Electronic Supplementary Information

Probing the magnetic and magnetothermal properties of M(II)-Ln(III) complexes (where M(II) = Ni or Zn; Ln(III) = La or Pr or Gd)

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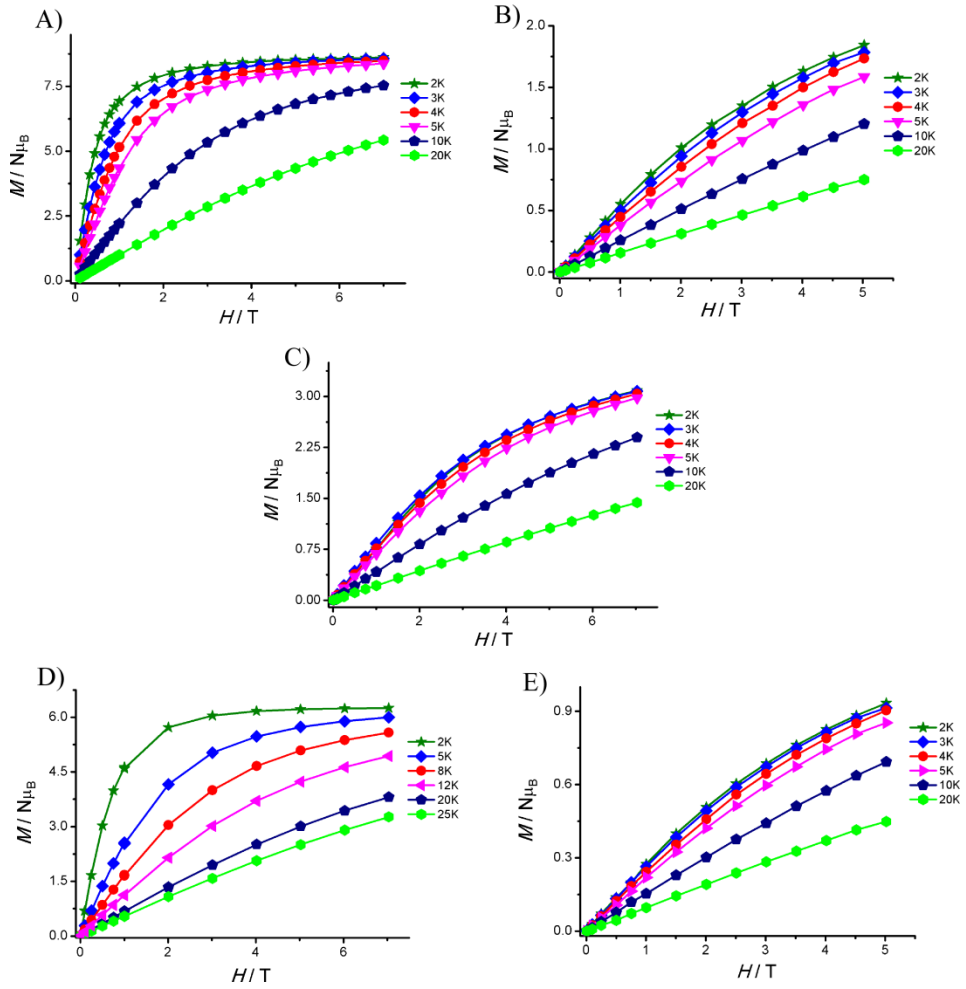

Fig S1. Field dependent magnetization data measured at the indicated temperatures of complexes **1** (A)**, 2** (B)**, 3** (C)**, 4** (D) **and 5** (E). Solid lines represent a guideline for the eye.

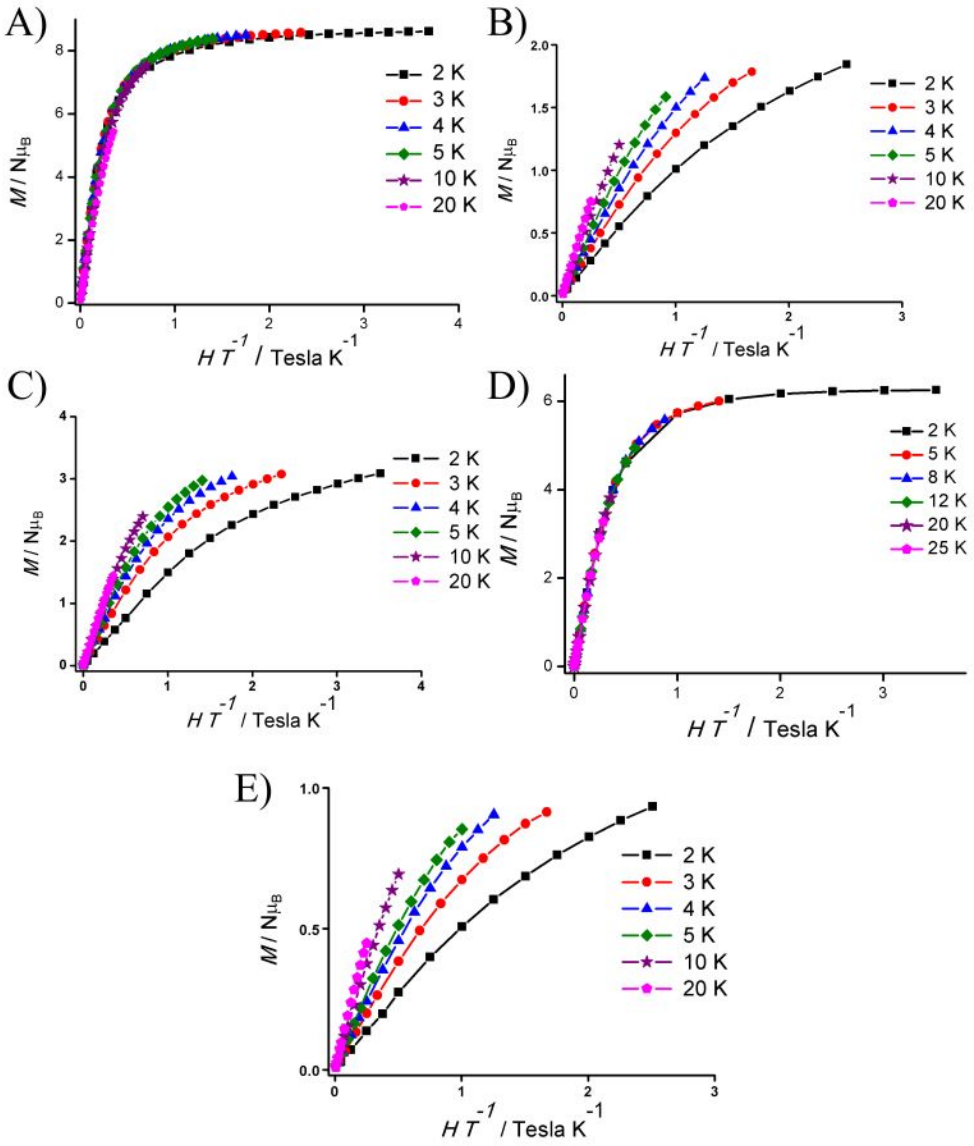

Fig S2. Reduced magnetization plots measured at the indicated temperatures of **1** (A)**, 2** (B)**, 3** (C)**, 4** (D) **and 5** (E). Solid lines represent a guideline for the eye.

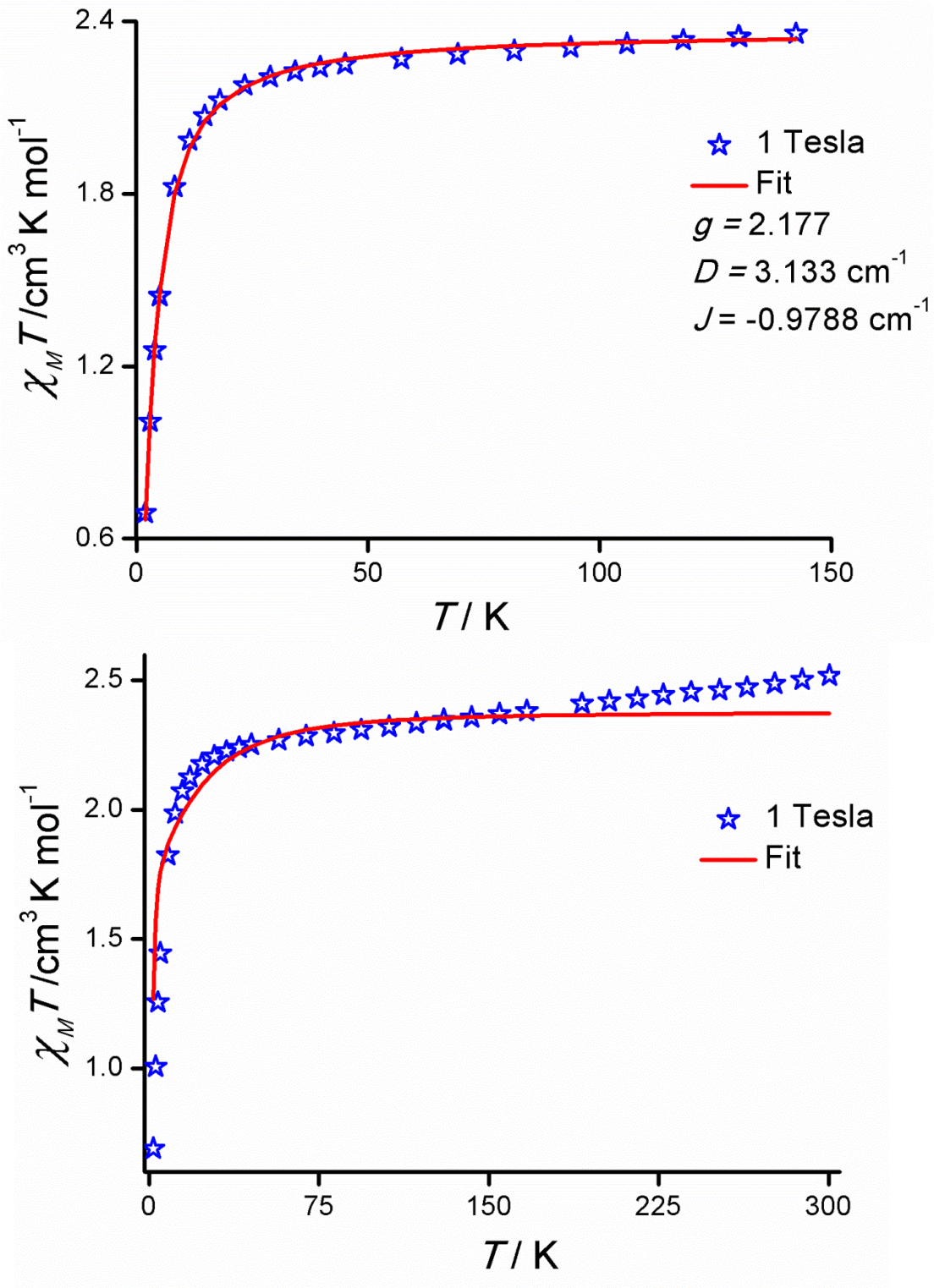

Fig S3. Fitting of the $\chi_M T(T)$ plot of **3** with (top panel) and without (bottom panel) the *J* parameter.

The parameters obtained without *J* appears non-realistic; D = -56 cm^{-1} and g = 2.18, and are therefore not considered.

Crystallographic information table

Complex 1:

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;
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R(int) was 0.3284 before and 0.1528 after correction
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Refinement of F^2^ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2^, conventional R-factors R are based on F, with F set to zero for negative F^2^. The threshold expression of F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2^ are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All the non-hydrogen atoms were refined anisotropically except the disordered nitrate groups.

For the disordered methanol solvent molecule hydrogen atoms were not added geometrically but to the molecular formula.

For the disordered group we have used several contrainsts and restraints such as DFIX, DANG, FLAT, ISOR, SIMU etc. for better convergence of the structure.
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N61 N 1.5929(8) 0.4806(3) 0.2569(6) 0.048(2) Uani 1 1 d . . .
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C16 C 1.3153(4) 0.32881(16) 0.4215(3) 0.0241(14) Uani 1 1 d G A .
C17 C 1.2513(6) 0.2394(3) 0.4291(5) 0.0214(14) Uani 1 1 d . . .
H17A H 1.2086 0.2173 0.4675 0.026 Uiso 1 1 calc R . .
C18 C 1.2341(6) 0.1757(3) 0.3023(6) 0.0243(15) Uani 1 1 d . . .
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C20 C 1.1366(8) 0.1250(3) 0.1621(7) 0.0358(18) Uani 1 1 d . . .
H20A H 1.1004 0.1210 0.0907 0.043 Uiso 1 1 calc R . .
C21 C 1.1454(8) 0.0845(3) 0.2306(7) 0.0371(19) Uani 1 1 d . . .
H21A H 1.1116 0.0536 0.2061 0.045 Uiso 1 1 calc R . .
C22 C 1.2018(7) 0.0886(3) 0.3321(7) 0.0345(18) Uani 1 1 d . . .
H22A H 1.2113 0.0604 0.3768 0.041 Uiso 1 1 calc R . .
C23 C 1.2453(7) 0.1346(3) 0.3695(6) 0.0277(15) Uani 1 1 d . . .
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C24 C 1.1643(7) 0.2121(3) 0.1150(6) 0.0282(16) Uani 1 1 d . . .
H24A H 1.1976 0.2000 0.0526 0.034 Uiso 1 1 calc R . .
H24B H 1.0771 0.2170 0.0929 0.034 Uiso 1 1 calc R . .
C25 C 1.3485(15) 0.4628(4) 0.4505(9) 0.082(5) Uani 1 1 d . . .

