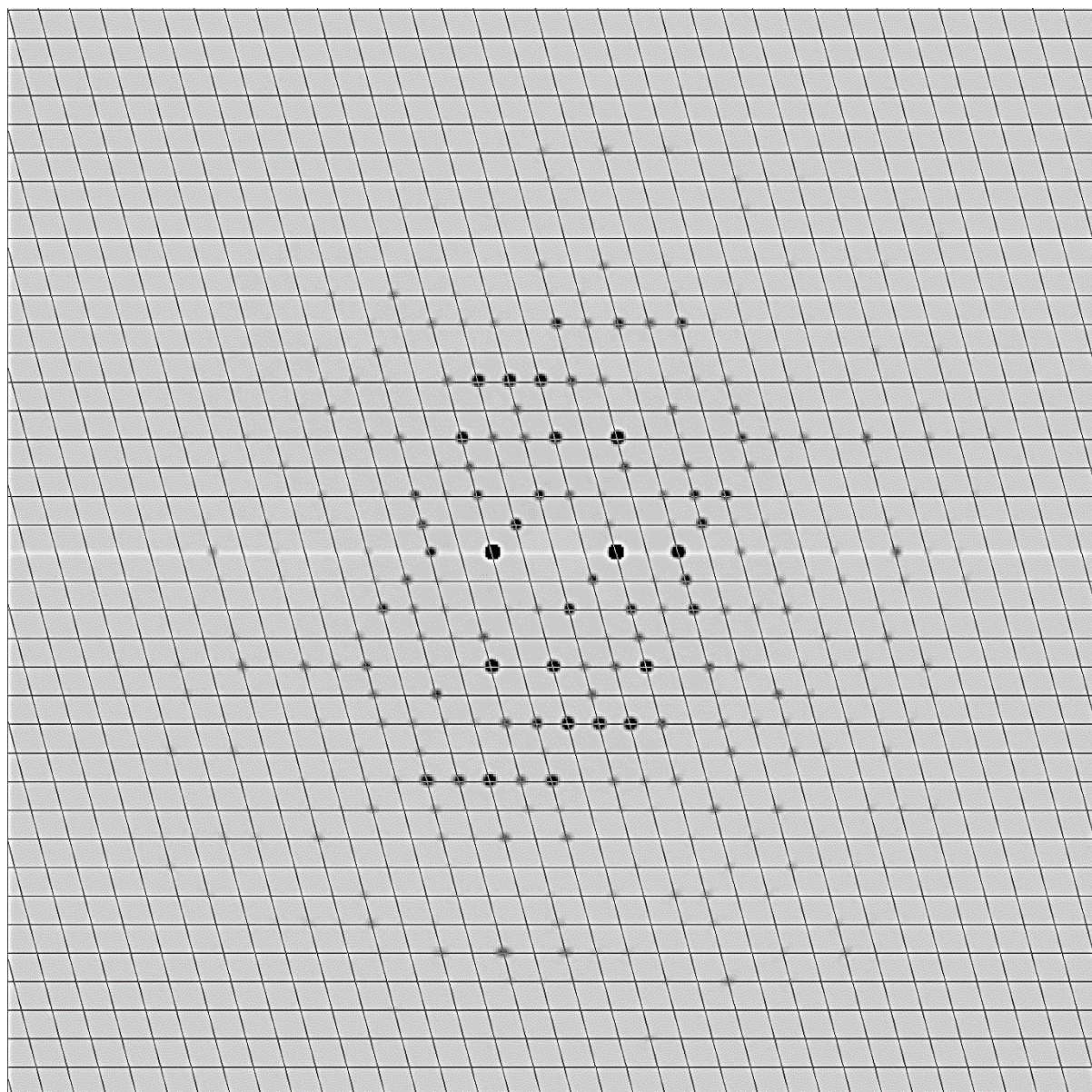


Fig. S1 Precession image 0kl

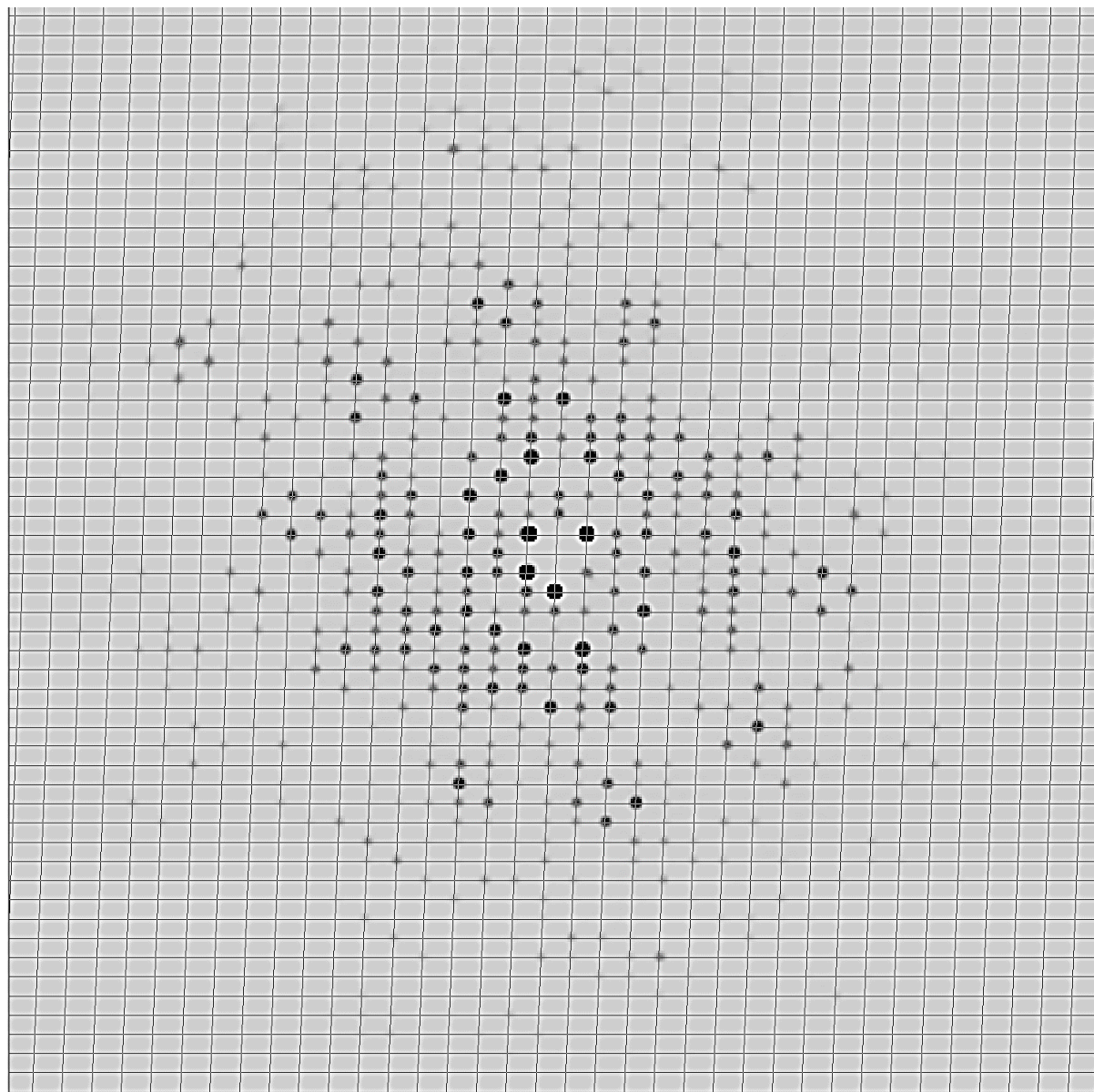


Fig. S2 Precession image h0l

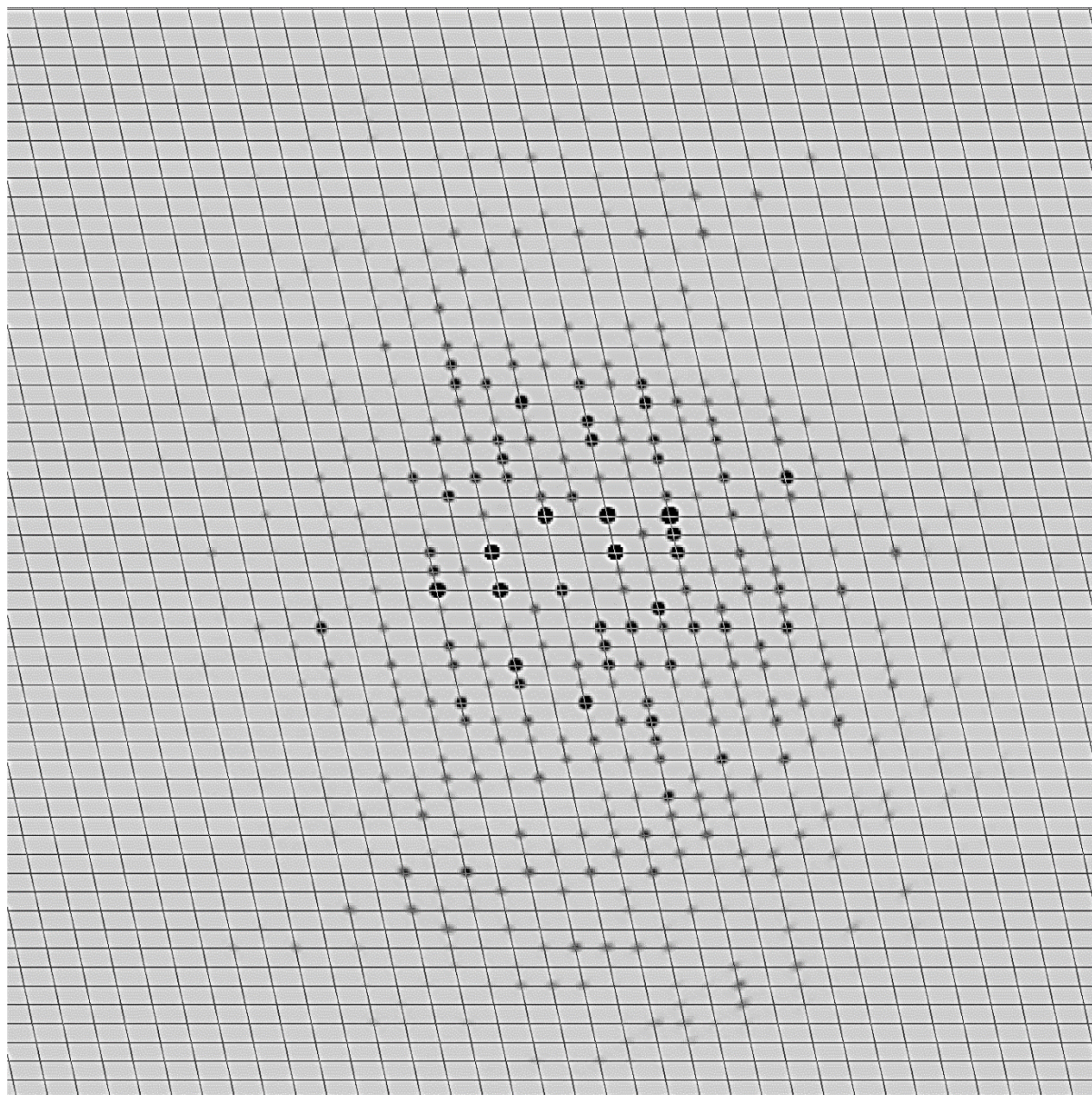


