Abstract

Table 1

Experimental details

Crystal data	
Chemical formula	$La_{1.75}Ni_{0.75}$
M_r	287.12
Crystal system, space group	Hexagonal, $P6_3mc$
Temperature (K)	300
a, *c* (Å)	10.0995 (18), 6.4490 (16)
V (Å^3)	569.7 (2)
Z	8
Radiation type	Mo *K*α
μ (mm^{-1})	30.37
Crystal size (mm)	0.10 × 0.08 × 0.02
Data collection	
Diffractometer	Bruker D8 Venture Photon 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Krause et al., 2015)
T_{min}, T_{max}	0.347, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4501, 388, 337
R_{int}	0.107
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.594
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.032, 0.062, 1.09
No. of reflections	388
No. of parameters	22
No. of restraints	1
	$w = 1/[\sigma^2(F_o^2) + (0.0062P)^2 + 13.2625P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.21, −1.12
Absolute structure	Flack x determined using 138 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	−1.0 (6)

Computer programs: *SHELXL2019*/1 (Sheldrick, 2019).

References

NOT FOUND

full crystallographic data

Computing details

Program(s) used to refine structure: *SHELXL2019*/1 (Sheldrick, 2019).

(20241004_a)

Crystal data

$La_{1.75}Ni_{0.75}$
M_r = 287.12
Hexagonal, $P6_3mc$
a = 10.0995 (18) Å
c = 6.4490 (16) Å
V = 569.7 (2) Å^3
Z = 8
F(000) = 966
D_x = 6.696 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3804 reflections
θ = 3.9–27.5°
μ = 30.37 mm^{-1}
T = 300 K
Lump, gray
0.10 × 0.08 × 0.02 mm

Data collection

Bruker D8 Venture Photon 100 CMOS diffractometer
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Krause et al., 2015)
T_{min} = 0.347, T_{max} = 0.746
4501 measured reflections
388 independent reflections
337 reflections with $I > 2\sigma(I)$
R_{int} = 0.107
θ_{max} = 25.0°, θ_{min} = 2.3°
h = −12→11
k = −12→11
l = −6→7

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.062
S = 1.09
388 reflections
22 parameters
1 restraint
$w = 1/[\sigma^2(F_o^2) + (0.0062P)^2 + 13.2625P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 1.21 e Å^{-3}
$\Delta\rho_{min}$ = −1.12 e Å^{-3}
Absolute structure: Flack x determined using 138 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter: −1.0 (6)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for (20241004_a)

	x	y	z	U_{iso}*/U_{eq}
La1	0.333333	0.666667	0.7870 (5)	0.0129 (7)
La2	0.12531 (11)	0.87469 (11)	0.0006 (2)	0.0145 (5)
La3	0.53923 (11)	0.46077 (11)	0.8123 (3)	0.0152 (5)
Ni1	0.8120 (2)	0.1880 (2)	0.0586 (6)	0.0173 (10)

Atomic displacement parameters (Å^2) for (20241004_a)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.0142 (10)	0.0142 (10)	0.0104 (17)	0.0071 (5)	0.000	0.000
La2	0.0143 (8)	0.0143 (8)	0.0151 (11)	0.0073 (9)	−0.0001 (5)	0.0001 (5)
La3	0.0156 (8)	0.0156 (8)	0.0139 (11)	0.0075 (8)	−0.0003 (5)	0.0003 (5)
Ni1	0.0150 (16)	0.0150 (16)	0.022 (2)	0.008 (2)	−0.0038 (9)	0.0038 (9)

Geometric parameters (Å, º) for (20241004_a)