H25A H 1.3722 0.4874 0.4013 0.122 Uiso 1 1 calc R A .
H25B H 1.4020 0.4652 0.5181 0.122 Uiso 1 1 calc R . .
H25C H 1.2658 0.4692 0.4615 0.122 Uiso 1 1 calc R . .
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C36 C 1.4443(6) 0.3043(3) 0.0542(5) 0.0267(16) Uani 1 1 d . A .
C37 C 1.4711(6) 0.2119(3) 0.0765(5) 0.0246(15) Uani 1 1 d . . .
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C38 C 1.4947(6) 0.1649(3) 0.2314(6) 0.0276(16) Uani 1 1 d . . .
C39 C 1.5701(6) 0.1707(3) 0.3279(6) 0.0290(16) Uani 1 1 d . . .
C40 C 1.6067(8) 0.1282(4) 0.3856(7) 0.042(2) Uani 1 1 d . . .
H40A H 1.6558 0.1311 0.4524 0.051 Uiso 1 1 calc R . .
C41 C 1.5724(9) 0.0818(4) 0.3467(9) 0.051(2) Uani 1 1 d . . .
H41A H 1.5999 0.0531 0.3858 0.061 Uiso 1 1 calc R . .
C42 C 1.4985(9) 0.0771(4) 0.2515(9) 0.050(2) Uani 1 1 d . . .
H42A H 1.4751 0.0450 0.2257 0.061 Uiso 1 1 calc R . .
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H44B H 1.6698 0.2328 0.3113 0.038 Uiso 1 1 calc R . .
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H45C H 1.3461 0.4292 -0.0862 0.054 Uiso 1 1 calc R . .
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H1S2 H 0.9035 0.2975 0.1340 0.079 Uiso 1 1 calc R . .
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O71 0.150(11) 0.079(7) 0.130(10) -0.012(7) -0.019(9) 0.027(7)
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C13 0.023(3) 0.039(4) 0.019(3) -0.008(3) 0.003(3) -0.001(3)
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C16 0.022(3) 0.032(4) 0.018(3) -0.002(3) -0.001(3) 0.001(3)
C17 0.017(3) 0.028(4) 0.019(3) 0.004(3) 0.002(2) 0.001(3)
C18 0.023(3) 0.025(4) 0.027(4) -0.003(3) 0.009(3) -0.006(3)
C19 0.024(3) 0.031(4) 0.026(4) -0.002(3) 0.006(3) -0.004(3)
C20 0.039(4) 0.038(4) 0.029(4) -0.009(4) 0.001(3) -0.005(4)
C21 0.040(4) 0.023(4) 0.048(5) -0.007(4) 0.008(4) -0.007(3)
C22 0.040(4) 0.018(4) 0.048(5) -0.004(3) 0.017(4) -0.002(3)
C23 0.027(4) 0.030(4) 0.027(4) 0.000(3) 0.005(3) -0.001(3)
C24 0.026(4) 0.034(4) 0.024(4) -0.004(3) 0.000(3) -0.005(3)
C25 0.181(15) 0.025(5) 0.050(6) -0.018(5) 0.053(8) -0.030(7)
C31 0.023(3) 0.047(5) 0.011(3) -0.003(3) 0.006(3) -0.007(3)
C32 0.025(4) 0.042(4) 0.018(4) -0.002(3) 0.002(3) -0.003(3)
C33 0.029(4) 0.059(5) 0.011(3) 0.005(3) 0.005(3) -0.002(4)
C34 0.029(4) 0.041(4) 0.019(3) 0.008(3) 0.001(3) -0.008(3)
C35 0.025(4) 0.039(4) 0.021(4) 0.005(3) 0.001(3) -0.013(3)

C36 0.021(3) 0.044(4) 0.015(3) 0.001(3) 0.003(3) -0.010(3)
C37 0.020(3) 0.038(4) 0.016(3) -0.006(3) 0.004(3) -0.003(3)
C38 0.026(3) 0.038(4) 0.021(4) -0.002(3) 0.009(3) 0.006(3)
C39 0.027(4) 0.042(4) 0.018(3) 0.001(3) 0.004(3) 0.006(3)
C40 0.044(5) 0.052(6) 0.029(4) 0.013(4) 0.002(4) 0.016(4)
C41 0.059(6) 0.040(5) 0.054(6) 0.021(5) 0.007(5) 0.015(5)
C42 0.055(6) 0.030(5) 0.067(7) 0.002(5) 0.012(5) 0.011(4)
C43 0.036(4) 0.033(4) 0.031(4) -0.004(3) 0.005(3) 0.006(3)
C44 0.026(4) 0.055(5) 0.014(3) -0.001(3) 0.005(3) 0.004(3)
C45 0.042(5) 0.035(4) 0.031(4) 0.007(4) 0.007(3) -0.006(4)

_geom_special_details
;
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.
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Gd1 O11 2.396(5) . ?
Gd1 O72 2.420(7) . ?
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_computing_publication_material   'Bruker SHELXTL'

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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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 'calc w=1/[\s^2^(Fo^2^)+(0.0574P)^2^+18.5424P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_site_symmetry_multiplicity
_atom_site_calc_flag
_atom_site_refinement_flags
_atom_site_disorder_assembly
_atom_site_disorder_group
Pr1 Pr 0.55010(3) 0.108674(10) 0.76454(2) 0.02171(9) Uani 1 1 d . . .
Ni2 Ni 0.60822(6) 0.23880(2) 0.74878(5) 0.01583(14) Uani 1 1 d . . .
C11 C 0.7078(4) 0.21551(18) 0.5236(4) 0.0173(9) Uani 1 1 d . . .
C12 C 0.7315(4) 0.20905(19) 0.4196(4) 0.0209(10) Uani 1 1 d . . .
H12A H 0.7565 0.2366 0.3827 0.025 Uiso 1 1 calc R . .
C13 C 0.7197(5) 0.1644(2) 0.3704(4) 0.0229(10) Uani 1 1 d . . .
H13A H 0.7350 0.1612 0.2997 0.028 Uiso 1 1 calc R . .
C14 C 0.6850(5) 0.1232(2) 0.4243(4) 0.0236(11) Uani 1 1 d . . .
H14A H 0.6779 0.0919 0.3910 0.028 Uiso 1 1 calc R . .
C15 C 0.6612(5) 0.12867(19) 0.5262(4) 0.0207(10) Uani 1 1 d . . .
C16 C 0.6711(4) 0.17464(18) 0.5790(4) 0.0188(9) Uani 1 1 d . . .
C17 C 0.7351(4) 0.26349(17) 0.5716(4) 0.0178(9) Uani 1 1 d . . .
H17A H 0.7781 0.2859 0.5343 0.021 Uiso 1 1 calc R . .
C18 C 0.7516(4) 0.32527(17) 0.6984(4) 0.0180(9) Uani 1 1 d . . .
C19 C 0.7409(5) 0.36648(18) 0.6319(4) 0.0216(10) Uani 1 1 d . . .
H19A H 0.7041 0.3633 0.5606 0.026 Uiso 1 1 calc R . .
C20 C 0.7840(5) 0.41208(19) 0.6698(5) 0.0263(11) Uani 1 1 d . . .
H20A H 0.7762 0.4400 0.6246 0.032 Uiso 1 1 calc R . .
C21 C 0.8379(5) 0.4167(2) 0.7729(5) 0.0308(12) Uani 1 1 d . . .

H21A H 0.8684 0.4477 0.7985 0.037 Uiso 1 1 calc R . .
C22 C 0.8479(5) 0.3764(2) 0.8391(5) 0.0284(12) Uani 1 1 d . . .
H22A H 0.8857 0.3802 0.9100 0.034 Uiso 1 1 calc R . .
C23 C 0.8035(4) 0.32990(18) 0.8047(4) 0.0197(10) Uani 1 1 d . . .
C24 C 0.8212(5) 0.28896(19) 0.8855(4) 0.0234(11) Uani 1 1 d . . .
H24A H 0.9083 0.2839 0.9057 0.028 Uiso 1 1 calc R . .
H24B H 0.7894 0.3004 0.9494 0.028 Uiso 1 1 calc R . .
C25 C 0.6308(8) 0.0420(2) 0.5404(5) 0.0477(18) Uani 1 1 d . . .
H25A H 0.6069 0.0174 0.5892 0.071 Uiso 1 1 calc R . .
H25B H 0.7119 0.0347 0.5262 0.071 Uiso 1 1 calc R . .
H25C H 0.5752 0.0410 0.4740 0.071 Uiso 1 1 calc R . .
N11 N 0.7066(4) 0.27844(14) 0.6596(3) 0.0163(8) Uani 1 1 d . . .
O11 O 0.6456(3) 0.17616(12) 0.6768(3) 0.0183(7) Uani 1 1 d . . .
O12 O 0.6287(4) 0.09037(13) 0.5869(3) 0.0277(8) Uani 1 1 d . . .
O13 O 0.7680(3) 0.24215(13) 0.8557(3) 0.0218(7) Uani 1 1 d . . .
C31 C 0.5310(4) 0.24609(19) 0.9875(4) 0.0197(10) Uani 1 1 d . . .
C32 C 0.5249(5) 0.2521(2) 1.0957(4) 0.0227(10) Uani 1 1 d . . .
H32A H 0.5161 0.2842 1.1232 0.027 Uiso 1 1 calc R . .
C33 C 0.5315(5) 0.2123(2) 1.1619(4) 0.0238(11) Uani 1 1 d . . .
H33A H 0.5290 0.2170 1.2350 0.029 Uiso 1 1 calc R . .
C34 C 0.5419(5) 0.16458(19) 1.1223(4) 0.0230(10) Uani 1 1 d . . .
H34A H 0.5458 0.1370 1.1683 0.028 Uiso 1 1 calc R . .
C35 C 0.5464(5) 0.15804(18) 1.0162(4) 0.0208(10) Uani 1 1 d . . .
C36 C 0.5413(4) 0.19851(19) 0.9455(4) 0.0194(10) Uani 1 1 d . . .
C37 C 0.5130(5) 0.28999(19) 0.9212(4) 0.0214(10) Uani 1 1 d . . .
H37A H 0.4882 0.3192 0.9527 0.026 Uiso 1 1 calc R . .
C38 C 0.4889(5) 0.33563(19) 0.7653(4) 0.0227(10) Uani 1 1 d . . .
C39 C 0.5226(5) 0.3822(2) 0.8031(5) 0.0289(12) Uani 1 1 d . . .
H39A H 0.5727 0.3860 0.8689 0.035 Uiso 1 1 calc R . .
C40 C 0.4819(6) 0.4235(2) 0.7433(6) 0.0402(15) Uani 1 1 d . . .
H40A H 0.5049 0.4556 0.7681 0.048 Uiso 1 1 calc R . .
C41 C 0.4084(6) 0.4177(2) 0.6482(5) 0.0400(15) Uani 1 1 d . . .
H41A H 0.3797 0.4458 0.6082 0.048 Uiso 1 1 calc R . .
C42 C 0.3762(5) 0.3711(2) 0.6110(5) 0.0335(13) Uani 1 1 d . . .
H42A H 0.3272 0.3674 0.5446 0.040 Uiso 1 1 calc R . .
C43 C 0.4148(5) 0.3293(2) 0.6697(4) 0.0244(11) Uani 1 1 d . . .
C44 C 0.3659(5) 0.2796(2) 0.6346(4) 0.0239(11) Uani 1 1 d . . .
H44A H 0.3154 0.2671 0.6858 0.029 Uiso 1 1 calc R . .
H44B H 0.3149 0.2827 0.5651 0.029 Uiso 1 1 calc R . .
C45 C 0.5713(5) 0.07032(19) 1.0371(4) 0.0265(11) Uani 1 1 d . . .
H45A H 0.5773 0.0406 0.9949 0.040 Uiso 1 1 calc R . .
H45B H 0.5024 0.0675 1.0751 0.040 Uiso 1 1 calc R . .
H45C H 0.6445 0.0741 1.0879 0.040 Uiso 1 1 calc R . .
N31 N 0.5278(4) 0.29242(15) 0.8237(3) 0.0190(8) Uani 1 1 d . . .
O31 O 0.5429(3) 0.18901(13) 0.8442(3) 0.0215(7) Uani 1 1 d . . .
O32 O 0.5560(4) 0.11306(13) 0.9679(3) 0.0250(8) Uani 1 1 d . . .
O33 O 0.4603(3) 0.24479(13) 0.6263(3) 0.0211(7) Uani 1 1 d . . .

N51 N 0.7753(6) 0.0605(2) 0.8353(5) 0.0456(14) Uani 1 1 d . . .
O51 O 0.8952(9) 0.0360(3) 0.8676(8) 0.121(3) Uani 1 1 d . . .
O52 O 0.7693(4) 0.10734(14) 0.8372(3) 0.0303(9) Uani 1 1 d . . .
O53 O 0.6837(4) 0.03541(15) 0.8062(4) 0.0372(10) Uani 1 1 d . . .
N61 N 0.3999(5) 0.01586(18) 0.7439(4) 0.0346(12) Uani 1 1 d . . .
O61 O 0.3392(5) -0.02164(17) 0.7312(4) 0.0488(13) Uani 1 1 d . . .
O62 O 0.4294(4) 0.03887(15) 0.6647(3) 0.0363(10) Uani 1 1 d . . .
O63 O 0.4332(4) 0.03401(16) 0.8345(3) 0.0380(11) Uani 1 1 d . . .
N71 N 0.3052(7) 0.1433(3) 0.6746(8) 0.078(2) Uani 1 1 d U . .
O71 O 0.2040(8) 0.1520(5) 0.6173(10) 0.172(5) Uani 1 1 d U . .
O72 O 0.3928(4) 0.14904(16) 0.6263(4) 0.0393(11) Uani 1 1 d U . .
O73 O 0.3235(5) 0.1246(2) 0.7687(5) 0.0619(15) Uani 1 1 d U . .
C1S C 1.0305(6) 0.1754(3) 0.8695(6) 0.0461(17) Uani 1 1 d . . .
O1S O 0.9219(4) 0.17971(15) 0.7969(3) 0.0320(9) Uani 1 1 d . . .
O1WS O 0.2041(15) 0.0521(9) 0.9061(11) 0.120(7) Uani 0.50 1 d P . .
O2S O 0.930(2) 0.0313(10) 0.5908(19) 0.076(7) Uiso 0.25 1 d PDU . .
C2S C 0.935(3) 0.0003(11) 0.504(2) 0.055(7) Uiso 0.25 1 d PDU . .

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Ni2 0.0221(3) 0.0141(3) 0.0114(3) 0.0003(2) 0.0029(2) -0.0018(2)
C11 0.015(2) 0.019(2) 0.017(2) -0.0007(18) 0.0021(18) 0.0010(17)
C12 0.019(2) 0.026(3) 0.019(2) -0.0013(19) 0.0049(19) -0.0017(19)
C13 0.023(3) 0.031(3) 0.015(2) -0.003(2) 0.0028(19) -0.002(2)
C14 0.026(3) 0.024(2) 0.020(2) -0.008(2) 0.002(2) -0.002(2)
C15 0.023(2) 0.020(2) 0.019(2) -0.0032(19) 0.004(2) -0.0020(19)
C16 0.021(2) 0.022(2) 0.013(2) -0.0027(18) 0.0015(18) 0.0027(18)
C17 0.019(2) 0.018(2) 0.016(2) 0.0036(17) 0.0010(18) -0.0006(17)
C18 0.019(2) 0.014(2) 0.022(2) -0.0003(18) 0.0052(19) -0.0009(17)
C19 0.024(3) 0.019(2) 0.023(2) 0.0012(19) 0.006(2) -0.0007(19)
C20 0.027(3) 0.017(2) 0.035(3) 0.005(2) 0.009(2) -0.003(2)
C21 0.038(3) 0.019(2) 0.037(3) -0.007(2) 0.008(3) -0.007(2)
C22 0.031(3) 0.025(3) 0.028(3) -0.009(2) -0.002(2) -0.007(2)
C23 0.020(2) 0.018(2) 0.021(2) -0.0020(18) 0.0025(19) 0.0002(18)
C24 0.028(3) 0.021(2) 0.019(2) -0.0029(19) -0.003(2) -0.003(2)
C25 0.093(6) 0.016(3) 0.038(3) -0.007(2) 0.024(4) -0.010(3)
N11 0.021(2) 0.0146(18) 0.0128(18) 0.0001(14) 0.0001(16) -0.0006(15)
O11 0.0267(18) 0.0152(15) 0.0135(15) 0.0002(12) 0.0048(14) -0.0003(13)
O12 0.049(2) 0.0143(17) 0.0210(18) -0.0059(14) 0.0090(17) -0.0046(16)
O13 0.0271(19) 0.0183(17) 0.0177(17) 0.0003(13) -0.0043(14) -0.0022(14)