Fig. S3 Precession image hk0

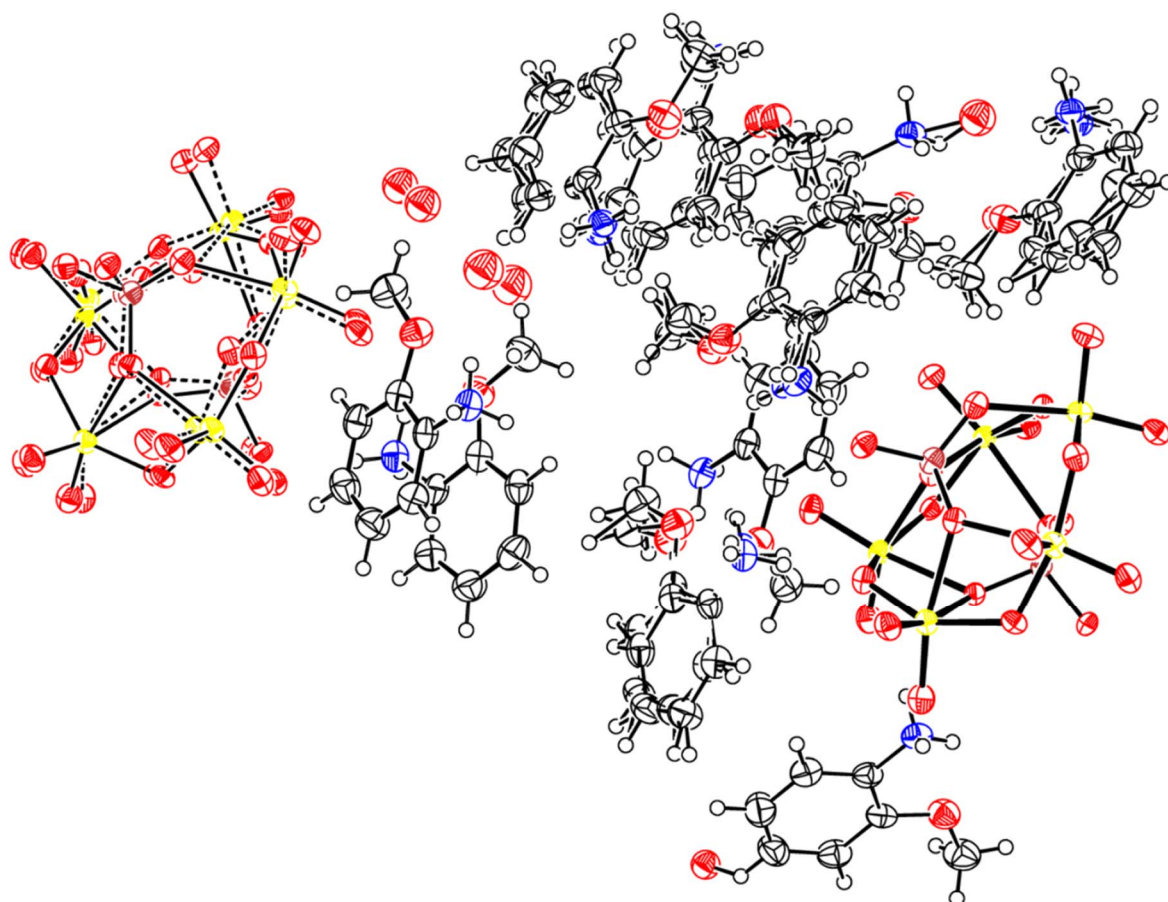


Fig. S4 The asymmetric unit of **1** with H atoms and thermal ellipsoids displayed.