La1—Ni1^{i}	2.938 (5)	La2—La3^{viii}	3.760 (2)
La1—Ni1^{ii}	2.938 (5)	La2—La3^{vii}	3.760 (2)
La1—Ni1^{iii}	2.938 (5)	La2—La2^{xiv}	3.797 (3)
La1—La3^{iv}	3.605 (2)	La2—La2^{xv}	3.797 (3)
La1—La3^{v}	3.605 (2)	La2—La3^{xvi}	3.8186 (15)
La1—La3	3.605 (2)	La2—La3^{xvii}	3.8186 (15)
La1—La3^{vi}	3.787 (3)	La2—La2^{xviii}	3.8990 (13)
La1—La3^{vii}	3.787 (3)	La2—La2^{xix}	3.8990 (13)
La1—La3^{viii}	3.787 (3)	La3—Ni1^{xx}	2.879 (3)
La1—La2^{ix}	3.891 (2)	La3—Ni1^{xxi}	2.879 (3)
La1—La2^{x}	3.891 (2)	La3—La3^{i}	3.5044 (17)
La1—La2^{xi}	3.891 (2)	La3—La3^{vi}	3.5044 (17)
La2—Ni1^{xii}	2.924 (3)	La3—Ni1^{ii}	3.599 (3)
La2—Ni1^{xiii}	2.924 (3)	La3—Ni1^{iii}	3.599 (3)
La2—Ni1^{vi}	3.054 (5)		
Ni1^{i}—La1—Ni1^{ii}	97.08 (13)	Ni1^{vi}—La2—La2^{xviii}	150.783 (18)
Ni1^{i}—La1—Ni1^{iii}	97.08 (13)	La3^{viii}—La2—La2^{xviii}	59.78 (3)
Ni1^{ii}—La1—Ni1^{iii}	97.08 (13)	La3^{vii}—La2—La2^{xviii}	89.80 (4)
Ni1^{i}—La1—La3^{iv}	65.83 (3)	La2^{xiv}—La2—La2^{xviii}	60.86 (2)
Ni1^{ii}—La1—La3^{iv}	152.52 (15)	La2^{xv}—La2—La2^{xviii}	90.0
Ni1^{iii}—La1—La3^{iv}	65.83 (3)	La3^{xvi}—La2—La2^{xviii}	90.03 (4)
Ni1^{i}—La1—La3^{v}	65.83 (3)	La3^{xvii}—La2—La2^{xviii}	142.75 (4)
Ni1^{ii}—La1—La3^{v}	65.83 (3)	La1^{xxii}—La2—La2^{xviii}	123.76 (4)
Ni1^{iii}—La1—La3^{v}	152.52 (15)	Ni1^{xii}—La2—La2^{xix}	108.40 (9)
La3^{iv}—La1—La3^{v}	119.797 (10)	Ni1^{xiii}—La2—La2^{xix}	50.75 (9)
Ni1^{i}—La1—La3	152.52 (15)	Ni1^{vi}—La2—La2^{xix}	150.783 (18)
Ni1^{ii}—La1—La3	65.83 (3)	La3^{viii}—La2—La2^{xix}	89.80 (4)
Ni1^{iii}—La1—La3	65.83 (3)	La3^{vii}—La2—La2^{xix}	59.78 (3)
La3^{iv}—La1—La3	119.795 (10)	La2^{xiv}—La2—La2^{xix}	90.0
La3^{v}—La1—La3	119.795 (10)	La2^{xv}—La2—La2^{xix}	60.86 (2)
Ni1^{i}—La1—La3^{vi}	95.99 (13)	La3^{xvi}—La2—La2^{xix}	142.75 (4)
Ni1^{ii}—La1—La3^{vi}	48.71 (7)	La3^{xvii}—La2—La2^{xix}	90.03 (4)
Ni1^{iii}—La1—La3^{vi}	48.71 (7)	La1^{xxii}—La2—La2^{xix}	123.76 (4)
La3^{iv}—La1—La3^{vi}	109.31 (7)	La2^{xviii}—La2—La2^{xix}	58.27 (4)
La3^{v}—La1—La3^{vi}	109.31 (7)	Ni1^{xx}—La3—Ni1^{xxi}	99.78 (18)
La3—La1—La3^{vi}	56.54 (4)	Ni1^{xx}—La3—La3^{i}	67.83 (7)
Ni1^{i}—La1—La3^{vii}	48.71 (7)	Ni1^{xxi}—La3—La3^{i}	67.83 (7)
Ni1^{ii}—La1—La3^{vii}	48.71 (7)	Ni1^{xx}—La3—La3^{vi}	129.64 (9)
Ni1^{iii}—La1—La3^{vii}	95.99 (13)	Ni1^{xxi}—La3—La3^{vi}	129.64 (9)
La3^{iv}—La1—La3^{vii}	109.31 (7)	La3^{i}—La3—La3^{vi}	133.89 (11)