C31 0.020(2) 0.024(2) 0.015(2) -0.0001(18) 0.0043(19) -0.0013(19)
C32 0.024(3) 0.027(3) 0.017(2) -0.0024(19) 0.004(2) -0.003(2)
C33 0.025(3) 0.036(3) 0.011(2) 0.002(2) 0.0028(19) -0.002(2)
C34 0.025(3) 0.026(3) 0.018(2) 0.0039(19) 0.002(2) -0.004(2)
C35 0.024(3) 0.019(2) 0.019(2) 0.0006(18) 0.004(2) -0.0028(19)
C36 0.020(2) 0.024(2) 0.015(2) 0.0009(18) 0.0047(18) -0.0028(18)
C37 0.023(2) 0.022(2) 0.020(2) -0.0042(19) 0.005(2) -0.0026(19)
C38 0.027(3) 0.020(2) 0.023(2) 0.0036(19) 0.010(2) 0.001(2)
C39 0.033(3) 0.021(3) 0.035(3) 0.001(2) 0.012(2) 0.000(2)
C40 0.052(4) 0.020(3) 0.051(4) 0.005(3) 0.017(3) 0.007(3)
C41 0.047(4) 0.031(3) 0.046(4) 0.018(3) 0.019(3) 0.011(3)
C42 0.032(3) 0.040(3) 0.030(3) 0.012(3) 0.010(2) 0.012(3)
C43 0.024(3) 0.029(3) 0.022(2) 0.004(2) 0.010(2) 0.005(2)
C44 0.022(3) 0.033(3) 0.017(2) 0.002(2) 0.003(2) 0.003(2)
C45 0.040(3) 0.020(2) 0.019(2) 0.0071(19) 0.004(2) -0.003(2)
N31 0.025(2) 0.0147(19) 0.0172(19) 0.0016(15) 0.0022(17) -0.0005(15)
O31 0.034(2) 0.0192(17) 0.0121(15) 0.0023(13) 0.0048(14) -0.0048(14)
O32 0.040(2) 0.0178(17) 0.0171(17) 0.0052(13) 0.0054(16) -0.0040(15)
O33 0.0243(18) 0.0227(17) 0.0162(16) 0.0017(13) 0.0029(14) -0.0023(14)
N51 0.058(4) 0.036(3) 0.043(3) -0.001(2) 0.009(3) 0.011(3)
O51 0.124(7) 0.075(6) 0.156(8) -0.016(5) -0.001(6) 0.037(5)
O52 0.036(2) 0.0197(18) 0.035(2) -0.0001(16) 0.0046(18) 0.0019(16)
O53 0.050(3) 0.0168(19) 0.043(2) -0.0012(17) 0.003(2) -0.0022(17)
N61 0.050(3) 0.024(2) 0.029(3) -0.0007(19) 0.004(2) -0.013(2)
O61 0.077(4) 0.032(2) 0.037(2) 0.0017(19) 0.007(2) -0.028(2)
O62 0.057(3) 0.029(2) 0.024(2) 0.0012(16) 0.0086(19) -0.0162(19)
O63 0.059(3) 0.030(2) 0.023(2) 0.0039(16) 0.000(2) -0.019(2)
N71 0.049(4) 0.069(4) 0.118(5) 0.040(4) 0.016(4) 0.007(3)
O71 0.072(5) 0.232(11) 0.212(10) 0.128(9) 0.020(6) 0.058(7)
O72 0.033(2) 0.031(2) 0.051(3) 0.0140(19) -0.004(2) -0.0098(17)
O73 0.053(3) 0.041(3) 0.100(4) 0.016(3) 0.037(3) 0.005(2)
C1S 0.038(4) 0.042(4) 0.055(4) 0.004(3) -0.006(3) -0.001(3)
O1S 0.032(2) 0.028(2) 0.036(2) -0.0020(17) 0.0038(18) 0.0021(16)
O1WS 0.097(12) 0.21(2) 0.058(9) -0.030(11) 0.028(8) -0.041(13)

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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.
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Pr1 O11 2.477(3) . ?
Pr1 O53 2.507(4) . ?
Pr1 O52 2.516(4) . ?
Pr1 O72 2.563(4) . ?
Pr1 O62 2.564(4) . ?
Pr1 O32 2.598(4) . ?
Pr1 O73 2.605(5) . ?
Pr1 O12 2.608(4) . ?
Pr1 O63 2.646(4) . ?
Pr1 N51 2.886(6) . ?
Pr1 N71 2.989(8) . ?
Ni2 O11 2.008(3) . ?
Ni2 N11 2.018(4) . ?
Ni2 N31 2.030(4) . ?
Ni2 O31 2.032(3) . ?
Ni2 O13 2.101(3) . ?
Ni2 O33 2.123(3) . ?
C11 C12 1.406(7) . ?
C11 C16 1.412(7) . ?
C11 C17 1.454(7) . ?
C12 C13 1.364(7) . ?
C12 H12A 0.9500 . ?
C13 C14 1.398(8) . ?
C13 H13A 0.9500 . ?
C14 C15 1.379(7) . ?
C14 H14A 0.9500 . ?
C15 O12 1.379(6) . ?
C15 C16 1.416(7) . ?
C16 O11 1.327(6) . ?
C17 N11 1.282(6) . ?
C17 H17A 0.9500 . ?
C18 C19 1.400(7) . ?
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H45A C45 H45B 109.5 . . ?
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O33 Ni2 N31 C38 -49.8(4) . . . . ?
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Complex 3:

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 'La'  'La'  -0.2871   2.4523
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_space_group_name_H-M    P2(1)/n

loop_
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 '-x, -y, -z'
 'x-1/2, -y-1/2, z-1/2'

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_cell_length_b                  14.595(3)
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_cell_angle_beta                 102.582(3)
_cell_angle_gamma                90.00
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_cell_measurement_reflns_used    16706
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_exptl_special_details
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 CrystalClear-SM Expert 2.1 b24 (Rigaku, 2012) was used for absorption correction.
R(int) was 0.1483 before and 0.1431 after correction
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Rigaku Saturn724+ (4x4 bin mode)
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_computing_publication_material   'Bruker SHELXTL'

_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.

 All the non-hydrogen atoms (except the disorded atoms and solvent molecule) were
refined anisotropically.The hydrogen atoms were added in its calculated
geometric position. The hydrogen atoms were refined as a riding model.

 For the better convergence of disordered solvents we have employed
several restraints and constraints such as DFIX, DANG, SIMU, FLAT etc.