Table S1. Hydrogen-bond geometry (Å, °) of compound **1**

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C1 <i>a</i> —H1 <i>c</i> 1 <i>a</i> ···O7 <i>b</i>	0.96	2.43	3.218 (11)	139.34
C5 <i>a</i> —H1 <i>c</i> 5 <i>a</i> ···O21 <i>b</i>	0.96	2.44	3.342 (11)	156.29
N1 <i>a</i> —H1 <i>n</i> 1 <i>a</i> ···O20 <i>a</i> ⁱⁱⁱ	0.87 (5)	2.10 (4)	2.819 (11)	140 (4)
N1 <i>a</i> —H2 <i>n</i> 1 <i>a</i> ···O24 <i>a</i>	0.87 (4)	2.36 (4)	2.658 (9)	100 (2)
N1 <i>a</i> —H2 <i>n</i> 1 <i>a</i> ···O6 <i>a</i> ^{iv}	0.87 (4)	2.34 (3)	3.187 (10)	163 (4)
N1 <i>a</i> —H2 <i>n</i> 1 <i>a</i> ···O18 <i>a</i> ^{iv}	0.87 (4)	2.45 (5)	2.858 (12)	109 (3)
O3 <i>w</i> —H1 <i>c</i> 1 <i>b</i> ···N1 <i>b</i> ⁱ	1.17	2.16	2.88 (5)	116.74
C1 <i>b</i> —H1 <i>c</i> 1 <i>b</i> ···O3 <i>w</i>	0.96	1.17	1.92 (5)	129.17
N1 <i>b</i> ⁱ —H1 <i>c</i> 5 <i>b</i> ···O19 <i>a</i> ⁱ	0.35	2.44	2.74 (4)	146.30
C5 <i>b</i> —H1 <i>c</i> 5 <i>b</i> ···O19 <i>a</i> ⁱ	0.96	2.44	3.33 (3)	154.60
C6 <i>b</i> —H2 <i>c</i> 6 <i>b</i> ···N1 <i>b</i> ⁱ	0.96	2.50	2.71 (8)	92.09
N1 <i>b</i> —H1 <i>n</i> 1 <i>b</i> ···O19 <i>a</i>	0.87 (6)	1.98 (6)	2.74 (4)	145 (7)
C5 <i>b</i> ⁱ —H1 <i>n</i> 1 <i>b</i> ···O19 <i>a</i>	1.36 (6)	1.98 (6)	3.33 (3)	175 (6)
N1 <i>b</i> —H2 <i>n</i> 1 <i>b</i> ···O3 <i>w</i> ⁱ	0.87 (10)	2.33 (7)	2.88 (5)	121 (4)
N1 <i>b</i> —H2 <i>n</i> 1 <i>b</i> ···O24 <i>b</i>	0.87 (10)	2.36 (7)	2.66 (5)	100 (6)
C1 <i>b</i> ⁱ —H2 <i>n</i> 1 <i>b</i> ···N1 <i>b</i>	1.18 (9)	0.87 (10)	1.81 (8)	124 (8)
C5 <i>b</i> ⁱ —H2 <i>n</i> 1 <i>b</i> ···O3 <i>w</i> ⁱ	0.99 (8)	2.33 (7)	2.83 (4)	110 (4)

C6c—H2c6c···O7a ⁱⁱⁱ	0.96	2.41	3.172 (11)	136.20
N1c—H1n1c···O7bx	0.87 (6)	2.22 (6)	3.07 (3)	166 (3)
N1c—H1n1c···O7b	0.87 (6)	1.95 (5)	2.799 (17)	164 (3)
N1c—H2n1c···O20bx	0.87 (4)	2.24 (5)	2.779 (19)	120 (4)
N1c—H2n1c···O24c	0.87 (4)	2.36 (4)	2.658 (12)	100 (2)
N1c—H2n1c···O20b	0.87 (4)	2.34 (4)	2.961 (13)	128 (5)
N1d—H1n1d···O21bx ^v	0.87 (5)	2.16 (5)	2.811 (17)	131 (4)
N1d—H1n1d···O9bx ^y	0.87 (5)	2.10 (5)	2.695 (17)	125 (5)
N1d—H1n1d···O21b ^v	0.87 (5)	2.43 (6)	2.996 (17)	123 (4)
N1d—H1n1d···O22b ^v	0.87 (5)	2.15 (4)	2.998 (13)	166 (5)
N1d—H2n1d···O24d	0.87 (4)	2.36 (5)	2.658 (11)	100 (3)
N1e—H1n1e···O23bx ^{vi}	0.87 (7)	1.70 (6)	2.55 (3)	162 (5)
N1e—H1n1e···O23b ^{vi}	0.87 (7)	1.97 (6)	2.82 (3)	164 (4)
N1f—H1n1e···O23bx ^{vi}	1.38 (6)	1.70 (6)	2.94 (3)	145 (3)
N1f—H1n1e···O23b ^{vi}	1.38 (6)	1.97 (6)	3.17 (2)	142 (3)
N1e—H2n1e···O4w	0.87 (5)	1.73 (5)	2.60 (3)	175 (4)
N1e—H2n1e···O24e	0.87 (5)	2.36 (5)	2.66 (2)	100 (3)
N1e—H2n1e···O24f	0.87 (5)	2.45 (4)	2.62 (2)	91 (3)
N1f—H2n1e···O4w	1.26 (4)	1.73 (5)	2.86 (3)	146 (4)
N1f—H2n1e···O24e	1.26 (4)	2.36 (5)	2.78 (2)	96 (2)
C3e—H1c3f···O2bx ^{vii}	1.16	2.44	3.23 (2)	123.90
C3f—H1c3f···O2bx ^{vii}	0.96	2.44	3.09 (2)	125.19
N1e—H1n1f···O23bx ^{vi}	0.75 (5)	2.08 (6)	2.55 (3)	120 (5)
N1e—H1n1f···O23b ^{vi}	0.75 (5)	2.31 (6)	2.82 (3)	126 (5)
N1f—H1n1f···O23bx ^{vi}	0.87 (6)	2.08 (6)	2.94 (3)	168 (4)
N1f—H1n1f···O23b ^{vi}	0.87 (6)	2.31 (6)	3.17 (2)	168 (4)
N1e—H2n1f···O4w	0.96 (6)	2.04 (4)	2.60 (3)	115 (3)
N1e—H2n1f···O24e	0.96 (6)	2.38 (4)	2.66 (2)	96 (3)
N1e—H2n1f···O24f	0.96 (6)	2.36 (4)	2.62 (2)	94 (3)
N1f—H2n1f···O4w	0.87 (5)	2.04 (4)	2.86 (3)	157 (5)
N1f—H2n1f···O24e	0.87 (5)	2.38 (4)	2.78 (2)	109 (3)
N1f—H2n1f···O24f	0.87 (5)	2.36 (4)	2.66 (2)	100 (3)
C6g—H1c6g···O3bx ^{viii}	0.96	2.46	3.39 (2)	163.83
C6g—H1c6g···O3b ^{viii}	0.96	1.85	2.78 (2)	163.77
C6k—H1c6g···O3bx ^{viii}	1.37	2.46	3.76 (2)	158.65
C6k—H1c6g···O3b ^{viii}	1.37	1.85	3.17 (2)	160.45
N1g—H1n1g···O16a ⁱⁱⁱ	0.87 (5)	2.47 (4)	3.219 (19)	145 (5)
N1g—H1n1g···O23a ⁱⁱⁱ	0.87 (5)	2.34 (6)	2.75 (3)	109 (4)
N1k—H1n1g···O16a ⁱⁱⁱ	0.83 (6)	2.47 (4)	3.074 (19)	131 (5)
N1k—H1n1g···O23a ⁱⁱⁱ	0.83 (6)	2.34 (6)	2.91 (3)	127 (4)
N1g—H2n1g···O24g	0.87 (4)	2.36 (5)	2.66 (2)	100 (3)
N1g—H2n1g···O24k	0.87 (4)	2.28 (5)	2.46 (2)	92 (3)