La3^{v}—La1—La3^{vii}	56.53 (4)
La3—La1—La3^{vii}	109.31 (7)
La3^{vi}—La1—La3^{vii}	61.31 (7)
Ni1^{i}—La1—La3^{viii}	48.71 (7)
Ni1^{ii}—La1—La3^{viii}	95.99 (13)
Ni1^{iii}—La1—La3^{viii}	48.71 (7)
La3^{iv}—La1—La3^{viii}	56.53 (4)
La3^{v}—La1—La3^{viii}	109.31 (7)
La3—La1—La3^{viii}	109.31 (7)
La3^{vi}—La1—La3^{viii}	61.31 (7)
La3^{vii}—La1—La3^{viii}	61.31 (7)
Ni1^{i}—La1—La2^{ix}	50.82 (9)
Ni1^{ii}—La1—La2^{ix}	125.599 (18)
Ni1^{iii}—La1—La2^{ix}	125.600 (18)
La3^{iv}—La1—La2^{ix}	61.107 (19)
La3^{v}—La1—La2^{ix}	61.107 (19)
La3—La1—La2^{ix}	156.66 (11)
La3^{vi}—La1—La2^{ix}	146.80 (9)
La3^{vii}—La1—La2^{ix}	90.63 (4)
La3^{viii}—La1—La2^{ix}	90.63 (4)
Ni1^{i}—La1—La2^{x}	125.599 (18)
Ni1^{ii}—La1—La2^{x}	125.598 (18)
Ni1^{iii}—La1—La2^{x}	50.82 (9)
La3^{iv}—La1—La2^{x}	61.105 (19)
La3^{v}—La1—La2^{x}	156.66 (11)
La3—La1—La2^{x}	61.106 (19)
La3^{vi}—La1—La2^{x}	90.63 (4)
La3^{vii}—La1—La2^{x}	146.81 (9)
La3^{viii}—La1—La2^{x}	90.63 (4)
La2^{ix}—La1—La2^{x}	108.17 (5)
Ni1^{i}—La1—La2^{xi}	125.599 (18)
Ni1^{ii}—La1—La2^{xi}	50.82 (9)
Ni1^{iii}—La1—La2^{xi}	125.598 (17)
La3^{iv}—La1—La2^{xi}	156.66 (11)
La3^{v}—La1—La2^{xi}	61.105 (19)
La3—La1—La2^{xi}	61.106 (19)
La3^{vi}—La1—La2^{xi}	90.63 (4)
La3^{vii}—La1—La2^{xi}	90.63 (4)
La3^{viii}—La1—La2^{xi}	146.81 (9)
La2^{ix}—La1—La2^{xi}	108.17 (5)
La2^{x}—La1—La2^{xi}	108.17 (5)
Ni1^{xii}—La2—Ni1^{xiii}	153.77 (15)
Ni1^{xii}—La2—Ni1^{vi}	100.76 (9)
Ni1^{xiii}—La2—Ni1^{vi}	100.76 (9)
Ni1^{xii}—La2—La3^{viii}	63.73 (8)
Ni1^{xiii}—La2—La3^{viii}	123.88 (9)
Ni1^{vi}—La2—La3^{viii}	104.95 (9)
Ni1^{xii}—La2—La3^{vii}	123.88 (9)
Ni1^{xiii}—La2—La3^{vii}	63.73 (8)
Ni1^{vi}—La2—La3^{vii}	104.95 (9)
La3^{viii}—La2—La3^{vii}	61.78 (6)
Ni1^{xx}—La3—Ni1^{ii}	159.08 (7)
Ni1^{xxi}—La3—Ni1^{ii}	89.90 (13)
La3^{i}—La3—Ni1^{ii}	99.48 (8)
La3^{vi}—La3—Ni1^{ii}	47.79 (7)
Ni1^{xx}—La3—Ni1^{iii}	89.90 (13)
Ni1^{xxi}—La3—Ni1^{iii}	159.08 (7)
La3^{i}—La3—Ni1^{iii}	99.48 (8)
La3^{vi}—La3—Ni1^{iii}	47.79 (7)
Ni1^{ii}—La3—Ni1^{iii}	75.43 (13)
Ni1^{xx}—La3—La1	110.94 (8)
Ni1^{xxi}—La3—La1	110.94 (8)
La3^{i}—La3—La1	69.54 (9)
La3^{vi}—La3—La1	64.34 (8)
Ni1^{ii}—La3—La1	48.13 (7)
Ni1^{iii}—La3—La1	48.13 (7)
Ni1^{xx}—La3—La2^{xxiii}	154.11 (8)
Ni1^{xxi}—La3—La2^{xxiii}	67.53 (9)
La3^{i}—La3—La2^{xxiii}	122.32 (4)
La3^{vi}—La3—La2^{xxiii}	63.31 (3)
Ni1^{ii}—La3—La2^{xxiii}	46.76 (6)
Ni1^{iii}—La3—La2^{xxiii}	109.89 (8)
La1—La3—La2^{xxiii}	94.85 (4)
Ni1^{xx}—La3—La2^{xxiv}	67.53 (9)
Ni1^{xxi}—La3—La2^{xxiv}	154.11 (8)
La3^{i}—La3—La2^{xxiv}	122.32 (4)
La3^{vi}—La3—La2^{xxiv}	63.31 (3)
Ni1^{ii}—La3—La2^{xxiv}	109.89 (8)
Ni1^{iii}—La3—La2^{xxiv}	46.76 (6)
La1—La3—La2^{xxiv}	94.85 (4)
La2^{xxiii}—La3—La2^{xxiv}	113.87 (7)
Ni1^{xx}—La3—La1^{i}	50.07 (9)
Ni1^{xxi}—La3—La1^{i}	50.07 (9)
La3^{i}—La3—La1^{i}	59.12 (5)
La3^{vi}—La3—La1^{i}	166.99 (9)
Ni1^{ii}—La3—La1^{i}	138.47 (7)
Ni1^{iii}—La3—La1^{i}	138.47 (7)
La1—La3—La1^{i}	128.67 (11)
La2^{xxiii}—La3—La1^{i}	111.59 (4)
La2^{xxiv}—La3—La1^{i}	111.59 (4)
Ni1^{xx}—La3—La2^{x}	49.36 (7)
Ni1^{xxi}—La3—La2^{x}	127.66 (9)
La3^{i}—La3—La2^{x}	61.62 (5)
La3^{vi}—La3—La2^{x}	96.30 (5)
Ni1^{ii}—La3—La2^{x}	110.32 (8)
Ni1^{iii}—La3—La2^{x}	48.51 (7)
La1—La3—La2^{x}	63.14 (5)
La2^{xxiii}—La3—La2^{x}	155.85 (6)
La2^{xxiv}—La3—La2^{x}	61.92 (4)
La1^{i}—La3—La2^{x}	91.02 (4)
Ni1^{xx}—La3—La2^{xi}	127.66 (9)
Ni1^{xxi}—La3—La2^{xi}	49.36 (7)