 The diffused electron density of the solvent molecules is not allowed us to model
these solvent molecules, hence SQUZZEE routine was employed to calculate the
```

solvent Void volume (1101 A^3) and the total number of electron (282) in this void space.

This void electrons are tentatively assigned for 15.5 molecules methanol solvent molecules in one unit cell.

The loop created in PLATON is appended at the end of cif file.
;

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_refine_ls_matrix_type full
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_atom_sites_solution_secondary difmap
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_atom_site_occupancy
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Ni1 Ni 0.29401(5) 0.37707(7) 0.16529(4) 0.0150(3) Uani 1 1 d . . .

Ni2 Ni 0.20895(5) 0.37458(7) -0.13948(4) 0.0140(3) Uani 1 1 d . . .
O11 O 0.3288(3) 0.4112(4) 0.0969(2) 0.0174(11) Uani 1 1 d . . .
O12 O 0.3269(3) 0.5025(4) 0.0066(2) 0.0204(12) Uani 1 1 d . . .
O13 O 0.3063(3) 0.2316(4) 0.1677(2) 0.0188(11) Uani 1 1 d . . .
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O33 O 0.2906(3) 0.5195(4) 0.1828(2) 0.0239(13) Uani 1 1 d . . .
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O73 O 0.2036(3) 0.2291(4) -0.1412(2) 0.0180(11) Uani 1 1 d . . .
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C11 C 0.4408(4) 0.4655(5) 0.1414(3) 0.0186(16) Uani 1 1 d . . .
C12 C 0.3851(4) 0.4606(5) 0.0962(3) 0.0162(15) Uani 1 1 d . . .
C13 C 0.3870(4) 0.5086(5) 0.0476(3) 0.0182(16) Uani 1 1 d . . .
C14 C 0.4438(4) 0.5567(6) 0.0410(3) 0.0268(19) Uani 1 1 d . . .
H14A H 0.4442 0.5873 0.0070 0.032 Uiso 1 1 calc R . .
C15 C 0.5017(4) 0.5596(6) 0.0858(4) 0.0247(18) Uani 1 1 d . . .
H15A H 0.5417 0.5919 0.0823 0.030 Uiso 1 1 calc R . .
C16 C 0.4991(4) 0.5147(6) 0.1346(3) 0.0232(18) Uani 1 1 d . . .
H16A H 0.5379 0.5169 0.1647 0.028 Uiso 1 1 calc R . .
C17 C 0.4440(4) 0.4194(6) 0.1933(3) 0.0218(17) Uani 1 1 d . . .
H17A H 0.4867 0.4194 0.2191 0.026 Uiso 1 1 calc R . .
C18 C 0.4082(4) 0.3277(6) 0.2600(3) 0.0222(18) Uani 1 1 d . . .
C19 C 0.3895(4) 0.2360(6) 0.2575(4) 0.0243(18) Uani 1 1 d . . .
C20 C 0.4012(4) 0.1870(7) 0.3067(4) 0.029(2) Uani 1 1 d . . .
H20A H 0.3898 0.1237 0.3057 0.035 Uiso 1 1 calc R . .
C21 C 0.4294(4) 0.2279(7) 0.3576(4) 0.035(2) Uani 1 1 d . . .
H21A H 0.4370 0.1932 0.3910 0.042 Uiso 1 1 calc R . .
C22 C 0.4465(4) 0.3223(7) 0.3586(3) 0.028(2) Uani 1 1 d . . .
H22A H 0.4653 0.3519 0.3929 0.033 Uiso 1 1 calc R . .
C23 C 0.4359(5) 0.3705(7) 0.3097(4) 0.0270(19) Uani 1 1 d . . .
H23A H 0.4476 0.4336 0.3100 0.032 Uiso 1 1 calc R . .
C24 C 0.3662(4) 0.1874(6) 0.2018(4) 0.0260(19) Uani 1 1 d . . .

H24A H 0.4038 0.1877 0.1816 0.031 Uiso 1 1 calc R . .
H24B H 0.3552 0.1228 0.2084 0.031 Uiso 1 1 calc R . .
C25 C 0.3227(5) 0.5562(6) -0.0419(3) 0.027(2) Uani 1 1 d . . .
H25A H 0.3554 0.6069 -0.0338 0.041 Uiso 1 1 calc R . .
H25B H 0.2764 0.5807 -0.0539 0.041 Uiso 1 1 calc R . .
H25C H 0.3336 0.5180 -0.0716 0.041 Uiso 1 1 calc R . .
C31 C 0.1413(4) 0.2835(6) 0.1639(3) 0.0211(17) Uani 1 1 d . . .
C32 C 0.1588(4) 0.2979(5) 0.1122(3) 0.0156(15) Uani 1 1 d . . .
C33 C 0.1164(4) 0.2536(5) 0.0654(3) 0.0176(16) Uani 1 1 d . . .
C34 C 0.0625(4) 0.1985(6) 0.0703(4) 0.0269(19) Uani 1 1 d . . .
H34A H 0.0363 0.1688 0.0384 0.032 Uiso 1 1 calc R . .
C35 C 0.0459(5) 0.1859(7) 0.1220(4) 0.035(2) Uani 1 1 d . . .
H35A H 0.0081 0.1488 0.1252 0.041 Uiso 1 1 calc R . .
C36 C 0.0850(4) 0.2280(7) 0.1683(4) 0.033(2) Uani 1 1 d . . .
H36A H 0.0739 0.2196 0.2036 0.039 Uiso 1 1 calc R . .
C37 C 0.1771(4) 0.3243(6) 0.2156(4) 0.0224(17) Uani 1 1 d . . .
H37A H 0.1559 0.3204 0.2465 0.027 Uiso 1 1 calc R . .
C38 C 0.2611(4) 0.4074(6) 0.2778(3) 0.0225(18) Uani 1 1 d . . .
C39 C 0.2753(5) 0.4997(6) 0.2785(4) 0.0281(19) Uani 1 1 d . . .
C40 C 0.3000(5) 0.5404(7) 0.3297(4) 0.041(3) Uani 1 1 d . . .
H40A H 0.3105 0.6039 0.3311 0.049 Uiso 1 1 calc R . .
C41 C 0.3098(5) 0.4910(7) 0.3792(4) 0.040(2) Uani 1 1 d . . .
H41A H 0.3265 0.5200 0.4140 0.048 Uiso 1 1 calc R . .
C42 C 0.2947(5) 0.3996(8) 0.3763(4) 0.036(2) Uani 1 1 d . . .
H42A H 0.3021 0.3653 0.4099 0.043 Uiso 1 1 calc R . .
C43 C 0.2694(5) 0.3549(6) 0.3269(4) 0.028(2) Uani 1 1 d . . .
H43 H 0.2580 0.2917 0.3259 0.033 Uiso 1 1 calc R . .
C44 C 0.2579(6) 0.5540(6) 0.2252(4) 0.037(2) Uani 1 1 d . . .
H44A H 0.2078 0.5529 0.2109 0.044 Uiso 1 1 calc R . .
H44B H 0.2718 0.6185 0.2332 0.044 Uiso 1 1 calc R . .
C45 C 0.0863(4) 0.2397(6) -0.0344(4) 0.0263(19) Uani 1 1 d . . .
H45A H 0.0895 0.1726 -0.0334 0.039 Uiso 1 1 calc R . .
H45B H 0.0998 0.2626 -0.0678 0.039 Uiso 1 1 calc R . .
H45C H 0.0392 0.2582 -0.0350 0.039 Uiso 1 1 calc R . .
C51 C 0.3619(4) 0.2852(5) -0.1381(3) 0.0180(16) Uani 1 1 d . . .
C52 C 0.3466(4) 0.3044(5) -0.0853(3) 0.0136(15) Uani 1 1 d . . .
C53 C 0.3909(4) 0.2655(5) -0.0389(3) 0.0170(16) Uani 1 1 d . . .
C54 C 0.4445(4) 0.2113(6) -0.0429(3) 0.0227(18) Uani 1 1 d . . .
H54A H 0.4728 0.1863 -0.0103 0.027 Uiso 1 1 calc R . .
C55 C 0.4580(4) 0.1924(6) -0.0948(4) 0.0280(19) Uani 1 1 d . . .
H55A H 0.4944 0.1526 -0.0980 0.034 Uiso 1 1 calc R . .
C56 C 0.4177(4) 0.2324(6) -0.1418(3) 0.0227(17) Uani 1 1 d . . .
H56A H 0.4287 0.2232 -0.1770 0.027 Uiso 1 1 calc R . .
C57 C 0.3256(4) 0.3274(5) -0.1895(3) 0.0176(16) Uani 1 1 d . . .
H57A H 0.3465 0.3234 -0.2205 0.021 Uiso 1 1 calc R . .
C58 C 0.2476(4) 0.4183(6) -0.2482(3) 0.0198(17) Uani 1 1 d . . .
C59 C 0.2338(4) 0.5117(6) -0.2458(3) 0.0214(17) Uani 1 1 d . . .

C60 C 0.2117(5) 0.5616(6) -0.2936(4) 0.032(2) Uani 1 1 d . . .
H60A H 0.2036 0.6255 -0.2913 0.038 Uiso 1 1 calc R . .
C61 C 0.2011(5) 0.5182(7) -0.3461(4) 0.037(2) Uani 1 1 d . . .
H61A H 0.1848 0.5522 -0.3792 0.044 Uiso 1 1 calc R . .
C62 C 0.2152(5) 0.4239(8) -0.3486(4) 0.039(2) Uani 1 1 d . . .
H62A H 0.2088 0.3945 -0.3838 0.047 Uiso 1 1 calc R . .
C63 C 0.2382(5) 0.3735(7) -0.3005(4) 0.028(2) Uani 1 1 d . . .
H63A H 0.2475 0.3099 -0.3024 0.033 Uiso 1 1 calc R . .
C64 C 0.2461(4) 0.5594(6) -0.1892(3) 0.0227(18) Uani 1 1 d . . .
H64A H 0.2949 0.5534 -0.1705 0.027 Uiso 1 1 calc R . .
H64B H 0.2357 0.6255 -0.1947 0.027 Uiso 1 1 calc R . .
C65 C 0.4210(4) 0.2555(6) 0.0608(3) 0.0241(18) Uani 1 1 d . . .
H65A H 0.4213 0.1884 0.0600 0.036 Uiso 1 1 calc R . .
H65B H 0.4058 0.2764 0.0939 0.036 Uiso 1 1 calc R . .
H65C H 0.4672 0.2785 0.0619 0.036 Uiso 1 1 calc R . .
C71 C 0.0622(4) 0.4624(5) -0.1217(3) 0.0216(17) Uani 1 1 d . . .
C72 C 0.1152(4) 0.4553(5) -0.0753(3) 0.0205(17) Uani 1 1 d . . .
C73 C 0.1123(4) 0.5077(6) -0.0279(3) 0.0243(18) Uani 1 1 d . . .
C74 C 0.0570(4) 0.5632(6) -0.0271(4) 0.030(2) Uani 1 1 d . . .
H74A H 0.0554 0.5979 0.0052 0.036 Uiso 1 1 calc R . .
C75 C 0.0034(5) 0.5685(7) -0.0738(4) 0.035(2) Uani 1 1 d . . .
H75A H -0.0350 0.6062 -0.0730 0.042 Uiso 1 1 calc R . .
C76 C 0.0061(4) 0.5206(6) -0.1195(4) 0.0263(19) Uani 1 1 d . . .
H76A H -0.0303 0.5256 -0.1513 0.032 Uiso 1 1 calc R . .
C77 C 0.0602(4) 0.4112(5) -0.1732(3) 0.0205(17) Uani 1 1 d . . .
H77A H 0.0181 0.4095 -0.1998 0.025 Uiso 1 1 calc R . .
C78 C 0.1012(4) 0.3155(5) -0.2351(3) 0.0198(17) Uani 1 1 d . . .
C79 C 0.1212(4) 0.2251(6) -0.2307(3) 0.0207(17) Uani 1 1 d . . .
C80 C 0.1149(4) 0.1731(6) -0.2788(4) 0.0283(19) Uani 1 1 d . . .
H80A H 0.1292 0.1109 -0.2764 0.034 Uiso 1 1 calc R . .
C81 C 0.0871(4) 0.2122(7) -0.3313(4) 0.031(2) Uani 1 1 d . . .
H81A H 0.0821 0.1764 -0.3642 0.038 Uiso 1 1 calc R . .
C82 C 0.0675(5) 0.3026(7) -0.3344(4) 0.036(2) Uani 1 1 d . . .
H82A H 0.0495 0.3294 -0.3697 0.043 Uiso 1 1 calc R . .
C83 C 0.0736(4) 0.3555(6) -0.2864(4) 0.026(2) Uani 1 1 d . . .
H83A H 0.0592 0.4177 -0.2886 0.031 Uiso 1 1 calc R . .
C84 C 0.1443(4) 0.1806(5) -0.1740(4) 0.0210(17) Uani 1 1 d . . .
H84A H 0.1065 0.1819 -0.1540 0.025 Uiso 1 1 calc R . .
H84B H 0.1565 0.1157 -0.1786 0.025 Uiso 1 1 calc R . .
C85 C 0.1719(5) 0.5536(6) 0.0635(4) 0.031(2) Uani 1 1 d . . .
H85A H 0.1384 0.6031 0.0544 0.047 Uiso 1 1 calc R . .
H85B H 0.2178 0.5798 0.0757 0.047 Uiso 1 1 calc R . .
H85C H 0.1612 0.5161 0.0935 0.047 Uiso 1 1 calc R . .
O101 O 0.0868(8) 0.5642(6) -0.2189(10) 0.143(13) Uiso 0.49(3) 1 d PDU A 1
O102 O 0.0068(5) 0.6844(10) -0.2491(6) 0.035(4) Uiso 0.49(3) 1 d PDU A 1
O103 O 0.1210(5) 0.7200(7) -0.2024(5) 0.026(4) Uiso 0.49(3) 1 d PDU A 1
N101 N 0.0715(4) 0.6562(6) -0.2235(4) 0.027(4) Uiso 0.49(3) 1 d PDU A 1

N10A N 0.0824(6) 0.6779(7) -0.2160(5) 0.062(6) Uiso 0.51(3) 1 d PDU A 2
O10A O 0.0833(5) 0.5836(7) -0.2164(5) 0.016(3) Uiso 0.51(3) 1 d PDU A 2
O10B O 0.0229(8) 0.7242(11) -0.2384(8) 0.071(6) Uiso 0.51(3) 1 d PDU A 2
O10C O 0.1409(9) 0.7259(10) -0.1933(14) 0.224(17) Uiso 0.51(3) 1 d PDU A 2
O111 O 0.5680(8) 0.0810(10) 0.0316(7) 0.087(6) Uiso 0.557(10) 1 d PDU B 1
N111 N 0.6063(7) 0.1554(10) 0.0225(7) 0.137(11) Uiso 0.557(10) 1 d PDU B 1
O112 O 0.6037(15) 0.2355(12) 0.0515(13) 0.222(15) Uiso 0.557(10) 1 d PDU B 1
O113 O 0.6473(13) 0.1498(18) -0.0156(11) 0.179(13) Uiso 0.557(10) 1 d PDU B 1
O11A O 0.0023(7) 0.0387(10) -0.0291(8) 0.072(6) Uiso 0.443(10) 1 d PDU . 2
O11B O 0.1091(7) -0.0144(14) -0.0444(9) 0.083(7) Uiso 0.443(10) 1 d PDU B 2
O11C O 0.0518(11) -0.0982(13) 0.0150(10) 0.117(9) Uiso 0.443(10) 1 d PDU . 2
N11A N 0.0544(6) -0.0246(9) -0.0195(5) 0.092(7) Uiso 0.443(10) 1 d PDU . 2

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La1 0.0145(3) 0.0112(3) 0.0156(3) 0.00105(16) 0.0030(2) 0.00015(15)
Ni1 0.0139(5) 0.0151(5) 0.0166(5) 0.0013(4) 0.0043(4) -0.0003(4)
Ni2 0.0151(5) 0.0123(5) 0.0141(5) 0.0013(4) 0.0024(4) 0.0007(4)
O11 0.020(3) 0.017(3) 0.016(3) 0.001(2) 0.004(2) -0.004(2)
O12 0.025(3) 0.018(3) 0.017(3) 0.001(2) 0.002(2) -0.004(2)
O13 0.017(3) 0.019(3) 0.019(3) -0.001(2) 0.002(2) 0.003(2)
O31 0.008(3) 0.015(3) 0.020(3) -0.002(2) -0.003(2) -0.0024(19)
O32 0.023(3) 0.021(3) 0.022(3) -0.002(2) 0.007(2) -0.002(2)
O33 0.031(3) 0.016(3) 0.026(3) 0.001(3) 0.007(2) 0.000(2)
O51 0.016(3) 0.012(3) 0.015(3) 0.002(2) 0.002(2) 0.000(2)
O52 0.019(3) 0.017(3) 0.017(3) 0.003(2) 0.000(2) 0.001(2)
O53 0.026(3) 0.011(3) 0.027(3) 0.001(2) 0.010(2) -0.001(2)
O71 0.016(3) 0.013(3) 0.020(3) -0.001(2) 0.006(2) 0.003(2)
O72 0.019(3) 0.021(3) 0.021(3) -0.002(2) 0.000(2) 0.005(2)
O73 0.015(3) 0.015(3) 0.021(3) -0.002(2) -0.002(2) 0.000(2)
O91 0.033(3) 0.018(3) 0.020(3) 0.000(2) 0.009(2) 0.002(2)
O92 0.025(3) 0.013(3) 0.020(3) 0.005(2) 0.007(2) 0.004(2)
O93 0.198(11) 0.039(5) 0.067(6) 0.001(5) 0.038(7) 0.036(7)
N11 0.019(4) 0.025(4) 0.016(3) 0.002(3) 0.005(3) 0.002(3)
N31 0.019(4) 0.019(3) 0.020(3) -0.002(3) 0.003(3) 0.006(3)
N51 0.015(3) 0.019(3) 0.015(3) -0.001(3) 0.003(3) -0.004(3)
N71 0.018(3) 0.019(3) 0.018(3) -0.002(3) 0.005(3) -0.002(3)
N91 0.034(4) 0.027(5) 0.046(5) -0.001(4) 0.019(4) -0.007(3)
C11 0.017(4) 0.016(4) 0.026(4) -0.004(3) 0.011(3) -0.005(3)
C12 0.015(4) 0.013(3) 0.023(4) -0.003(3) 0.011(3) -0.004(3)
C13 0.017(4) 0.018(4) 0.018(4) -0.006(3) 0.000(3) -0.006(3)

C14 0.029(5) 0.033(5) 0.021(4) 0.002(4) 0.010(3) -0.010(4)
C15 0.023(4) 0.021(4) 0.032(4) 0.003(4) 0.010(4) -0.008(3)
C16 0.019(4) 0.029(4) 0.022(4) -0.005(4) 0.005(3) -0.005(3)
C17 0.017(4) 0.024(4) 0.024(4) -0.002(4) 0.003(3) 0.001(3)
C18 0.017(4) 0.029(4) 0.020(4) 0.009(4) 0.003(3) 0.008(4)
C19 0.021(4) 0.025(4) 0.029(4) 0.009(4) 0.010(3) 0.009(3)
C20 0.027(5) 0.031(5) 0.032(5) 0.014(4) 0.010(4) 0.005(4)
C21 0.027(5) 0.050(6) 0.029(5) 0.022(5) 0.005(4) 0.009(4)