N1g—H2n1g···O2a	0.87 (4)	2.42 (5)	2.95 (2)	120 (5)
N1k—H2n1g···O24g	1.09 (4)	2.36 (5)	2.87 (2)	107 (3)
N1k—H2n1g···O24k	1.09 (4)	2.28 (5)	2.66 (2)	98 (3)
N1k—H2n1g···O2a	1.09 (4)	2.42 (5)	3.00 (2)	112 (4)
C4h—H1c4h···O2w'	0.96	2.44	3.38 (3)	167.92
C4l—H1c4h···O2w'	1.29	2.44	3.71 (3)	167.42
C6h—H2c6h···O24i	0.96	2.46	3.34 (3)	153.24
C6l—H2c6h···O24i	1.25	2.46	3.65 (3)	157.76
N1h—H1n1h···O10b ^{ix}	0.87 (6)	2.04 (5)	2.77 (3)	141 (4)
N1h—H1n1h···O10b ^{ix}	0.87 (6)	2.16 (5)	2.82 (3)	133 (4)
N1l—H1n1h···O10b ^{ix}	1.00 (6)	2.04 (5)	2.78 (3)	129 (3)
N1l—H1n1h···O10b ^{ix}	1.00 (6)	2.16 (5)	2.81 (3)	121 (3)
N1h—H2n1h···O6b ^{vii}	0.87 (5)	2.22 (6)	2.90 (3)	135 (4)
N1h—H2n1h···O24h	0.87 (5)	2.36 (5)	2.66 (2)	100 (4)
N1h—H2n1h···O24l	0.87 (5)	2.46 (5)	2.85 (2)	108 (4)
N1h—H2n1h···O6b ^{vii}	0.87 (5)	2.23 (6)	2.95 (3)	140 (4)
N1l—H2n1h···O6b ^{vii}	0.65 (5)	2.22 (6)	2.76 (3)	142 (5)
N1l—H2n1h···O24h	0.65 (5)	2.36 (5)	2.48 (2)	93 (4)
N1l—H2n1h···O24l	0.65 (5)	2.46 (5)	2.66 (2)	101 (5)
N1l—H2n1h···O6b ^{vii}	0.65 (5)	2.23 (6)	2.80 (3)	148 (5)
C6i—H3c6i···O23b ^{ix}	0.96	2.38	3.132 (19)	134.79
C6j—H3c6i···O23b ^{ix}	0.85	2.38	3.097 (19)	141.76
N1i—H1n1i···O7a ⁱⁱⁱ	0.87 (5)	2.28 (4)	3.084 (17)	154 (5)
N1i—H1n1i···O10a ⁱⁱⁱ	0.87 (5)	2.04 (6)	2.68 (3)	129 (5)
N1j—H1n1i···O7a ⁱⁱⁱ	1.14 (5)	2.28 (4)	3.372 (17)	160 (5)
N1j—H1n1i···O10a ⁱⁱⁱ	1.14 (5)	2.04 (6)	2.82 (3)	122 (4)
N1i—H2n1i···O3w ^x	0.87 (4)	2.37 (4)	3.20 (2)	159 (6)
N1i—H2n1i···O24i	0.87 (4)	2.36 (5)	2.66 (2)	100 (3)
N1i—H2n1i···O24j	0.87 (4)	2.44 (5)	2.83 (2)	108 (3)
N1j—H2n1i···O3w ^x	0.58 (5)	2.37 (4)	2.88 (2)	147 (7)
N1j—H2n1i···O24i	0.58 (5)	2.36 (5)	2.52 (2)	100 (4)
N1j—H2n1i···O24j	0.58 (5)	2.44 (5)	2.66 (2)	106 (4)
C5i—H1c5j···O23b ^{ix}	1.17	2.46	3.51 (2)	148.52
C5j—H1c5j···O23b ^{ix}	0.96	2.46	3.33 (2)	152.17
C6i—H3c6j···O23b ^{ix}	1.20	2.37	3.132 (19)	119.15
C6j—H3c6j···O23b ^{ix}	0.96	2.37	3.097 (19)	132.21
N1i—H1n1j···O5a ⁱⁱⁱ	0.68 (5)	2.46 (4)	2.795 (19)	113 (5)
N1i—H1n1j···O10a ⁱⁱⁱ	0.68 (5)	2.09 (6)	2.68 (3)	146 (6)
N1j—H1n1j···O5a ⁱⁱⁱ	0.87 (5)	2.46 (4)	2.694 (19)	96 (3)
N1j—H1n1j···O10a ⁱⁱⁱ	0.87 (5)	2.09 (6)	2.82 (3)	141 (5)
N1i—H2n1j···O3w ^x	1.19 (4)	2.02 (4)	3.20 (2)	169 (4)
N1i—H2n1j···O24i	1.19 (4)	2.35 (5)	2.66 (2)	91 (2)

N1i—H2n1j···O24j	1.19 (4)	2.36 (5)	2.83 (2)	101 (2)
N1j—H2n1j···O3w ^x	0.87 (4)	2.02 (4)	2.88 (2)	167 (5)
N1j—H2n1j···O24i	0.87 (4)	2.35 (5)	2.52 (2)	91 (3)
N1j—H2n1j···O24j	0.87 (4)	2.36 (5)	2.66 (2)	100 (3)
C1g—H1c1k···O6bx ^{vii}	1.10	2.46	3.39 (2)	141.18
C1g—H1c1k···O13bx ^{vii}	1.10	2.38	3.39 (3)	151.16
C1k—H1c1k···O6bx ^{vii}	0.96	2.46	3.23 (2)	136.73
C1k—H1c1k···O13bx ^{vii}	0.96	2.38	3.25 (3)	150.31
C6g—H1c6k···O3b ^{viii}	0.59	2.22	2.78 (2)	162.75
C6k—H1c6k···O3b ^{viii}	0.96	2.22	3.17 (2)	171.45
N1g—H1n1k···O9a	0.99 (5)	2.29 (5)	2.873 (18)	117 (4)
N1g—H1n1k···O16a ⁱⁱⁱ	0.99 (5)	2.32 (4)	3.219 (19)	151 (4)
N1k—H1n1k···O9a	0.87 (5)	2.29 (5)	2.690 (18)	108 (5)
N1k—H1n1k···O16a ⁱⁱⁱ	0.87 (5)	2.32 (4)	3.074 (19)	146 (4)
N1g—H2n1k···O24g	0.67 (4)	2.47 (5)	2.66 (2)	99 (5)
N1g—H2n1k···O24k	0.67 (4)	2.36 (5)	2.46 (2)	91 (4)
N1g—H2n1k···O2a	0.67 (4)	2.44 (5)	2.95 (2)	135 (6)
N1k—H2n1k···O24g	0.87 (4)	2.47 (5)	2.87 (2)	108 (4)
N1k—H2n1k···O24k	0.87 (4)	2.36 (5)	2.66 (2)	100 (3)
N1k—H2n1k···O2a	0.87 (4)	2.44 (5)	3.00 (2)	122 (5)
N1h—H1n1l···O10bx ^{ix}	0.80 (6)	1.98 (5)	2.77 (3)	166 (4)
N1h—H1n1l···O10b ^{ix}	0.80 (6)	2.07 (5)	2.82 (3)	157 (4)
N1l—H1n1l···O10bx ^{ix}	0.87 (6)	1.98 (5)	2.78 (3)	151 (4)
N1l—H1n1l···O10b ^{ix}	0.87 (6)	2.07 (5)	2.81 (3)	142 (4)
N1h—H2n1l···O6bx ^{vii}	1.09 (5)	2.09 (6)	2.90 (3)	129 (4)
N1h—H2n1l···O24h	1.09 (5)	2.29 (5)	2.66 (2)	97 (3)
N1h—H2n1l···O24l	1.09 (5)	2.36 (5)	2.85 (2)	105 (3)
N1h—H2n1l···O6b ^{vii}	1.09 (5)	2.08 (6)	2.95 (3)	134 (4)
N1l—H2n1l···O6bx ^{vii}	0.87 (5)	2.09 (6)	2.76 (3)	134 (4)
N1l—H2n1l···O24h	0.87 (5)	2.29 (5)	2.48 (2)	92 (3)
N1l—H2n1l···O24l	0.87 (5)	2.36 (5)	2.66 (2)	100 (4)
N1l—H2n1l···O6b ^{vii}	0.87 (5)	2.08 (6)	2.80 (3)	140 (4)
C1m—H1c1m···O4a ^{xi}	0.96	2.43	3.367 (17)	164.69
C1n—H1c1m···O4a ^{xi}	1.12	2.43	3.494 (17)	158.50
C6m—H2c6m···O2bx ^{viii}	0.96	2.28	2.81 (2)	114.26
C6n—H2c6m···O2bx ^{viii}	1.38	2.28	3.00 (2)	107.84
N1m—H1n1m···O12a	0.87 (6)	1.98 (6)	2.76 (3)	149 (4)
N1n—H1n1m···O12a	0.84 (6)	1.98 (6)	2.76 (3)	154 (4)
N1m—H2n1m···O24m	0.87 (5)	2.36 (4)	2.658 (19)	100 (3)
N1m—H2n1m···O24n	0.87 (5)	2.11 (4)	2.506 (19)	107 (3)
N1n—H2n1m···O24m	1.04 (5)	2.36 (4)	2.796 (19)	104 (2)
N1n—H2n1m···O24n	1.04 (5)	2.11 (4)	2.658 (19)	110 (3)