Ni1^{xii}—La2—La2^{xiv}	49.52 (7)	La3^{i}—La3—La2^{xi}	61.62 (5)
Ni1^{xiii}—La2—La2^{xiv}	108.95 (7)	La3^{vi}—La3—La2^{xi}	96.30 (5)
Ni1^{vi}—La2—La2^{xiv}	108.11 (8)	Ni1^{ii}—La3—La2^{xi}	48.51 (7)
La3^{viii}—La2—La2^{xiv}	108.94 (3)	Ni1^{iii}—La3—La2^{xi}	110.32 (8)
La3^{vii}—La2—La2^{xiv}	146.93 (3)	La1—La3—La2^{xi}	63.14 (5)
Ni1^{xii}—La2—La2^{xv}	108.95 (7)	La2^{xxiii}—La3—La2^{xi}	61.92 (4)
Ni1^{xiii}—La2—La2^{xv}	49.52 (7)	La2^{xxiv}—La3—La2^{xi}	155.85 (6)
Ni1^{vi}—La2—La2^{xv}	108.11 (8)	La1^{i}—La3—La2^{xi}	91.02 (4)
La3^{viii}—La2—La2^{xv}	146.93 (3)	La2^{x}—La3—La2^{xi}	111.23 (8)
La3^{vii}—La2—La2^{xv}	108.94 (3)	La3^{xxv}—Ni1—La3^{xxvi}	84.22 (12)
La2^{xiv}—La2—La2^{xv}	60.0	La3^{xxv}—Ni1—La2^{xxvii}	82.29 (7)
Ni1^{xii}—La2—La3^{xvi}	48.35 (7)	La3^{xxvi}—Ni1—La2^{xxvii}	137.44 (16)
Ni1^{xiii}—La2—La3^{xvi}	157.88 (10)	La3^{xxv}—Ni1—La2^{xxviii}	137.44 (16)
Ni1^{vi}—La2—La3^{xvi}	61.99 (5)	La3^{xxvi}—Ni1—La2^{xxviii}	82.29 (7)
La3^{viii}—La2—La3^{xvi}	55.08 (3)	La2^{xxvii}—Ni1—La2^{xxviii}	80.97 (14)
La3^{vii}—La2—La3^{xvi}	105.44 (4)	La3^{xxv}—Ni1—La1^{vi}	81.22 (11)
La2^{xiv}—La2—La3^{xvi}	90.48 (4)	La3^{xxvi}—Ni1—La1^{vi}	81.22 (11)
La2^{xv}—La2—La3^{xvi}	145.62 (4)	La2^{xxvii}—Ni1—La1^{vi}	135.47 (10)
Ni1^{xii}—La2—La3^{xvii}	157.88 (10)	La2^{xxviii}—Ni1—La1^{vi}	135.47 (10)
Ni1^{xiii}—La2—La3^{xvii}	48.35 (7)	La3^{xxv}—Ni1—La2^{i}	133.87 (8)
Ni1^{vi}—La2—La3^{xvii}	61.99 (5)	La3^{xxvi}—Ni1—La2^{i}	133.87 (8)
La3^{viii}—La2—La3^{xvii}	105.44 (4)	La2^{xxvii}—Ni1—La2^{i}	81.39 (10)
La3^{vii}—La2—La3^{xvii}	55.08 (3)	La2^{xxviii}—Ni1—La2^{i}	81.39 (10)
La2^{xiv}—La2—La3^{xvii}	145.62 (4)	La1^{vi}—Ni1—La2^{i}	80.96 (13)
La2^{xv}—La2—La3^{xvii}	90.48 (4)	La3^{xxv}—Ni1—La3^{xxix}	136.86 (13)
La3^{xvi}—La2—La3^{xvii}	109.54 (8)	La3^{xxvi}—Ni1—La3^{xxix}	64.37 (4)
Ni1^{xii}—La2—La1^{xxii}	102.74 (7)	La2^{xxvii}—Ni1—La3^{xxix}	140.83 (13)
Ni1^{xiii}—La2—La1^{xxii}	102.74 (7)	La2^{xxviii}—Ni1—La3^{xxix}	69.52 (6)
Ni1^{vi}—La2—La1^{xxii}	48.22 (10)	La1^{vi}—Ni1—La3^{xxix}	66.04 (7)
La3^{viii}—La2—La1^{xxii}	63.99 (6)	La2^{i}—Ni1—La3^{xxix}	69.50 (7)
La3^{vii}—La2—La1^{xxii}	63.99 (5)	La3^{xxv}—Ni1—La3^{xxx}	64.37 (4)
La2^{xiv}—La2—La1^{xxii}	144.09 (3)	La3^{xxvi}—Ni1—La3^{xxx}	136.86 (13)
La2^{xv}—La2—La1^{xxii}	144.09 (3)	La2^{xxvii}—Ni1—La3^{xxx}	69.52 (6)
La3^{xvi}—La2—La1^{xxii}	55.75 (4)	La2^{xxviii}—Ni1—La3^{xxx}	140.83 (13)
La3^{xvii}—La2—La1^{xxii}	55.75 (4)	La1^{vi}—Ni1—La3^{xxx}	66.04 (7)
Ni1^{xii}—La2—La2^{xviii}	50.75 (9)	La2^{i}—Ni1—La3^{xxx}	69.50 (7)
Ni1^{xiii}—La2—La2^{xviii}	108.40 (9)	La3^{xxix}—Ni1—La3^{xxx}	120.12 (12)