C22 0.021(4) 0.046(6) 0.013(4) 0.006(4) -0.002(3) -0.002(4)
C23 0.027(5) 0.033(5) 0.020(4) -0.001(4) 0.000(4) 0.004(4)
C24 0.022(4) 0.025(4) 0.032(5) 0.003(4) 0.010(4) 0.007(4)
C25 0.042(5) 0.015(4) 0.020(4) 0.009(3) -0.004(4) -0.007(4)
C31 0.016(4) 0.020(4) 0.028(4) 0.001(4) 0.006(3) -0.005(3)
C32 0.009(3) 0.018(4) 0.021(4) 0.002(3) 0.005(3) 0.003(3)
C33 0.012(4) 0.015(4) 0.028(4) 0.002(3) 0.007(3) 0.001(3)
C34 0.030(5) 0.022(4) 0.030(4) -0.001(4) 0.007(4) -0.003(4)
C35 0.029(5) 0.041(6) 0.037(5) 0.000(5) 0.015(4) -0.022(4)
C36 0.028(5) 0.040(5) 0.033(5) -0.005(4) 0.014(4) -0.019(4)
C37 0.018(4) 0.025(4) 0.026(4) 0.002(4) 0.008(3) 0.001(3)
C38 0.018(4) 0.029(5) 0.023(4) -0.002(4) 0.010(3) 0.003(3)
C39 0.030(5) 0.023(4) 0.036(5) 0.000(4) 0.017(4) 0.008(4)
C40 0.043(6) 0.040(6) 0.044(6) -0.024(5) 0.023(5) -0.010(5)
C41 0.037(6) 0.048(6) 0.036(5) -0.017(5) 0.011(4) -0.006(5)
C42 0.027(5) 0.056(7) 0.026(5) 0.003(5) 0.007(4) 0.010(5)
C43 0.027(5) 0.031(5) 0.026(5) 0.000(4) 0.009(4) -0.003(4)
C44 0.059(7) 0.020(4) 0.038(5) 0.003(4) 0.023(5) 0.013(4)
C45 0.023(4) 0.025(4) 0.029(4) 0.002(4) 0.003(3) -0.007(4)
C51 0.021(4) 0.016(4) 0.017(4) -0.002(3) 0.004(3) -0.002(3)
C52 0.015(4) 0.013(3) 0.013(3) -0.003(3) 0.003(3) -0.004(3)
C53 0.019(4) 0.015(4) 0.018(4) 0.002(3) 0.005(3) -0.002(3)
C54 0.015(4) 0.028(4) 0.024(4) -0.002(4) 0.002(3) 0.005(3)
C55 0.025(4) 0.031(5) 0.029(4) 0.000(4) 0.007(4) 0.009(4)
C56 0.023(4) 0.026(4) 0.019(4) -0.007(4) 0.005(3) -0.003(3)
C57 0.023(4) 0.011(3) 0.021(4) -0.002(3) 0.011(3) -0.002(3)
C58 0.023(4) 0.021(4) 0.017(4) 0.001(3) 0.008(3) -0.006(3)
C59 0.022(4) 0.018(4) 0.024(4) -0.002(4) 0.006(3) -0.008(3)
C60 0.038(5) 0.024(4) 0.037(5) 0.008(4) 0.017(4) 0.003(4)
C61 0.037(5) 0.048(6) 0.024(4) 0.013(5) 0.002(4) 0.005(5)
C62 0.042(6) 0.061(7) 0.015(4) -0.001(5) 0.009(4) 0.003(5)
C63 0.036(5) 0.031(5) 0.017(4) -0.009(4) 0.008(4) -0.005(4)
C64 0.031(5) 0.017(4) 0.021(4) 0.003(3) 0.006(3) -0.005(3)
C65 0.025(4) 0.023(4) 0.021(4) 0.002(4) 0.000(3) 0.007(3)
C71 0.024(4) 0.014(4) 0.025(4) 0.002(3) 0.000(3) 0.001(3)
C72 0.020(4) 0.017(4) 0.025(4) 0.003(3) 0.006(3) 0.000(3)
C73 0.025(4) 0.023(4) 0.024(4) 0.001(4) 0.003(3) 0.005(4)
C74 0.027(5) 0.028(5) 0.032(5) -0.012(4) 0.001(4) 0.010(4)
C75 0.030(5) 0.038(5) 0.034(5) -0.002(4) 0.000(4) 0.021(4)

C76 0.019(4) 0.023(4) 0.033(5) -0.002(4) -0.003(3) 0.007(3)
C77 0.019(4) 0.019(4) 0.021(4) 0.004(3) 0.000(3) 0.003(3)
C78 0.025(4) 0.016(4) 0.018(4) -0.004(3) 0.002(3) -0.006(3)
C79 0.009(4) 0.028(4) 0.023(4) -0.005(4) 0.000(3) -0.002(3)
C80 0.024(5) 0.025(4) 0.034(5) -0.004(4) 0.004(4) 0.000(4)
C81 0.023(5) 0.044(6) 0.025(4) -0.010(4) 0.001(4) -0.002(4)
C82 0.033(5) 0.050(6) 0.024(4) 0.002(5) 0.004(4) -0.014(5)
C83 0.024(5) 0.027(5) 0.026(5) 0.002(4) 0.002(4) 0.003(3)
C84 0.015(4) 0.014(4) 0.033(5) -0.002(4) 0.002(3) -0.001(3)
C85 0.039(5) 0.024(5) 0.028(4) -0.009(4) 0.001(4) 0.000(4)

_geom_special_details
;
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.
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O12 La1 O31 C32 163.5(5) . . . . ?
N91 La1 O31 C32 -50.1(5) . . . . ?
O71 La1 O31 Ni1 -149.53(19) . . . . ?
O11 La1 O31 Ni1 -12.11(19) . . . . ?
O51 La1 O31 Ni1 -6(12) . . . . ?
O92 La1 O31 Ni1 114.7(2) . . . . ?
O91 La1 O31 Ni1 84.2(2) . . . . ?
O32 La1 O31 Ni1 163.5(3) . . . . ?
O52 La1 O31 Ni1 35.0(3) . . . . ?
O72 La1 O31 Ni1 -111.2(2) . . . . ?
O12 La1 O31 Ni1 -48.5(2) . . . . ?
N91 La1 O31 Ni1 98.0(2) . . . . ?
O71 La1 O32 C33 -154.9(5) . . . . ?
O11 La1 O32 C33 -12.7(6) . . . . ?
O31 La1 O32 C33 -17.4(5) . . . . ?
O51 La1 O32 C33 162.5(5) . . . . ?
O92 La1 O32 C33 113.8(5) . . . . ?
O91 La1 O32 C33 60.6(5) . . . . ?
O52 La1 O32 C33 86.0(5) . . . . ?
O72 La1 O32 C33 -92.6(5) . . . . ?
O12 La1 O32 C33 -98.2(6) . . . . ?
N91 La1 O32 C33 87.0(5) . . . . ?
O71 La1 O32 C45 40.1(5) . . . . ?
O11 La1 O32 C45 -177.7(5) . . . . ?
O31 La1 O32 C45 177.6(6) . . . . ?
O51 La1 O32 C45 -2.5(6) . . . . ?

O92 La1 O32 C45 -51.2(5) . . . . ?
O91 La1 O32 C45 -104.4(6) . . . . ?
O52 La1 O32 C45 -79.0(6) . . . . ?
O72 La1 O32 C45 102.4(6) . . . . ?
O12 La1 O32 C45 96.8(6) . . . . ?
N91 La1 O32 C45 -78.0(6) . . . . ?
O11 Ni1 O33 C44 169.5(6) . . . . ?
N31 Ni1 O33 C44 3.4(6) . . . . ?
O31 Ni1 O33 C44 91.1(6) . . . . ?
N11 Ni1 O33 C44 -103.3(6) . . . . ?
O13 Ni1 O33 C44 -51.6(12) . . . . ?
O71 Ni2 O51 C52 157.7(6) . . . . ?
N51 Ni2 O51 C52 -33.2(6) . . . . ?
N71 Ni2 O51 C52 108.3(9) . . . . ?
O73 Ni2 O51 C52 56.1(5) . . . . ?
O53 Ni2 O51 C52 -118.5(5) . . . . ?
O71 Ni2 O51 La1 11.4(2) . . . . ?
N51 Ni2 O51 La1 -179.6(2) . . . . ?
N71 Ni2 O51 La1 -38.0(9) . . . . ?
O73 Ni2 O51 La1 -90.3(2) . . . . ?
O53 Ni2 O51 La1 95.1(2) . . . . ?
O71 La1 O51 C52 -157.5(5) . . . . ?
O11 La1 O51 C52 64.8(5) . . . . ?
O31 La1 O51 C52 58(12) . . . . ?
O92 La1 O51 C52 -62.2(5) . . . . ?
O91 La1 O51 C52 -31.2(5) . . . . ?
O32 La1 O51 C52 -110.7(5) . . . . ?
O52 La1 O51 C52 17.5(5) . . . . ?
O72 La1 O51 C52 163.7(5) . . . . ?
O12 La1 O51 C52 101.4(5) . . . . ?
N91 La1 O51 C52 -45.3(5) . . . . ?
O71 La1 O51 Ni2 -10.42(18) . . . . ?
O11 La1 O51 Ni2 -148.15(19) . . . . ?
O31 La1 O51 Ni2 -155(12) . . . . ?
O92 La1 O51 Ni2 84.8(2) . . . . ?
O91 La1 O51 Ni2 115.8(2) . . . . ?
O32 La1 O51 Ni2 36.4(3) . . . . ?
O52 La1 O51 Ni2 164.5(3) . . . . ?
O72 La1 O51 Ni2 -49.3(2) . . . . ?
O12 La1 O51 Ni2 -111.5(2) . . . . ?
N91 La1 O51 Ni2 101.8(2) . . . . ?
O71 La1 O52 C53 -13.6(6) . . . . ?
O11 La1 O52 C53 -155.6(5) . . . . ?
O31 La1 O52 C53 161.7(5) . . . . ?
O51 La1 O52 C53 -18.9(5) . . . . ?
O92 La1 O52 C53 57.6(5) . . . . ?
O91 La1 O52 C53 111.0(5) . . . . ?

O32 La1 O52 C53 84.8(5) . . . . ?
O72 La1 O52 C53 -97.7(5) . . . . ?
O12 La1 O52 C53 -93.0(5) . . . . ?
N91 La1 O52 C53 83.8(5) . . . . ?
O71 La1 O52 C65 -176.2(5) . . . . ?
O11 La1 O52 C65 41.8(5) . . . . ?
O31 La1 O52 C65 -0.9(6) . . . . ?
O51 La1 O52 C65 178.5(6) . . . . ?
O92 La1 O52 C65 -105.0(5) . . . . ?
O91 La1 O52 C65 -51.6(5) . . . . ?
O32 La1 O52 C65 -77.7(6) . . . . ?
O72 La1 O52 C65 99.7(6) . . . . ?
O12 La1 O52 C65 104.5(5) . . . . ?
N91 La1 O52 C65 -78.7(5) . . . . ?
O71 Ni2 O53 C64 160.7(5) . . . . ?
O51 Ni2 O53 C64 81.6(5) . . . . ?
N51 Ni2 O53 C64 -6.8(5) . . . . ?
N71 Ni2 O53 C64 -111.3(5) . . . . ?
O73 Ni2 O53 C64 -68.3(13) . . . . ?
O51 Ni2 O71 C72 154.8(6) . . . . ?
N51 Ni2 O71 C72 106.7(10) . . . . ?
N71 Ni2 O71 C72 -38.7(6) . . . . ?
O73 Ni2 O71 C72 -122.8(5) . . . . ?
O53 Ni2 O71 C72 49.0(5) . . . . ?
O51 Ni2 O71 La1 -12.4(2) . . . . ?
N51 Ni2 O71 La1 -60.5(10) . . . . ?
N71 Ni2 O71 La1 154.2(3) . . . . ?
O73 Ni2 O71 La1 70.1(2) . . . . ?
O53 Ni2 O71 La1 -118.2(2) . . . . ?
O11 La1 O71 C72 -56.1(7) . . . . ?
O31 La1 O71 C72 24.0(6) . . . . ?
O51 La1 O71 C72 -155.4(6) . . . . ?
O92 La1 O71 C72 135.3(6) . . . . ?
O91 La1 O71 C72 112.2(6) . . . . ?
O32 La1 O71 C72 65.9(6) . . . . ?
O52 La1 O71 C72 -160.6(5) . . . . ?
O72 La1 O71 C72 -18.5(5) . . . . ?
O12 La1 O71 C72 -89.3(6) . . . . ?
N91 La1 O71 C72 126.9(6) . . . . ?
O11 La1 O71 Ni2 110.1(3) . . . . ?
O31 La1 O71 Ni2 -169.79(19) . . . . ?
O51 La1 O71 Ni2 10.75(19) . . . . ?
O92 La1 O71 Ni2 -58.6(2) . . . . ?
O91 La1 O71 Ni2 -81.6(3) . . . . ?
O32 La1 O71 Ni2 -127.9(3) . . . . ?
O52 La1 O71 Ni2 5.6(3) . . . . ?
O72 La1 O71 Ni2 147.7(3) . . . . ?

O12 La1 O71 Ni2 76.9(2) . . . . ?
N91 La1 O71 Ni2 -66.9(3) . . . . ?
O71 La1 O72 C73 17.9(5) . . . . ?
O11 La1 O72 C73 176.2(5) . . . . ?
O31 La1 O72 C73 -122.9(6) . . . . ?
O51 La1 O72 C73 57.9(6) . . . . ?
O92 La1 O72 C73 -22.3(6) . . . . ?
O91 La1 O72 C73 -100.4(6) . . . . ?
O32 La1 O72 C73 -59.7(5) . . . . ?
O52 La1 O72 C73 122.2(5) . . . . ?
O12 La1 O72 C73 117.4(6) . . . . ?
N91 La1 O72 C73 -60.4(7) . . . . ?
O71 La1 O72 C85 -177.1(7) . . . . ?
O11 La1 O72 C85 -18.9(6) . . . . ?
O31 La1 O72 C85 42.0(6) . . . . ?
O51 La1 O72 C85 -137.1(6) . . . . ?
O92 La1 O72 C85 142.6(6) . . . . ?
O91 La1 O72 C85 64.5(7) . . . . ?
O32 La1 O72 C85 105.3(6) . . . . ?
O52 La1 O72 C85 -72.9(7) . . . . ?
O12 La1 O72 C85 -77.7(6) . . . . ?
N91 La1 O72 C85 104.5(7) . . . . ?
O71 Ni2 O73 C84 92.6(6) . . . . ?
O51 Ni2 O73 C84 171.7(6) . . . . ?
N51 Ni2 O73 C84 -98.6(6) . . . . ?
N71 Ni2 O73 C84 5.8(6) . . . . ?
O53 Ni2 O73 C84 -37.4(14) . . . . ?
O71 La1 O91 N91 34.7(6) . . . . ?
O11 La1 O91 N91 -152.5(5) . . . . ?
O31 La1 O91 N91 145.8(5) . . . . ?
O51 La1 O91 N91 -35.1(5) . . . . ?
O92 La1 O91 N91 4.0(4) . . . . ?
O32 La1 O91 N91 81.3(5) . . . . ?
O52 La1 O91 N91 -79.7(5) . . . . ?
O72 La1 O91 N91 123.3(5) . . . . ?
O12 La1 O91 N91 -113.8(5) . . . . ?
O71 La1 O92 N91 -161.0(5) . . . . ?
O11 La1 O92 N91 28.2(6) . . . . ?
O31 La1 O92 N91 -42.7(5) . . . . ?
O51 La1 O92 N91 136.5(5) . . . . ?
O91 La1 O92 N91 -4.0(4) . . . . ?
O32 La1 O92 N91 -87.5(5) . . . . ?
O52 La1 O92 N91 72.4(5) . . . . ?
O72 La1 O92 N91 -126.8(5) . . . . ?
O12 La1 O92 N91 114.7(5) . . . . ?
O11 Ni1 N11 C17 21.2(7) . . . . ?
N31 Ni1 N11 C17 -149.2(7) . . . . ?

O31 Ni1 N11 C17 68.3(11) . . . . ?
O33 Ni1 N11 C17 -66.7(7) . . . . ?
O13 Ni1 N11 C17 123.6(7) . . . . ?
O11 Ni1 N11 C18 -160.0(6) . . . . ?
N31 Ni1 N11 C18 29.6(7) . . . . ?
O31 Ni1 N11 C18 -112.9(8) . . . . ?
O33 Ni1 N11 C18 112.1(6) . . . . ?
O13 Ni1 N11 C18 -57.6(6) . . . . ?
O11 Ni1 N31 C37 68.2(12) . . . . ?
O31 Ni1 N31 C37 20.0(7) . . . . ?
N11 Ni1 N31 C37 -148.1(7) . . . . ?
O33 Ni1 N31 C37 126.1(7) . . . . ?
O13 Ni1 N31 C37 -64.6(7) . . . . ?
O11 Ni1 N31 C38 -111.5(10) . . . . ?
O31 Ni1 N31 C38 -159.7(6) . . . . ?
N11 Ni1 N31 C38 32.2(7) . . . . ?
O33 Ni1 N31 C38 -53.6(6) . . . . ?
O13 Ni1 N31 C38 115.7(6) . . . . ?
O71 Ni2 N51 C57 72.4(12) . . . . ?
O51 Ni2 N51 C57 25.2(6) . . . . ?
N71 Ni2 N51 C57 -143.5(6) . . . . ?
O73 Ni2 N51 C57 -59.2(6) . . . . ?
O53 Ni2 N51 C57 130.2(6) . . . . ?
O71 Ni2 N51 C58 -104.3(10) . . . . ?
O51 Ni2 N51 C58 -151.5(6) . . . . ?
N71 Ni2 N51 C58 39.9(6) . . . . ?
O73 Ni2 N51 C58 124.1(6) . . . . ?
O53 Ni2 N51 C58 -46.4(6) . . . . ?
O71 Ni2 N71 C77 27.6(7) . . . . ?
O51 Ni2 N71 C77 76.1(11) . . . . ?
N51 Ni2 N71 C77 -143.8(7) . . . . ?
O73 Ni2 N71 C77 128.3(7) . . . . ?
O53 Ni2 N71 C77 -59.0(7) . . . . ?
O71 Ni2 N71 C78 -156.0(6) . . . . ?
O51 Ni2 N71 C78 -107.5(9) . . . . ?
N51 Ni2 N71 C78 32.6(6) . . . . ?
O73 Ni2 N71 C78 -55.3(6) . . . . ?
O53 Ni2 N71 C78 117.4(6) . . . . ?
La1 O91 N91 O92 -7.4(8) . . . . ?
La1 O91 N91 O93 169.9(8) . . . . ?
La1 O92 N91 O91 7.5(8) . . . . ?
La1 O92 N91 O93 -169.8(8) . . . . ?
O71 La1 N91 O91 -152.7(4) . . . . ?
O11 La1 N91 O91 29.2(5) . . . . ?
O31 La1 N91 O91 -32.1(5) . . . . ?
O51 La1 N91 O91 147.1(5) . . . . ?
O92 La1 N91 O91 -172.8(8) . . . . ?

O32 La1 N91 O91 -89.9(5) . . . . ?
O52 La1 N91 O91 89.4(5) . . . . ?
O72 La1 N91 O91 -89.1(6) . . . . ?
O12 La1 N91 O91 94.2(5) . . . . ?
O71 La1 N91 O92 20.1(5) . . . . ?
O11 La1 N91 O92 -158.1(4) . . . . ?
O31 La1 N91 O92 140.7(5) . . . . ?
O51 La1 N91 O92 -40.1(5) . . . . ?
O91 La1 N91 O92 172.8(8) . . . . ?
O32 La1 N91 O92 82.9(5) . . . . ?
O52 La1 N91 O92 -97.8(5) . . . . ?
O72 La1 N91 O92 83.7(6) . . . . ?
O12 La1 N91 O92 -93.0(5) . . . . ?
O71 La1 N91 O93 110(4) . . . . ?
O11 La1 N91 O93 -69(4) . . . . ?
O31 La1 N91 O93 -130(4) . . . . ?
O51 La1 N91 O93 49(4) . . . . ?
O92 La1 N91 O93 90(4) . . . . ?
O91 La1 N91 O93 -98(4) . . . . ?
O32 La1 N91 O93 172(4) . . . . ?
O52 La1 N91 O93 -8(4) . . . . ?
O72 La1 N91 O93 173(4) . . . . ?