C6m—H2c6n···O2bx ^{viii}	0.85	2.33	2.81 (2)	116.61
C6n—H2c6n···O2bx ^{viii}	0.96	2.33	3.00 (2)	127.12
N1m—H1n1n···O12a	0.95 (6)	2.01 (6)	2.76 (3)	134 (4)
N1n—H1n1n···O12a	0.87 (6)	2.01 (6)	2.76 (3)	144 (4)
N1m—H2n1n···O24n	0.73 (5)	2.36 (4)	2.506 (19)	93 (3)
N1n—H2n1n···O24n	0.87 (5)	2.36 (4)	2.658 (19)	100 (3)
C1o—H1c1o···O16bx ^{viii}	0.96	2.33	3.23 (5)	155.69
C1o—H1c1o···O4w ⁱⁱ	0.96	2.46	3.04 (4)	118.70
C3o—H1c3o···O1w ^{vii}	0.96	2.41	3.21 (4)	140.93
N1o ⁱⁱ —H1c5o···O24o ⁱⁱ	1.11	1.77	2.66 (4)	133.58
C2o ⁱⁱ —H1c5o···O4w ⁱⁱ	0.77	2.35	2.90 (3)	129.12
C2o ⁱⁱ —H1c5o···O24o ⁱⁱ	0.77	1.77	2.31 (3)	126.07
C2o ⁱⁱ —H1c5o···N1o ⁱⁱ	0.77	1.11	1.46 (5)	100.28
C5o—H1c5o···O4w ⁱⁱ	0.96	2.35	2.98 (3)	122.49
C5o—H1c5o···N1o ⁱⁱ	0.96	1.11	2.01 (4)	151.27
C7o ⁱⁱ —H1c5o···O4w ⁱⁱ	1.34	2.35	3.61 (2)	154.93
C7o ⁱⁱ —H1c5o···N1o ⁱⁱ	1.34	1.11	2.45 (4)	175.85
N1o—H1n1o···O13bx ^{vii}	0.87 (5)	2.25 (5)	2.99 (3)	143 (6)
N1o—H1n1o···O24e	0.87 (5)	2.47 (6)	3.11 (3)	131 (6)
O4w—H2n1o···O24o	1.07 (6)	2.36 (6)	3.28 (3)	144 (5)
O4w—H2n1o···N1o	1.07 (6)	0.87 (7)	1.48 (5)	99 (5)
N1o—H2n1o···O4w	0.87 (7)	1.07 (6)	1.48 (5)	99 (5)
N1o—H2n1o···O24o	0.87 (7)	2.36 (6)	2.66 (4)	100 (5)

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

Table S2. The relevant bond distances (Å)

Bond	Bond distances	Bond	Bond distances
Mo1bx—O1bx	1.897 (8)	O24h—C7l	1.079 (17)
Mo1bx—O6bx	1.712 (13)	N1h—C2h	1.46 (2)

Mo1bx—O18bx	1.937 (10)	N1h—H1n1h	0.87 (6)
Mo1bx—O13bx	1.694 (14)	N1h—H2n1h	0.87 (5)
Mo1bx—Mo1b	0.427 (2)	N1h—N1l	0.25 (3)
Mo1bx—O1b	1.598 (5)	N1h—C2l	1.44 (2)
Mo1bx—O6b	1.724 (6)	N1h—H1n1l	0.80 (6)
Mo1bx—O13b	1.606 (7)	C1h—C4h	1.38 (3)
Mo4bx—O1bx	1.919 (9)	C1h—C5h	1.39 (2)
Mo4bx—O20bx	1.722 (16)	C1h—H1c1h	0.96
Mo4bx—O21bx	1.944 (10)	C1h—C1l	0.38 (3)
Mo4bx—O4bx	1.697 (11)	C1h—C4l	1.10 (3)
Mo4bx—Mo4b	0.211 (3)	C1h—H1c1l	0.988
Mo4bx—O1b	1.929 (5)	C2h—C3h	1.39 (2)
Mo4bx—O4b	1.895 (6)	C2h—C7h	1.373 (17)
Mo4bx—O20b	1.625 (8)	C2h—N1l	1.53 (3)
Mo4bx—O21b	1.893 (6)	C2h—C2l	0.291 (19)
Mo5bx—O23bx	1.716 (14)	C2h—C3l	1.12 (3)
Mo5bx—O10bx	1.959 (8)	C3h—C4h	1.38 (3)
Mo5bx—O7bx	1.712 (17)	C3h—H1c3h	0.96
Mo5bx—O21bx	1.913 (7)	C3h—C3l	0.33 (2)
Mo5bx—Mo5b	0.342 (3)	C3h—C4l	1.42 (3)
Mo5bx—O7b	1.950 (8)	C3h—H1c3l	0.7268
Mo5bx—O10b	1.698 (5)	C4h—H1c4h	0.96
Mo5bx—O15b	2.028 (6)	C4h—C3l	1.43 (3)
Mo5bx—O21b	2.132 (6)	C4h—C4l	0.37 (3)
Mo5bx—O23b	1.728 (7)	C4h—H1c4l	0.6897
Mo3bx—O10bx	1.935 (11)	C5h—C7h	1.401 (19)
Mo3bx—O19bx	1.730 (11)	C5h—H1c5h	0.96
Mo3bx—O16bx	1.698 (15)	C5h—C1l	1.04 (2)
Mo3bx—O12bx	1.922 (10)	C5h—C5l	0.37 (2)
Mo3bx—Mo3b	0.461 (2)	C5h—C7l	1.52 (2)
Mo3bx—O12b	1.738 (6)	C6h—H1c6h	0.96
Mo3bx—O16b	2.044 (7)	C6h—H2c6h	0.96
Mo3bx—O17b	2.078 (6)	C6h—H3c6h	0.96
Mo3bx—O19b	1.481 (6)	C6h—O24l	1.281 (19)
Mo2bx—O3bx	1.701 (10)	C6h—C6l	0.41 (3)
Mo2bx—O18bx	1.923 (12)	C6h—H2c6l	0.8114
Mo2bx—O12bx	1.960 (13)	C7h—C2l	1.166 (17)
Mo2bx—O2bx	1.717 (16)	C7h—C5l	1.358 (19)
Mo2bx—Mo2b	0.346 (3)	C7h—C7l	0.325 (19)
Mo2bx—O2b	1.493 (8)	H1c1h—H1c1l	0.4102
Mo2bx—O3b	1.822 (6)	H1c3h—H1c3l	0.3333
Mo2bx—O18b	1.753 (7)	H1c4h—H1c4l	0.4068