Symmetry codes: (i) −*x*+1, −*y*+1, *z*+1/2; (ii) *y*, −*x*+*y*+1, *z*+1/2; (iii) *x*−*y*, *x*, *z*+1/2; (iv) −*y*+1, *x*−*y*+1, *z*; (v) −*x*+*y*, −*x*+1, *z*; (vi) −*x*+1, −*y*+1, *z*−1/2; (vii) *x*−*y*, *x*, *z*−1/2; (viii) *y*, −*x*+*y*+1, *z*−1/2; (ix) *x*, *y*, *z*+1; (x) −*x*+*y*, −*x*+1, *z*+1; (xi) −*y*+1, *x*−*y*+1, *z*+1; (xii) −*x*+*y*+1, −*x*+2, *z*; (xiii) −*y*, *x*−*y*, *z*; (xiv) −*y*+1, *x*−*y*+2, *z*; (xv) −*x*+*y*−1, −*x*+1, *z*; (xvi) −*y*+1, *x*−*y*+1, *z*−1; (xvii) −*x*+*y*, −*x*+1, *z*−1; (xviii) *x*−*y*+1, *x*+1, *z*+1/2; (xix) *y*−1, −*x*+*y*, *z*+1/2; (xx) −*y*+1, *x*−*y*, *z*+1; (xxi) −*x*+*y*+1, −*x*+1, *z*+1; (xxii) *x*, *y*, *z*−1; (xxiii) *x*−*y*+1, *x*, *z*+1/2; (xxiv) *y*, −*x*+*y*, *z*+1/2; (xxv) −*y*+1, *x*−*y*, *z*−1; (xxvi) −*x*+*y*+1, −*x*+1, *z*−1; (xxvii) −*x*+*y*, −*x*, *z*; (xxviii) −*y*+2, *x*−*y*+1, *z*; (xxix) *x*−*y*+1, *x*, *z*−1/2; (xxx) *y*, −*x*+*y*, *z*−1/2.