O12 La1 N91 O93 -3(4) . . . . ?
Ni1 O11 C12 C13 -154.3(6) . . . . ?
La1 O11 C12 C13 23.9(9) . . . . ?
Ni1 O11 C12 C11 25.8(10) . . . . ?
La1 O11 C12 C11 -156.0(6) . . . . ?
C16 C11 C12 O11 175.8(7) . . . . ?
C17 C11 C12 O11 -0.5(12) . . . . ?
C16 C11 C12 C13 -4.0(11) . . . . ?
C17 C11 C12 C13 179.7(8) . . . . ?
O11 C12 C13 C14 -175.7(7) . . . . ?
C11 C12 C13 C14 4.1(12) . . . . ?
O11 C12 C13 O12 3.6(10) . . . . ?
C11 C12 C13 O12 -176.6(7) . . . . ?
C25 O12 C13 C14 -6.3(12) . . . . ?
La1 O12 C13 C14 154.4(7) . . . . ?
C25 O12 C13 C12 174.4(7) . . . . ?
La1 O12 C13 C12 -24.9(8) . . . . ?
C12 C13 C14 C15 -1.9(13) . . . . ?
O12 C13 C14 C15 178.9(8) . . . . ?
C13 C14 C15 C16 -0.3(13) . . . . ?
C14 C15 C16 C11 0.3(13) . . . . ?
C12 C11 C16 C15 1.9(12) . . . . ?
C17 C11 C16 C15 178.5(8) . . . . ?
C18 N11 C17 C11 174.4(8) . . . . ?
Ni1 N11 C17 C11 -6.8(12) . . . . ?

C12 C11 C17 N11 -9.5(14) . . . . ?
C16 C11 C17 N11 174.2(8) . . . . ?
C17 N11 C18 C23 58.3(11) . . . . ?
Ni1 N11 C18 C23 -120.6(8) . . . . ?
C17 N11 C18 C19 -124.8(9) . . . . ?
Ni1 N11 C18 C19 56.3(9) . . . . ?
C23 C18 C19 C20 -1.9(13) . . . . ?
N11 C18 C19 C20 -178.8(7) . . . . ?
C23 C18 C19 C24 -173.3(8) . . . . ?
N11 C18 C19 C24 9.8(12) . . . . ?
C18 C19 C20 C21 1.6(13) . . . . ?
C24 C19 C20 C21 173.1(8) . . . . ?
C19 C20 C21 C22 -0.2(14) . . . . ?
C20 C21 C22 C23 -0.8(14) . . . . ?
C21 C22 C23 C18 0.5(14) . . . . ?
C19 C18 C23 C22 0.9(14) . . . . ?
N11 C18 C23 C22 177.6(8) . . . . ?
Ni1 O13 C24 C19 38.1(9) . . . . ?
C20 C19 C24 O13 129.6(8) . . . . ?
C18 C19 C24 O13 -59.2(10) . . . . ?
Ni1 O31 C32 C31 26.8(10) . . . . ?
La1 O31 C32 C31 169.4(6) . . . . ?
Ni1 O31 C32 C33 -155.4(5) . . . . ?
La1 O31 C32 C33 -12.8(9) . . . . ?
C36 C31 C32 O31 178.0(8) . . . . ?
C37 C31 C32 O31 -0.6(13) . . . . ?
C36 C31 C32 C33 0.1(12) . . . . ?
C37 C31 C32 C33 -178.4(7) . . . . ?
C45 O32 C33 C34 -0.4(11) . . . . ?
La1 O32 C33 C34 -166.5(6) . . . . ?
C45 O32 C33 C32 -175.4(6) . . . . ?
La1 O32 C33 C32 18.5(8) . . . . ?
O31 C32 C33 C34 -179.3(7) . . . . ?
C31 C32 C33 C34 -1.3(11) . . . . ?
O31 C32 C33 O32 -4.1(10) . . . . ?
C31 C32 C33 O32 173.9(6) . . . . ?
O32 C33 C34 C35 -172.8(8) . . . . ?
C32 C33 C34 C35 1.9(13) . . . . ?
C33 C34 C35 C36 -1.2(14) . . . . ?
C34 C35 C36 C31 0.0(15) . . . . ?
C32 C31 C36 C35 0.5(14) . . . . ?
C37 C31 C36 C35 179.2(9) . . . . ?
C38 N31 C37 C31 176.2(8) . . . . ?
Ni1 N31 C37 C31 -3.5(12) . . . . ?
C32 C31 C37 N31 -12.5(14) . . . . ?
C36 C31 C37 N31 168.9(8) . . . . ?
C37 N31 C38 C39 -123.0(9) . . . . ?

Ni1 N31 C38 C39 56.7(9) . . . . ?
C37 N31 C38 C43 56.4(11) . . . . ?
Ni1 N31 C38 C43 -123.9(7) . . . . ?
C43 C38 C39 C40 1.4(13) . . . . ?
N31 C38 C39 C40 -179.2(8) . . . . ?
C43 C38 C39 C44 -173.1(8) . . . . ?
N31 C38 C39 C44 6.3(12) . . . . ?
C38 C39 C40 C41 -0.5(15) . . . . ?
C44 C39 C40 C41 173.9(9) . . . . ?
C39 C40 C41 C42 0.3(16) . . . . ?
C40 C41 C42 C43 -1.0(15) . . . . ?
C41 C42 C43 C38 1.8(14) . . . . ?
C39 C38 C43 C42 -2.0(13) . . . . ?
N31 C38 C43 C42 178.6(8) . . . . ?
Ni1 O33 C44 C39 44.6(10) . . . . ?
C38 C39 C44 O33 -58.3(12) . . . . ?
C40 C39 C44 O33 127.4(9) . . . . ?
Ni2 O51 C52 C53 -156.4(5) . . . . ?
La1 O51 C52 C53 -15.5(9) . . . . ?
Ni2 O51 C52 C51 22.7(10) . . . . ?
La1 O51 C52 C51 163.6(5) . . . . ?
C56 C51 C52 O51 180.0(7) . . . . ?
C57 C51 C52 O51 7.2(12) . . . . ?
C56 C51 C52 C53 -0.8(11) . . . . ?
C57 C51 C52 C53 -173.6(7) . . . . ?
C65 O52 C53 C54 2.0(11) . . . . ?
La1 O52 C53 C54 -161.7(6) . . . . ?
C65 O52 C53 C52 -176.8(6) . . . . ?
La1 O52 C53 C52 19.5(8) . . . . ?
O51 C52 C53 C54 178.0(7) . . . . ?
C51 C52 C53 C54 -1.2(11) . . . . ?
O51 C52 C53 O52 -3.1(10) . . . . ?
C51 C52 C53 O52 177.6(6) . . . . ?
O52 C53 C54 C55 -178.3(8) . . . . ?
C52 C53 C54 C55 0.4(13) . . . . ?
C53 C54 C55 C56 2.4(13) . . . . ?
C52 C51 C56 C55 3.7(13) . . . . ?
C57 C51 C56 C55 176.9(8) . . . . ?
C54 C55 C56 C51 -4.5(13) . . . . ?
C58 N51 C57 C51 170.0(7) . . . . ?
Ni2 N51 C57 C51 -6.9(11) . . . . ?
C56 C51 C57 N51 170.8(8) . . . . ?
C52 C51 C57 N51 -16.1(13) . . . . ?
C57 N51 C58 C59 -123.3(8) . . . . ?
Ni2 N51 C58 C59 53.6(9) . . . . ?
C57 N51 C58 C63 60.1(10) . . . . ?
Ni2 N51 C58 C63 -123.0(8) . . . . ?

N51 C58 C59 C60 -177.3(7) . . . . ?
C63 C58 C59 C60 -0.7(13) . . . . ?
N51 C58 C59 C64 5.0(11) . . . . ?
C63 C58 C59 C64 -178.4(8) . . . . ?
C58 C59 C60 C61 1.5(14) . . . . ?
C64 C59 C60 C61 179.2(8) . . . . ?
C59 C60 C61 C62 -1.6(15) . . . . ?
C60 C61 C62 C63 0.9(15) . . . . ?
C61 C62 C63 C58 -0.1(15) . . . . ?
C59 C58 C63 C62 0.0(13) . . . . ?
N51 C58 C63 C62 176.5(8) . . . . ?
Ni2 O53 C64 C59 53.6(8) . . . . ?
C60 C59 C64 O53 121.1(8) . . . . ?
C58 C59 C64 O53 -61.2(10) . . . . ?
Ni2 O71 C72 C71 32.4(10) . . . . ?
La1 O71 C72 C71 -162.8(6) . . . . ?
Ni2 O71 C72 C73 -147.9(6) . . . . ?
La1 O71 C72 C73 16.9(10) . . . . ?
C76 C71 C72 O71 178.4(8) . . . . ?
C77 C71 C72 O71 -0.4(13) . . . . ?
C76 C71 C72 C73 -1.3(12) . . . . ?
C77 C71 C72 C73 179.9(8) . . . . ?
C85 O72 C73 C74 -2.9(13) . . . . ?
La1 O72 C73 C74 163.2(8) . . . . ?
C85 O72 C73 C72 176.2(8) . . . . ?
La1 O72 C73 C72 -17.7(9) . . . . ?
O71 C72 C73 C74 -178.2(8) . . . . ?
C71 C72 C73 C74 1.6(13) . . . . ?
O71 C72 C73 O72 2.7(11) . . . . ?
C71 C72 C73 O72 -177.5(7) . . . . ?
O72 C73 C74 C75 178.5(9) . . . . ?
C72 C73 C74 C75 -0.5(15) . . . . ?
C73 C74 C75 C76 -0.9(16) . . . . ?
C74 C75 C76 C71 1.1(16) . . . . ?
C72 C71 C76 C75 0.0(14) . . . . ?
C77 C71 C76 C75 178.8(9) . . . . ?
C78 N71 C77 C71 175.8(7) . . . . ?
Ni2 N71 C77 C71 -8.0(12) . . . . ?
C72 C71 C77 N71 -13.4(13) . . . . ?
C76 C71 C77 N71 167.8(8) . . . . ?
C77 N71 C78 C79 -126.1(9) . . . . ?
Ni2 N71 C78 C79 57.3(9) . . . . ?
C77 N71 C78 C83 55.3(11) . . . . ?
Ni2 N71 C78 C83 -121.3(8) . . . . ?
C83 C78 C79 C80 1.2(13) . . . . ?
N71 C78 C79 C80 -177.4(7) . . . . ?
C83 C78 C79 C84 -173.7(8) . . . . ?

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N71 C78 C79 C84 7.7(11) . . . . ?
C78 C79 C80 C81 -1.1(13) . . . . ?
C84 C79 C80 C81 173.8(8) . . . . ?
C79 C80 C81 C82 1.0(14) . . . . ?
C80 C81 C82 C83 -1.0(14) . . . . ?
C79 C78 C83 C82 -1.2(13) . . . . ?
N71 C78 C83 C82 177.3(8) . . . . ?
C81 C82 C83 C78 1.1(14) . . . . ?
Ni2 O73 C84 C79 42.6(8) . . . . ?
C78 C79 C84 O73 -59.6(10) . . . . ?
C80 C79 C84 O73 125.5(8) . . . . ?
O11A O11C N11A O11B 165.6(16) 3 . . . ?
O11A O11C N11A O11A -14.4(16) 3 . . . ?
O11C O11A N11A O11B -142(4) 3 . . . ?
N11A O11A N11A O11B -167.7(14) 3 . . . ?
O11C O11A N11A O11C 38(4) 3 . . . ?
N11A O11A N11A O11C 12.3(14) 3 . . . ?
O11C O11A N11A O11A 25(2) 3 . . 3 ?
N11A O11A N11A O11A 0.001(2) 3 . . 3 ?

_diffrn_measured_fraction_theta_max    0.997
_diffrn_reflns_theta_full              26.37
_diffrn_measured_fraction_theta_full   0.997
_refine_diff_density_max    2.983
_refine_diff_density_min   -1.482
_refine_diff_density_rms    0.257
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 _platon_squeeze_void_nr
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 _platon_squeeze_void_average_z
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 _platon_squeeze_void_count_electrons
 _platon_squeeze_void_content
  1  0.276 -0.159  1.024      278       68 ' '
  2  0.724  0.159  0.976      277       74 ' '
  3  0.223  0.343  0.475      273       73 ' '
  4  0.777  0.657  0.525      273       67 ' '
_platon_squeeze_details                  ?
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Complex **4**:

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;
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;
_chemical_name_common           ?
_chemical_melting_point         ?
_chemical_formula_moiety        ?
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 'C61 H60 Gd N7 O22 Zn2'
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 _atom_type_symbol
 _atom_type_description
 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Gd'  'Gd'  -0.1653   3.9035
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'  'N'   0.0061   0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Zn'  'Zn'   0.2839   1.4301
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting          Triclinic
_symmetry_space_group_name_H-M    P-1

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-x, -y, -z'

_cell_length_a                  12.714(3)
_cell_length_b                  13.200(3)
_cell_length_c                  21.782(6)
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_cell_angle_alpha                85.876(12)
_cell_angle_beta                 87.692(12)
_cell_angle_gamma                61.678(5)
_cell_volume                     3209.6(14)
_cell_formula_units_Z            2
_cell_measurement_temperature    100(2)
_cell_measurement_reflns_used    10104
_cell_measurement_theta_min      3.07
_cell_measurement_theta_max      25.0

_exptl_crystal_description       Needle
_exptl_crystal_colour            Colourless
_exptl_crystal_size_max          0.16
_exptl_crystal_size_mid          0.16
_exptl_crystal_size_min          0.09
_exptl_crystal_density_meas      ?
_exptl_crystal_density_diffrn    1.584
_exptl_crystal_density_method    'not measured'
_exptl_crystal_F_000             1550
_exptl_absorpt_coefficient_mu    1.845
_exptl_absorpt_correction_type   Numerical
_exptl_absorpt_correction_T_min  0.7567
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_exptl_special_details
;
 CrystalClear-SM Expert 2.1 b24 (Rigaku, 2012) was used for absorption correction.
R(int) was 0.2093 before and 0.0637 after correction
;

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_diffrn_radiation_wavelength     0.71070
_diffrn_radiation_type           MoK\a
_diffrn_radiation_source         'fine-focus sealed tube'
_diffrn_radiation_monochromator  graphite
_diffrn_measurement_device_type
;
Rigaku Saturn724+ (4x4 bin mode)
;
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_diffrn_reflns_number            35802
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_diffrn_reflns_av_sigmaI/netI    0.0659
_diffrn_reflns_limit_h_min       -14
_diffrn_reflns_limit_h_max       15
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_diffrn_reflns_limit_k_min       -15
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_reflns_number_gt                9728
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;
CrystalClear-SM Expert 2.1 b24 (Rigaku, 2012)
;
_computing_cell_refinement
;
CrystalClear-SM Expert 2.1 b24 (Rigaku, 2012)
;
_computing_data_reduction
;
CrystalClear-SM Expert 2.1 b24 (Rigaku, 2012)
;
_computing_structure_solution     'SHELXS-97 (Sheldrick, 2008)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 2008)'
_computing_molecular_graphics     'Bruker SHELXTL'
_computing_publication_material   'Bruker SHELXTL'

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.

 All the non-hydrogen atoms (except the disorded and solvent molecule) were
refined anisotropically and the hydrogen atoms were added in its calculated
geometric position. The hydrogen atoms were refined as a riding model.

 For the better convergence of disordered nitrate ions we have employed
several restraints and constraints such as DFIX, DANG, SIMU etc.

 Due to the diffused electron density some of the solvent molecules are
heavily disorded which is not allowed us to model them, hence SQUZZEE routine
was used to calculated remaining electrons in the void.
```