P1bx—O5bx	1.569 (14)	H1c5h—C5l	0.7522
P1bx—O14bx	1.525 (13)	H1c5h—H1c5l	0.3978
P1bx—O17bx	1.532 (13)	H1c6h—C6l	0.6592
P1bx—O11bx	1.537 (8)	H1c6h—H1c6l	0.4299
P1bx—P1b	0.176 (5)	H2c6h—H2c6l	0.4678
P1bx—O14b	1.352 (8)	H3c6h—C6l	0.951
P1bx—O17b	1.582 (8)	H3c6h—H3c6l	0.3824
P2bx—O15bx	1.560 (9)	H1n1h—H1n1l	0.28 (6)
P2bx—O22bx	1.562 (14)	H2n1h—N1l	0.65 (5)
P2bx—O9bx	1.535 (10)	H2n1h—H2n1l	0.23 (6)
P2bx—O8bx	1.519 (11)	O24i—C6i	1.44 (2)
P2bx—P2b	0.157 (6)	O24i—C7i	1.372 (18)
P2bx—O8b	1.471 (7)	O24i—O24j	0.402 (17)
P2bx—O9b	1.451 (9)	O24i—C7j	1.102 (19)
O3bx—Mo2b	1.662 (10)	N1i—C2i	1.46 (2)
O3bx—O3b	0.645 (16)	N1i—H1n1i	0.87 (5)
O5bx—P1b	1.514 (13)	N1i—H2n1i	0.87 (4)
O5bx—O5b	0.347 (16)	N1i—N1j	0.33 (2)
O14bx—Mo1b	2.151 (11)	N1i—C2j	1.38 (2)
O14bx—O14b	0.218 (13)	N1i—H1n1j	0.68 (5)
O15bx—Mo3b	2.053 (6)	C1i—C4i	1.38 (3)
O15bx—P2b	1.533 (7)	C1i—C5i	1.39 (3)
O15bx—O15b	0.383 (9)	C1i—H1c1i	0.96
O1bx—Mo4b	1.924 (9)	C1i—C1j	0.35 (4)
O1bx—O1b	0.547 (15)	C1i—C4j	1.22 (3)
O6bx—Mo1b	1.764 (14)	C1i—H1c1j	0.9213
O6bx—O6b	0.317 (16)	C2i—C3i	1.39 (2)
O23bx—Mo5b	1.794 (14)	C2i—C7i	1.373 (18)
O23bx—O23b	0.47 (2)	C2i—C2j	0.291 (17)
O17bx—Mo2b	2.107 (9)	C2i—C3j	1.11 (2)
O17bx—P1b	1.523 (12)	C2i—C7j	1.567 (17)
O17bx—O17b	0.380 (11)	C3i—C4i	1.38 (2)
O18bx—Mo1b	1.544 (11)	C3i—H1c3i	0.96
O18bx—Mo2b	2.147 (12)	C3i—C3j	0.30 (3)
O18bx—O18b	0.648 (12)	C3i—C4j	1.33 (3)
O11bx—P1b	1.444 (7)	C3i—H1c3j	0.809
O11bx—O11b	0.244 (8)	C4i—H1c4i	0.96
O10bx—Mo3b	1.726 (12)	C4i—C3j	1.50 (3)
O10bx—O10b	0.330 (10)	C4i—C4j	0.36 (4)
O13bx—Mo1b	1.941 (13)	C4i—H1c4j	0.7152
O13bx—O13b	0.724 (15)	C5i—C7i	1.401 (19)
O7bx—Mo5b	1.487 (16)	C5i—H1c5i	0.96

O7bx—O7b	0.29 (2)	C5i—C1j	1.08 (2)
O19bx—Mo3b	2.050 (11)	C5i—C5j	0.31 (2)
O19bx—O19b	0.540 (15)	C5i—C7j	1.543 (18)
O16bx—Mo3b	1.464 (16)	C6i—H1c6i	0.96
O16bx—O16b	0.629 (15)	C6i—H2c6i	0.96
O20bx—Mo4b	1.813 (16)	C6i—H3c6i	0.96
O20bx—O20b	0.486 (14)	C6i—O24j	1.32 (2)
O12bx—Mo2b	1.681 (13)	C6i—C6j	0.45 (2)
O12bx—O12b	0.571 (11)	C6i—H2c6j	0.7224
O21bx—Mo4b	1.992 (10)	C7i—C2j	1.225 (18)
O21bx—Mo5b	1.768 (8)	C7i—C5j	1.313 (19)
O21bx—O21b	0.533 (15)	C7i—C7j	0.316 (15)
O4bx—Mo4b	1.492 (11)	H1c1i—H1c1j	0.3989
O4bx—O4b	0.465 (17)	H1c3i—H1c3j	0.2971
O2bx—Mo2b	1.944 (16)	H1c4i—H1c4j	0.4287
O2bx—O2b	0.477 (15)	H1c5i—C5j	0.8152
O22bx—P2b	1.513 (13)	H1c5i—H1c5j	0.3174
O22bx—O8b	1.398 (11)	H1c6i—C6j	0.7461
O22bx—O22b	1.433 (10)	H1c6i—H1c6j	0.5292
O9bx—P2b	1.489 (9)	H2c6i—H2c6j	0.4962
O9bx—O9b	1.277 (17)	H3c6i—C6j	0.8535
O8bx—O8b	1.393 (13)	H3c6i—H3c6j	0.3611
O1w—O1w'	0.63 (5)	H1n1i—H1n1j	0.38 (6)
O2w—O2w'	0.71 (6)	H2n1i—N1j	0.58 (5)
O24a—C6a	1.441 (9)	H2n1i—H2n1j	0.38 (6)
O24a—C7a	1.372 (9)	O24j—C6j	1.44 (2)
N1a—C2a	1.462 (11)	O24j—C7j	1.372 (17)
N1a—H1n1a	0.87 (5)	N1j—C2j	1.46 (2)
N1a—H2n1a	0.87 (4)	N1j—H1n1j	0.87 (5)
C1a—C4a	1.381 (15)	N1j—H2n1j	0.87 (4)
C1a—C5a	1.386 (12)	C1j—C4j	1.38 (3)
C1a—H1c1a	0.96	C1j—C5j	1.39 (2)
C2a—C3a	1.387 (12)	C1j—H1c1j	0.96
C2a—C7a	1.373 (11)	C2j—C3j	1.39 (2)
C3a—C4a	1.382 (13)	C2j—C7j	1.373 (18)
C3a—H1c3a	0.96	C3j—C4j	1.38 (2)
C4a—H1c4a	0.96	C3j—H1c3j	0.96
C5a—C7a	1.401 (11)	C4j—H1c4j	0.96
C5a—H1c5a	0.96	C5j—C7j	1.401 (18)
C6a—H1c6a	0.96	C5j—H1c5j	0.96
C6a—H2c6a	0.96	C6j—H1c6j	0.96
C6a—H3c6a	0.96	C6j—H2c6j	0.96