The calculated solvent void volume is 281 A^3 with 45 electrons in total, which would account for ~2.5 molecules of methanol for one unit cell.

The loop generated from PLATON is appended at the end of the cif file
;

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_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type           full
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_refine_ls_weighting_details
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_atom_sites_solution_primary     direct
_atom_sites_solution_secondary   difmap
_atom_sites_solution_hydrogens   geom
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_refine_ls_extinction_method     none
_refine_ls_extinction_coef       ?
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_refine_ls_number_restraints     18
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 _atom_site_U_iso_or_equiv
 _atom_site_adp_type
 _atom_site_occupancy
 _atom_site_symmetry_multiplicity
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 _atom_site_refinement_flags
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 _atom_site_disorder_group
Gd1 Gd 0.885768(19) 0.387954(18) 0.261267(10) 0.01423(8) Uani 1 1 d . . .
Zn2 Zn 1.06882(5) 0.52367(4) 0.21245(2) 0.01528(13) Uani 1 1 d . . .
Zn3 Zn 0.74850(5) 0.20800(4) 0.31032(2) 0.01600(13) Uani 1 1 d . . .
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O33 O 0.5717(3) 0.3652(3) 0.30407(14) 0.0197(7) Uani 1 1 d . . .
H33 H 0.5436 0.4043 0.2651 0.024 Uiso 1 1 calc R . .
O11 O 0.7786(3) 0.2860(3) 0.23074(13) 0.0168(7) Uani 1 1 d . . .
O73 O 0.9025(3) 0.6979(3) 0.22154(14) 0.0194(7) Uani 1 1 d . . .
H73 H 0.8671 0.7183 0.2610 0.023 Uiso 1 1 calc R . .
O52 O 0.8543(3) 0.4667(3) 0.37238(14) 0.0180(7) Uani 1 1 d . . .
O31 O 0.8678(3) 0.2576(3) 0.33470(13) 0.0167(7) Uani 1 1 d . . .
O94 O 0.7639(3) 0.5988(3) 0.24775(15) 0.0196(7) Uani 1 1 d . . .
O51 O 1.0046(3) 0.4813(3) 0.29266(13) 0.0173(7) Uani 1 1 d . . .
O13 O 0.8995(3) 0.0193(3) 0.32998(15) 0.0221(8) Uani 1 1 d . . .
H13 H 0.9689 0.0061 0.3514 0.027 Uiso 1 1 calc R . .
O12 O 0.7831(3) 0.4414(3) 0.15351(14) 0.0180(7) Uani 1 1 d . . .
O32 O 1.0759(3) 0.2378(3) 0.32216(14) 0.0185(7) Uani 1 1 d . . .
O113 O 1.3740(3) 0.2602(3) 0.09182(16) 0.0270(8) Uani 1 1 d . . .
O53 O 1.2571(3) 0.3831(3) 0.19153(14) 0.0186(7) Uani 1 1 d . . .
H53 H 1.2697 0.3166 0.1715 0.022 Uiso 1 1 calc R . .
O71 O 1.0109(3) 0.4137(3) 0.18700(13) 0.0158(7) Uani 1 1 d . . .
O92 O 0.5501(5) 0.7118(4) 0.2645(3) 0.0803(17) Uani 1 1 d . . .
O112 O 1.3230(3) 0.4280(3) 0.04534(16) 0.0288(8) Uani 1 1 d . . .
O72 O 1.0179(3) 0.2165(2) 0.19038(14) 0.0173(7) Uani 1 1 d . . .
N101 N 1.2045(5) -0.1072(5) 0.3536(3) 0.0237(16) Uiso 0.758(9) 1 d PDU A 1
O101 O 1.3051(4) -0.1156(5) 0.3634(3) 0.0465(17) Uiso 0.758(9) 1 d PDU A 1
O102 O 1.1720(5) -0.1758(4) 0.3812(2) 0.0352(15) Uiso 0.758(9) 1 d PDU A 1
O103 O 1.1341(4) -0.0310(4) 0.3161(2) 0.0313(15) Uiso 0.758(9) 1 d PDU A 1
N10A N 1.231(2) -0.116(3) 0.3531(14) 0.098(10) Uiso 0.242(9) 1 d PDU A 2
O10A O 1.2345(18) -0.0486(17) 0.3106(8) 0.067(7) Uiso 0.242(9) 1 d PDU A 2
O10B O 1.1354(14) -0.1218(17) 0.3631(8) 0.049(5) Uiso 0.242(9) 1 d PDU A 2
O10C O 1.3128(16) -0.1604(19) 0.3927(9) 0.078(7) Uiso 0.242(9) 1 d PDU A 2
O111 O 1.4268(4) 0.2735(3) -0.00347(16) 0.0382(10) Uani 1 1 d . . .
O93 O 0.6686(3) 0.5046(3) 0.28286(15) 0.0202(7) Uani 1 1 d . . .
N51 N 1.1597(3) 0.5840(3) 0.26127(17) 0.0148(8) Uani 1 1 d . . .
N71 N 1.0538(3) 0.5836(3) 0.12064(16) 0.0150(8) Uani 1 1 d . . .
N111 N 1.3754(4) 0.3211(4) 0.04405(19) 0.0248(10) Uani 1 1 d . . .
N11 N 0.6887(3) 0.1225(3) 0.25950(17) 0.0169(8) Uani 1 1 d . . .
N31 N 0.7054(3) 0.2065(3) 0.40396(17) 0.0169(8) Uani 1 1 d . . .
N91 N 0.6664(4) 0.5998(4) 0.2653(2) 0.0383(12) Uani 1 1 d . . .
C51 C 1.0551(4) 0.5933(4) 0.3586(2) 0.0180(10) Uani 1 1 d . . .
C54 C 0.8938(4) 0.5771(4) 0.4452(2) 0.0181(10) Uani 1 1 d . . .
H54A H 0.8373 0.5736 0.4740 0.022 Uiso 1 1 calc R . .
C35 C 1.0539(4) 0.1962(4) 0.3782(2) 0.0164(10) Uani 1 1 d . . .
C65 C 0.7625(4) 0.4690(4) 0.4147(2) 0.0238(11) Uani 1 1 d . . .
H65A H 0.7981 0.4340 0.4549 0.036 Uiso 1 1 calc R . .
H65B H 0.7260 0.4255 0.3986 0.036 Uiso 1 1 calc R . .
H65C H 0.7011 0.5490 0.4192 0.036 Uiso 1 1 calc R . .
C11 C 0.6824(4) 0.2245(4) 0.1597(2) 0.0159(10) Uani 1 1 d . . .
C45 C 1.1971(4) 0.2130(5) 0.3077(3) 0.0326(13) Uani 1 1 d . . .
H45A H 1.2514 0.1536 0.3375 0.049 Uiso 1 1 calc R . .

H45B H 1.2045 0.2833 0.3097 0.049 Uiso 1 1 calc R . .
H45C H 1.2178 0.1852 0.2662 0.049 Uiso 1 1 calc R . .
C73 C 1.1291(4) 0.2272(4) 0.0312(2) 0.0214(11) Uani 1 1 d . . .
H73A H 1.1560 0.1834 -0.0042 0.026 Uiso 1 1 calc R . .
C24 C 0.8892(4) -0.0775(4) 0.3102(2) 0.0219(11) Uani 1 1 d . . .
H24A H 0.9458 -0.1488 0.3336 0.026 Uiso 1 1 calc R . .
H24B H 0.9100 -0.0869 0.2660 0.026 Uiso 1 1 calc R . .
C20 C 0.5304(4) -0.0277(4) 0.3361(2) 0.0237(11) Uani 1 1 d . . .
H20A H 0.4514 -0.0173 0.3413 0.028 Uiso 1 1 calc R . .
C55 C 0.9120(4) 0.5264(4) 0.3897(2) 0.0173(10) Uani 1 1 d . . .
C75 C 1.0853(4) 0.4009(4) 0.0827(2) 0.0162(10) Uani 1 1 d . . .
C19 C 0.5510(4) 0.0527(4) 0.3014(2) 0.0233(11) Uani 1 1 d . . .
H19A H 0.4857 0.1190 0.2830 0.028 Uiso 1 1 calc R . .
C13 C 0.6428(4) 0.3185(4) 0.0569(2) 0.0209(11) Uani 1 1 d . . .
H13A H 0.6136 0.3260 0.0165 0.025 Uiso 1 1 calc R . .
C71 C 1.0556(4) 0.2484(4) 0.1357(2) 0.0156(10) Uani 1 1 d . . .
C63 C 1.3352(4) 0.5214(4) 0.1961(2) 0.0211(11) Uani 1 1 d . . .
C21 C 0.6268(5) -0.1249(4) 0.3634(2) 0.0249(11) Uani 1 1 d . . .
H21A H 0.6133 -0.1805 0.3877 0.030 Uiso 1 1 calc R . .
C60 C 1.2980(5) 0.7476(4) 0.1776(2) 0.0274(12) Uani 1 1 d . . .
H60A H 1.2861 0.8243 0.1714 0.033 Uiso 1 1 calc R . .
C56 C 0.9930(4) 0.5325(3) 0.34486(19) 0.0144(10) Uani 1 1 d . . .
C52 C 1.0375(4) 0.6407(4) 0.4166(2) 0.0187(10) Uani 1 1 d . . .
H52A H 1.0819 0.6784 0.4264 0.022 Uiso 1 1 calc R . .
C74 C 1.1244(4) 0.3330(4) 0.0308(2) 0.0197(11) Uani 1 1 d . . .
H74A H 1.1480 0.3617 -0.0054 0.024 Uiso 1 1 calc R . .
C78 C 1.0411(4) 0.6965(4) 0.1050(2) 0.0158(10) Uani 1 1 d . . .
C23 C 0.7640(4) -0.0589(4) 0.3206(2) 0.0194(11) Uani 1 1 d . . .
C32 C 0.9815(4) 0.1273(4) 0.4883(2) 0.0202(11) Uani 1 1 d . . .
H32A H 0.9563 0.1075 0.5269 0.024 Uiso 1 1 calc R . .
C57 C 1.1363(4) 0.6121(4) 0.3174(2) 0.0165(10) Uani 1 1 d . . .
H57A H 1.1768 0.6492 0.3333 0.020 Uiso 1 1 calc R . .
C16 C 0.7329(4) 0.2936(4) 0.1765(2) 0.0177(10) Uani 1 1 d . . .
C84 C 0.8501(4) 0.7771(4) 0.1698(2) 0.0199(11) Uani 1 1 d . . .
H84A H 0.7910 0.8529 0.1844 0.024 Uiso 1 1 calc R . .
H84B H 0.8072 0.7489 0.1447 0.024 Uiso 1 1 calc R . .
C59 C 1.2233(4) 0.7234(4) 0.2172(2) 0.0214(11) Uani 1 1 d . . .
H59A H 1.1603 0.7835 0.2384 0.026 Uiso 1 1 calc R . .
C82 C 0.9294(4) 0.9012(4) 0.1137(2) 0.0198(11) Uani 1 1 d . . .
H82A H 0.8645 0.9664 0.1305 0.024 Uiso 1 1 calc R . .
C34 C 1.1341(4) 0.1449(4) 0.4260(2) 0.0209(11) Uani 1 1 d . . .
H34A H 1.2141 0.1317 0.4211 0.025 Uiso 1 1 calc R . .
C40 C 0.4644(5) 0.1519(5) 0.4762(2) 0.0309(13) Uani 1 1 d . . .
H40A H 0.4560 0.0964 0.5032 0.037 Uiso 1 1 calc R . .
C77 C 1.0761(4) 0.5153(4) 0.0759(2) 0.0160(10) Uani 1 1 d . . .
H77A H 1.0873 0.5424 0.0359 0.019 Uiso 1 1 calc R . .
C39 C 0.5781(5) 0.1363(5) 0.4598(2) 0.0276(12) Uani 1 1 d . . .