O24b—C2b ⁱ	1.32 (5)	C6j—H3c6j	0.96
O24b—C3b ⁱ	0.89 (5)	O24k—C6k	1.44 (2)
O24b—C4b ⁱ	1.12 (8)	O24k—C7k	1.372 (18)
O24b—C6b	1.44 (5)	N1k—C2k	1.46 (2)
O24b—C7b	1.37 (4)	N1k—H1n1k	0.87 (5)
N1b—C2b	1.46 (7)	N1k—H2n1k	0.87 (4)
N1b—C5b ⁱ	0.76 (6)	C1k—C4k	1.38 (3)
N1b—H1c5b ⁱ	0.3454	C1k—C5k	1.39 (3)
N1b—H1n1b	0.87 (6)	C1k—H1c1k	0.96
N1b—H2n1b	0.87 (10)	C2k—C3k	1.39 (3)
C1b—C4b	1.38 (8)	C2k—C7k	1.373 (17)
C1b—C5b	1.39 (8)	C3k—C4k	1.38 (3)
C1b—H1c1b	0.96	C3k—H1c3k	0.96
C2b—C3b	1.39 (6)	C4k—H1c4k	0.96
C2b—C5b ⁱ	1.19 (5)	C5k—C7k	1.401 (19)
C2b—C7b	1.37 (2)	C5k—H1c5k	0.96
C2b—C7b ⁱ	0.74 (3)	C6k—H1c6k	0.96
C3b—C4b	1.38 (8)	C6k—H2c6k	0.96
C3b—C6b ⁱ	0.65 (5)	C6k—H3c6k	0.96
C3b—H1c3b	0.96	O24l—C6l	1.44 (2)
C4b—H1c4b	0.96	O24l—C7l	1.372 (18)
C5b—C7b	1.40 (3)	N1l—C2l	1.46 (2)
C5b—H1c5b	0.96	N1l—H1n1l	0.87 (6)
C5b—H2n1b ⁱ	0.99 (8)	N1l—H2n1l	0.87 (5)
C6b—H1c3b ⁱ	0.4713	C1l—C4l	1.38 (3)
C6b—H1c6b	0.96	C1l—C5l	1.39 (2)
C6b—H2c6b	0.96	C1l—H1c1l	0.96
C6b—H3c6b	0.96	C2l—C3l	1.39 (2)
C7b—C7b ⁱ	0.705 (13)	C2l—C7l	1.373 (17)
H1c3b—H2c6b ⁱ	0.6223	C3l—C4l	1.38 (3)
H1c5b—H1n1b ⁱ	0.5574	C3l—H1c3l	0.96
O24c—C6c	1.441 (12)	C4l—H1c4l	0.96
O24c—C7c	1.372 (10)	C5l—C7l	1.40 (2)
N1c—C2c	1.462 (15)	C5l—H1c5l	0.96
N1c—H1n1c	0.87 (6)	C6l—H1c6l	0.96
N1c—H2n1c	0.87 (4)	C6l—H2c6l	0.96
C1c—C4c	1.381 (19)	C6l—H3c6l	0.96
C1c—C5c	1.386 (16)	O24m—C6m	1.441 (18)
C1c—H1c1c	0.96	O24m—C7m	1.372 (17)
C2c—C3c	1.387 (14)	O24m—O24n	0.365 (15)
C2c—C7c	1.373 (11)	O24m—C6n	1.390 (19)
C3c—C4c	1.382 (17)	O24m—C7n	1.131 (17)

C3c—H1c3c	0.96	N1m—C2m	1.46 (2)
C4c—H1c4c	0.96	N1m—H1n1m	0.87 (6)
C5c—C7c	1.401 (12)	N1m—H2n1m	0.87 (5)
C5c—H1c5c	0.96	N1m—N1n	0.19 (2)
C6c—H1c6c	0.96	N1m—C2n	1.49 (2)
C6c—H2c6c	0.96	N1m—H2n1n	0.73 (5)
C6c—H3c6c	0.96	C1m—C4m	1.38 (3)
O24d—C6d	1.441 (11)	C1m—C5m	1.39 (2)
O24d—C7d	1.372 (9)	C1m—H1c1m	0.96
N1d—C2d	1.462 (14)	C1m—C1n	0.54 (3)
N1d—H1n1d	0.87 (5)	C1m—C4n	0.91 (3)
N1d—H2n1d	0.87 (4)	C2m—C3m	1.39 (2)
C1d—C4d	1.381 (19)	C2m—C7m	1.373 (17)
C1d—C5d	1.386 (14)	C2m—N1n	1.43 (2)
C1d—H1c1d	0.96	C2m—C2n	0.072 (18)
C2d—C3d	1.387 (14)	C2m—C3n	1.35 (2)
C2d—C7d	1.373 (11)	C2m—C7n	1.444 (17)
C3d—C4d	1.382 (15)	C3m—C4m	1.38 (2)
C3d—H1c3d	0.96	C3m—H1c3m	0.96
C4d—H1c4d	0.96	C3m—C2n	1.43 (2)
C5d—C7d	1.401 (11)	C3m—C3n	0.30 (2)
C5d—H1c5d	0.96	C3m—H1c3n	0.7107
C6d—H1c6d	0.96	C4m—H1c4m	0.96
C6d—H2c6d	0.96	C4m—C3n	1.18 (2)
C6d—H3c6d	0.96	C4m—C4n	0.48 (3)
O24e—C6e	1.44 (2)	C4m—H1c4n	0.8707
O24e—C7e	1.372 (15)	C5m—C7m	1.401 (17)
O24e—O24f	0.444 (14)	C5m—H1c5m	0.96
O24e—C6f	1.40 (2)	C5m—C1n	0.95 (2)
N1e—C2e	1.46 (2)	C5m—C5n	0.45 (2)
N1e—H1n1e	0.87 (7)	C6m—H1c6m	0.96
N1e—H2n1e	0.87 (5)	C6m—H2c6m	0.96
N1e—N1f	0.67 (3)	C6m—H3c6m	0.96
N1e—H1n1f	0.75 (5)	C6m—C6n	0.60 (2)
C1e—C4e	1.38 (3)	C6m—H2c6n	0.852
C1e—C5e	1.39 (2)	C6m—H3c6n	0.8146
C1e—H1c1e	0.96	C7m—C2n	1.303 (16)
C1e—C1f	0.59 (3)	C7m—C5n	1.261 (17)
C1e—C5f	1.03 (2)	C7m—C7n	0.249 (16)
C2e—C3e	1.39 (2)	H1c1m—H1c1n	0.6993
C2e—C7e	1.373 (18)	H1c3m—H1c3n	0.3898
C2e—N1f	1.26 (2)	H1c4m—H1c4n	0.6248

C2e—C2f	0.461 (17)	H1c5m—C5n	0.815
C2e—C7f	1.328 (18)	H1c5m—H1c5n	0.5917
C3e—C4e	1.38 (2)	H1c6m—C6n	0.5957
C3e—H1c3e	0.96	H1c6m—H1c6n	0.6989
C3e—C2f	1.02 (2)	H2c6m—H2c6n	0.6626
C3e—C3f	0.42 (2)	H3c6m—H3c6n	0.6239
C4e—H1c4e	0.96	H1n1m—N1n	0.84 (6)
C4e—C1f	1.33 (3)	H1n1m—H1n1n	0.26 (6)
C4e—C3f	1.15 (2)	H2n1m—H2n1n	0.28 (6)
C4e—C4f	0.45 (3)	O24n—C6n	1.441 (18)
C5e—C7e	1.401 (17)	O24n—C7n	1.372 (16)
C5e—H1c5e	0.96	N1n—C2n	1.46 (2)
C5e—C5f	0.55 (2)	N1n—H1n1n	0.87 (6)
C5e—C7f	1.142 (18)	N1n—H2n1n	0.87 (5)
C5e—H1c5f	1.021	C1n—C4n	1.38 (3)
C6e—H1c6e	0.96	C1n—C5n	1.39 (2)
C6e—H2c6e	0.96	C1n—H1c1n	0.96
C6e—H3c6e	0.96	C2n—C3n	1.39 (2)
C6e—C6f	0.47 (2)	C2n—C7n	1.373 (16)
C6e—H1c6f	0.5045	C3n—C4n	1.38 (2)
C7e—O24f	0.956 (15)	C3n—H1c3n	0.96
C7e—C2f	1.534 (16)	C4n—H1c4n	0.96
C7e—C7f	0.427 (14)	C5n—C7n	1.401 (17)
H1c1e—C1f	0.8986	C5n—H1c5n	0.96
H1c1e—H1c1f	0.7592	C6n—H1c6n	0.96
H1c3e—C3f	0.9386	C6n—H2c6n	0.96
H1c3e—H1c3f	0.4889	C6n—H3c6n	0.96
H1c4e—C4f	0.5858	O24o—C1o ⁱⁱ	0.65 (6)
H1c4e—H1c4f	0.4701	O24o—C4o ⁱⁱ	1.51 (5)
H1c5e—H1c5f	0.665	O24o—C5o ⁱⁱ	0.90 (3)
H1c6e—H1c6f	0.467	O24o—C6o	1.44 (4)
H2c6e—C6f	0.7948	O24o—C7o	1.37 (3)
H2c6e—H2c6f	0.4598	N1o—C2o	1.46 (5)
H3c6e—C6f	1.0063	N1o—H1n1o	0.87 (5)
H3c6e—H3c6f	0.6338	N1o—H2n1o	0.87 (7)
H1n1e—H1n1f	0.73 (7)	C1o—C4o	1.38 (6)
H2n1e—H2n1f	0.73 (6)	C1o—C5o	1.39 (6)
O24f—C6f	1.441 (19)	C1o—C6o ⁱⁱ	1.56 (5)
O24f—C7f	1.372 (15)	C1o—H1c1o	0.96
N1f—C2f	1.46 (2)	C2o—C3o	1.39 (4)
N1f—H1n1f	0.87 (6)	C2o—C5o ⁱⁱ	1.41 (3)
N1f—H2n1f	0.87 (5)	C2o—C7o	1.37 (2)

C1f—C4f	1.38 (3)	C2o—H1c5o ⁱⁱ	0.7728
C1f—C5f	1.39 (2)	C3o—C4o	1.38 (7)
C1f—H1c1f	0.96	C3o—C6o ⁱⁱ	0.88 (5)
C2f—C3f	1.387 (19)	C3o—H1c3o	0.96
C2f—C7f	1.373 (17)	C3o—H2c6o ⁱⁱ	0.8673
C3f—C4f	1.38 (2)	C3o—H3c6o ⁱⁱ	0.8408
C3f—H1c3f	0.96	C4o—C6o ⁱⁱ	0.58 (7)
C4f—H1c4f	0.96	C4o—H1c4o	0.96
C5f—C7f	1.401 (16)	C4o—H1c6o ⁱⁱ	0.4922
C5f—H1c5f	0.96	C5o—C7o	1.40 (3)
C6f—H1c6f	0.96	C5o—C7o ⁱⁱ	0.74 (3)
C6f—H2c6f	0.96	C5o—H1c5o	0.96
C6f—H3c6f	0.96	C6o—H1c6o	0.96
O24g—C6g	1.44 (2)	C6o—H2c6o	0.96
O24g—C7g	1.372 (17)	C6o—H3c6o	0.96
O24g—O24k	0.358 (16)	C7o—C7o ⁱⁱ	0.731 (14)
O24g—C6k	1.26 (2)	H1c4o—H1c6o ⁱⁱ	0.5119
N1g—C2g	1.46 (2)	Mo1a—O1a	1.898 (5)
N1g—H1n1g	0.87 (5)	Mo1a—O6a	1.712 (5)
N1g—H2n1g	0.87 (4)	Mo1a—O13a	1.695 (7)
N1g—N1k	0.26 (3)	Mo1a—O18a	1.942 (6)
N1g—C2k	1.52 (2)	Mo2a—O2a	1.717 (7)
N1g—H2n1k	0.67 (4)	Mo2a—O3a	1.701 (5)
C1g—C4g	1.38 (3)	Mo2a—O12a	1.960 (5)
C1g—C5g	1.39 (2)	Mo2a—O18a	1.929 (6)
C1g—H1c1g	0.96	Mo3a—O10a	1.936 (6)
C1g—C1k	0.45 (3)	Mo3a—O12a	1.922 (6)
C1g—C5k	0.99 (3)	Mo3a—O16a	1.697 (6)
C2g—C3g	1.39 (2)	Mo3a—O19a	1.730 (6)
C2g—C7g	1.373 (17)	Mo4a—O1a	1.919 (5)
C2g—N1k	1.46 (2)	Mo4a—O4a	1.696 (6)
C2g—C2k	0.33 (2)	Mo4a—O20a	1.724 (7)
C2g—C7k	1.130 (17)	Mo4a—O21a	1.943 (5)
C3g—C4g	1.38 (3)	Mo5a—O7a	1.712 (8)
C3g—H1c3g	0.96	Mo5a—O10a	1.961 (5)
C3g—C2k	1.10 (2)	Mo5a—O21a	1.913 (6)
C3g—C3k	0.36 (3)	Mo5a—O23a	1.716 (6)
C3g—C4k	1.41 (3)	P1a—O5a	1.569 (7)
C4g—H1c4g	0.96	P1a—O11a	1.537 (5)
C4g—C1k	1.03 (3)	P1a—O14a	1.524 (5)
C4g—C3k	1.46 (3)	P1a—O17a	1.534 (6)
C4g—C4k	0.42 (3)	P2a—O8a	1.556 (5)

C5g—C7g	1.401 (19)	P2a—O9a	1.534 (7)
C5g—H1c5g	0.96	P2a—O15a	1.560 (5)
C5g—C5k	0.44 (2)	P2a—O22a	1.517 (6)
C5g—C7k	1.372 (19)	Mo1b—O1b	1.898 (5)
C5g—H1c5k	0.7209	Mo1b—O6b	1.712 (7)
C6g—H1c6g	0.96	Mo1b—O13b	1.695 (7)
C6g—H2c6g	0.96	Mo1b—O18b	1.942 (6)
C6g—H3c6g	0.96	Mo2b—O2b	1.717 (7)
C6g—C6k	0.43 (2)	Mo2b—O3b	1.701 (6)
C6g—H1c6k	0.5852	Mo2b—O12b	1.960 (6)
C6g—H3c6k	1.0302	Mo2b—O18b	1.929 (7)
C7g—O24k	1.040 (18)	Mo3b—O10b	1.936 (6)
C7g—C5k	1.537 (19)	Mo3b—O12b	1.922 (6)
C7g—C7k	0.369 (16)	Mo3b—O16b	1.697 (7)
H1c1g—C1k	1.0369	Mo3b—O19b	1.730 (6)
H1c1g—H1c1k	0.4991	Mo4b—O1b	1.919 (5)
H1c3g—C3k	0.6632	Mo4b—O4b	1.696 (6)
H1c3g—H1c3k	0.3586	Mo4b—O20b	1.724 (8)
H1c4g—C4k	0.6612	Mo4b—O21b	1.943 (6)
H1c4g—H1c4k	0.451	Mo5b—O7b	1.712 (8)
H1c5g—H1c5k	0.4779	Mo5b—O10b	1.961 (5)
H1c6g—H1c6k	0.4329	Mo5b—O21b	1.913 (6)
H2c6g—C6k	0.8591	Mo5b—O23b	1.716 (7)
H2c6g—H2c6k	0.4866	P1b—O5b	1.569 (6)
H3c6g—H3c6k	0.4395	P1b—O11b	1.537 (5)
H1n1g—N1k	0.83 (6)	P1b—O14b	1.524 (6)
H1n1g—H1n1k	0.28 (7)	P1b—O17b	1.534 (6)
H2n1g—H2n1k	0.24 (6)	P2b—O8b	1.556 (5)
O24h—C6h	1.441 (19)	P2b—O9b	1.534 (8)
O24h—C7h	1.372 (17)	P2b—O15b	1.560 (6)
O24h—O24l	0.34 (2)	P2b—O22b	1.517 (7)