H39A H 0.6470 0.0701 0.4755 0.033 Uiso 1 1 calc R . .
C33 C 1.0962(4) 0.1123(4) 0.4817(2) 0.0224(11) Uani 1 1 d . . .
H33A H 1.1500 0.0797 0.5153 0.027 Uiso 1 1 calc R . .
C72 C 1.0941(4) 0.1837(4) 0.0843(2) 0.0195(11) Uani 1 1 d . . .
H72A H 1.0968 0.1105 0.0850 0.023 Uiso 1 1 calc R . .
C41 C 0.3640(5) 0.2478(4) 0.4533(2) 0.0302(13) Uani 1 1 d . . .
H41A H 0.2867 0.2584 0.4648 0.036 Uiso 1 1 calc R . .
C81 C 1.0077(5) 0.9171(4) 0.0738(2) 0.0231(11) Uani 1 1 d . . .
H81A H 0.9945 0.9929 0.0620 0.028 Uiso 1 1 calc R . .
C64 C 1.3562(4) 0.3982(4) 0.2097(2) 0.0238(11) Uani 1 1 d . . .
H64A H 1.4290 0.3449 0.1875 0.029 Uiso 1 1 calc R . .
H64B H 1.3700 0.3779 0.2543 0.029 Uiso 1 1 calc R . .
C76 C 1.0509(4) 0.3580(4) 0.1352(2) 0.0155(10) Uani 1 1 d . . .
C18 C 0.6658(4) 0.0380(4) 0.2931(2) 0.0163(10) Uani 1 1 d . . .
C79 C 1.1226(4) 0.7118(4) 0.0671(2) 0.0197(10) Uani 1 1 d . . .
H79A H 1.1903 0.6466 0.0521 0.024 Uiso 1 1 calc R . .
C42 C 0.3763(5) 0.3279(4) 0.4138(2) 0.0264(12) Uani 1 1 d . . .
H42A H 0.3068 0.3932 0.3978 0.032 Uiso 1 1 calc R . .
C43 C 0.4889(4) 0.3152(4) 0.3966(2) 0.0204(11) Uani 1 1 d . . .
C31 C 0.9013(4) 0.1717(4) 0.4386(2) 0.0200(11) Uani 1 1 d . . .
C85 C 1.0240(5) 0.1042(4) 0.1948(2) 0.0250(11) Uani 1 1 d . . .
H85A H 1.0792 0.0566 0.1634 0.037 Uiso 1 1 calc R . .
H85B H 0.9443 0.1125 0.1883 0.037 Uiso 1 1 calc R . .
H85C H 1.0524 0.0672 0.2358 0.037 Uiso 1 1 calc R . .
C14 C 0.6894(4) 0.3901(4) 0.0733(2) 0.0200(11) Uani 1 1 d . . .
H14A H 0.6902 0.4475 0.0446 0.024 Uiso 1 1 calc R . .
C44 C 0.4990(4) 0.4090(4) 0.3580(2) 0.0235(11) Uani 1 1 d . . .
H44A H 0.4183 0.4693 0.3453 0.028 Uiso 1 1 calc R . .
H44B H 0.5345 0.4450 0.3828 0.028 Uiso 1 1 calc R . .
C58 C 1.2408(4) 0.6118(4) 0.2257(2) 0.0186(10) Uani 1 1 d . . .
C62 C 1.4094(4) 0.5455(4) 0.1567(2) 0.0256(12) Uani 1 1 d . . .
H62A H 1.4733 0.4852 0.1362 0.031 Uiso 1 1 calc R . .
C15 C 0.7341(4) 0.3756(4) 0.1319(2) 0.0163(10) Uani 1 1 d . . .
C12 C 0.6393(4) 0.2379(4) 0.0989(2) 0.0192(10) Uani 1 1 d . . .
H12A H 0.6074 0.1901 0.0872 0.023 Uiso 1 1 calc R . .
C36 C 0.9375(4) 0.2089(4) 0.3837(2) 0.0169(10) Uani 1 1 d . . .
C80 C 1.1063(4) 0.8222(4) 0.0505(2) 0.0230(11) Uani 1 1 d . . .
H80A H 1.1617 0.8328 0.0237 0.028 Uiso 1 1 calc R . .
C37 C 0.7822(4) 0.1835(4) 0.4466(2) 0.0201(11) Uani 1 1 d . . .
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C22 C 0.7418(4) -0.1399(4) 0.3552(2) 0.0206(11) Uani 1 1 d . . .
H22A H 0.8069 -0.2066 0.3734 0.025 Uiso 1 1 calc R . .
C61 C 1.3903(5) 0.6590(5) 0.1472(2) 0.0289(12) Uani 1 1 d . . .
H61A H 1.4408 0.6755 0.1196 0.035 Uiso 1 1 calc R . .
C53 C 0.9587(4) 0.6339(4) 0.4590(2) 0.0195(11) Uani 1 1 d . . .
H53A H 0.9479 0.6673 0.4975 0.023 Uiso 1 1 calc R . .
C25 C 0.7741(5) 0.5359(4) 0.1119(2) 0.0247(11) Uani 1 1 d . . .

H25A H 0.8147 0.5058 0.0731 0.037 Uiso 1 1 calc R . .
H25B H 0.8118 0.5759 0.1306 0.037 Uiso 1 1 calc R . .
H25C H 0.6897 0.5900 0.1040 0.037 Uiso 1 1 calc R . .
C38 C 0.5904(4) 0.2176(4) 0.4207(2) 0.0187(10) Uani 1 1 d . . .
C83 C 0.9430(4) 0.7917(4) 0.1302(2) 0.0163(10) Uani 1 1 d . . .
C17 C 0.6652(4) 0.1428(4) 0.2012(2) 0.0188(11) Uani 1 1 d . . .
H17A H 0.6332 0.0994 0.1838 0.023 Uiso 1 1 calc R . .
O1S O 0.6557(5) 0.3660(5) 0.5523(3) 0.0738(15) Uiso 1 1 d . . .
H1S H 0.7062 0.3178 0.5773 0.111 Uiso 1 1 calc R . .
C1S C 0.5456(7) 0.3587(6) 0.5585(3) 0.062(2) Uiso 1 1 d . . .
H1S1 H 0.5221 0.3613 0.6020 0.093 Uiso 1 1 calc R . .
H1S2 H 0.5577 0.2861 0.5428 0.093 Uiso 1 1 calc R . .
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O33 0.0181(17) 0.0191(16) 0.0212(17) -0.0008(13) 0.0000(14) -0.0083(15)
O11 0.0186(17) 0.0158(16) 0.0160(16) 0.0004(13) -0.0040(13) -0.0079(14)
O73 0.0222(17) 0.0154(16) 0.0169(16) -0.0012(13) 0.0022(14) -0.0059(14)
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O31 0.0156(16) 0.0202(16) 0.0160(16) -0.0008(13) -0.0009(13) -0.0098(14)
O94 0.0136(17) 0.0161(16) 0.0288(18) -0.0031(14) 0.0018(14) -0.0068(14)
O51 0.0201(17) 0.0147(15) 0.0162(16) -0.0038(13) 0.0009(13) -0.0071(14)
O13 0.0178(17) 0.0185(17) 0.0308(19) -0.0034(14) -0.0054(15) -0.0085(15)
O12 0.0216(17) 0.0198(16) 0.0174(16) 0.0027(13) -0.0024(13) -0.0140(15)
O32 0.0158(16) 0.0209(17) 0.0219(17) 0.0010(13) 0.0001(13) -0.0115(14)
O113 0.028(2) 0.0233(18) 0.029(2) 0.0041(15) -0.0018(16) -0.0125(16)
O53 0.0162(16) 0.0160(16) 0.0238(17) -0.0067(13) -0.0006(14) -0.0071(14)
O71 0.0155(16) 0.0162(15) 0.0185(16) -0.0062(13) 0.0035(13) -0.0094(14)
O92 0.051(3) 0.055(3) 0.108(4) -0.011(3) -0.007(3) -0.002(3)
O112 0.0230(19) 0.0212(19) 0.036(2) 0.0021(15) 0.0030(16) -0.0058(16)
O72 0.0239(18) 0.0127(15) 0.0175(16) -0.0016(12) 0.0029(14) -0.0107(14)
O111 0.041(2) 0.045(2) 0.026(2) -0.0131(18) 0.0057(18) -0.017(2)
O93 0.0179(17) 0.0139(16) 0.0306(19) -0.0002(14) 0.0011(14) -0.0091(14)
N51 0.0124(19) 0.0129(18) 0.018(2) -0.0026(15) -0.0015(16) -0.0050(16)
N71 0.0129(19) 0.0134(18) 0.017(2) -0.0024(15) 0.0001(15) -0.0047(16)
N111 0.019(2) 0.025(2) 0.028(2) -0.0047(19) -0.0024(18) -0.0080(19)
N11 0.016(2) 0.0152(19) 0.019(2) 0.0000(16) -0.0006(16) -0.0074(17)

N31 0.017(2) 0.0168(19) 0.017(2) -0.0001(16) 0.0001(16) -0.0079(17)
N91 0.032(3) 0.039(3) 0.039(3) -0.012(2) 0.000(2) -0.011(2)
C51 0.019(2) 0.015(2) 0.017(2) -0.0004(18) -0.0010(19) -0.005(2)
C54 0.020(2) 0.016(2) 0.015(2) 0.0018(18) 0.0026(19) -0.006(2)
C35 0.023(2) 0.010(2) 0.017(2) -0.0036(18) 0.0013(19) -0.007(2)
C65 0.024(3) 0.026(3) 0.027(3) -0.008(2) 0.010(2) -0.016(2)
C11 0.012(2) 0.018(2) 0.019(2) -0.0048(19) 0.0018(18) -0.0070(19)
C45 0.017(3) 0.037(3) 0.040(3) 0.007(3) 0.001(2) -0.011(2)
C73 0.027(3) 0.022(2) 0.020(2) -0.008(2) 0.001(2) -0.014(2)
C24 0.019(3) 0.015(2) 0.031(3) -0.005(2) -0.003(2) -0.007(2)
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C55 0.019(2) 0.007(2) 0.023(2) -0.0001(18) -0.001(2) -0.0045(19)
C75 0.013(2) 0.016(2) 0.018(2) -0.0001(18) -0.0034(18) -0.0058(19)
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C13 0.016(2) 0.026(3) 0.017(2) -0.008(2) 0.0024(19) -0.007(2)
C71 0.012(2) 0.014(2) 0.022(2) -0.0030(18) 0.0017(19) -0.0077(19)
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C21 0.034(3) 0.023(3) 0.022(3) -0.001(2) 0.002(2) -0.017(2)
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C52 0.019(2) 0.012(2) 0.022(3) 0.0001(19) -0.006(2) -0.004(2)
C74 0.016(2) 0.026(3) 0.014(2) -0.0019(19) 0.0012(19) -0.008(2)
C78 0.021(2) 0.014(2) 0.015(2) -0.0002(18) -0.0029(19) -0.010(2)
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C32 0.033(3) 0.013(2) 0.018(2) -0.0017(18) 0.001(2) -0.013(2)
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C84 0.020(2) 0.013(2) 0.023(3) -0.0006(19) -0.001(2) -0.005(2)
C59 0.021(3) 0.021(2) 0.025(3) -0.005(2) -0.001(2) -0.012(2)
C82 0.021(3) 0.015(2) 0.021(2) -0.0053(19) 0.001(2) -0.007(2)
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C77 0.009(2) 0.023(2) 0.013(2) -0.0006(19) -0.0005(18) -0.006(2)
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C33 0.027(3) 0.017(2) 0.023(3) 0.001(2) -0.010(2) -0.010(2)
C72 0.018(2) 0.015(2) 0.024(3) -0.0077(19) 0.001(2) -0.007(2)
C41 0.027(3) 0.033(3) 0.040(3) -0.022(3) 0.018(2) -0.020(3)
C81 0.033(3) 0.016(2) 0.023(3) -0.003(2) -0.001(2) -0.014(2)
C64 0.015(2) 0.025(3) 0.028(3) -0.005(2) -0.002(2) -0.006(2)
C76 0.013(2) 0.016(2) 0.015(2) -0.0012(18) -0.0039(18) -0.0051(19)
C18 0.022(2) 0.015(2) 0.013(2) -0.0008(18) 0.0020(19) -0.011(2)
C79 0.018(2) 0.018(2) 0.022(3) -0.0026(19) 0.002(2) -0.008(2)
C42 0.020(3) 0.026(3) 0.034(3) -0.011(2) 0.004(2) -0.010(2)
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C31 0.025(3) 0.016(2) 0.019(2) -0.0016(19) -0.004(2) -0.009(2)
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C14 0.018(2) 0.021(2) 0.019(2) -0.0008(19) 0.004(2) -0.008(2)

C44 0.019(3) 0.018(2) 0.031(3) -0.006(2) 0.004(2) -0.006(2)
C58 0.014(2) 0.025(2) 0.020(2) -0.005(2) 0.0003(19) -0.011(2)
C62 0.018(3) 0.034(3) 0.028(3) -0.013(2) 0.007(2) -0.014(2)
C15 0.009(2) 0.019(2) 0.020(2) -0.0039(19) 0.0028(18) -0.0067(19)
C12 0.017(2) 0.017(2) 0.022(2) -0.0071(19) 0.002(2) -0.006(2)
C36 0.021(2) 0.013(2) 0.015(2) -0.0041(18) -0.0023(19) -0.006(2)
C80 0.026(3) 0.027(3) 0.020(3) 0.001(2) 0.002(2) -0.017(2)
C37 0.026(3) 0.014(2) 0.016(2) -0.0044(18) 0.003(2) -0.006(2)
C22 0.027(3) 0.015(2) 0.020(2) 0.0050(19) -0.007(2) -0.011(2)
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C53 0.025(3) 0.014(2) 0.015(2) -0.0020(18) -0.003(2) -0.006(2)
C25 0.031(3) 0.022(3) 0.024(3) 0.006(2) -0.001(2) -0.016(2)
C38 0.015(2) 0.024(2) 0.022(2) -0.006(2) 0.0040(19) -0.013(2)
C83 0.018(2) 0.016(2) 0.016(2) -0.0017(18) -0.0032(19) -0.008(2)
C17 0.010(2) 0.014(2) 0.028(3) -0.008(2) 0.0005(19) -0.0017(19)

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;
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.
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Gd1 O32 2.620(3) . ?
Gd1 O52 2.643(3) . ?
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Gd1 N91 2.867(5) . ?
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Zn2 N71 2.079(4) . ?

Zn2 O53 2.280(3) . ?
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O31 C36 1.331(5) . ?
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O51 C56 1.332(5) . ?
O13 C24 1.441(5) . ?
O13 H13 0.9500 . ?
O12 C15 1.399(5) . ?
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O32 C35 1.376(5) . ?
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O113 N111 1.273(5) . ?
O53 C64 1.440(6) . ?
O53 H53 0.9500 . ?
O71 C76 1.339(5) . ?
O92 N91 1.515(6) . ?
O112 N111 1.244(5) . ?
O72 C71 1.379(5) . ?
O72 C85 1.444(5) . ?
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N101 O102 1.269(6) . ?
N10A O10A 1.254(9) . ?
N10A O10B 1.259(9) . ?
N10A O10C 1.263(9) . ?
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O93 N91 1.274(6) . ?
N51 C57 1.285(5) . ?
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C54 H54A 0.9500 . ?
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C55 C56 1.417(6) . ?
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C75 C77 1.456(6) . ?
C19 C18 1.384(7) . ?
C19 H19A 0.9500 . ?
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C71 C76 1.418(6) . ?
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C21 H21A 0.9500 . ?
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C52 C53 1.365(7) . ?

C52 H52A 0.9500 . ?
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C78 C79 1.380(7) . ?
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C23 C22 1.393(7) . ?
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C40 H40A 0.9500 . ?
C77 H77A 0.9500 . ?
C39 C38 1.386(7) . ?
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C79 C80 1.394(7) . ?
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C42 C43 1.399(7) . ?
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C43 C44 1.501(7) . ?
C31 C36 1.405(7) . ?
C31 C37 1.451(7) . ?
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C85 H85C 0.9800 . ?
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C12 H12A 0.9500 . ?
C80 H80A 0.9500 . ?
C37 H37A 0.9500 . ?
C22 H22A 0.9500 . ?
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C53 H53A 0.9500 . ?
C25 H25A 0.9800 . ?
C25 H25B 0.9800 . ?
C25 H25C 0.9800 . ?
C17 H17A 0.9500 . ?
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O31 Gd1 O94 129.56(10) . . ?
O11 Gd1 O94 112.27(10) . . ?
O71 Gd1 O93 131.64(11) . . ?
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H65B C65 H65C 109.5 . . ?
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O1S C1S H1S3 109.5 . . ?
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H1S2 C1S H1S3 109.5 . . ?

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O51 Gd1 O94 N91 -142.4(3) . . . . ?
O12 Gd1 O94 N91 84.0(3) . . . . ?
O32 Gd1 O94 N91 -122.9(3) . . . . ?
O52 Gd1 O94 N91 -78.5(3) . . . . ?
O72 Gd1 O94 N91 118.8(3) . . . . ?
O71 Zn2 O51 C56 -172.0(3) . . . . ?
N51 Zn2 O51 C56 24.9(3) . . . . ?
N71 Zn2 O51 C56 -118.7(4) . . . . ?
O53 Zn2 O51 C56 107.1(3) . . . . ?
O73 Zn2 O51 C56 -63.0(3) . . . . ?
O71 Zn2 O51 Gd1 -14.06(11) . . . . ?
N51 Zn2 O51 Gd1 -177.24(13) . . . . ?
N71 Zn2 O51 Gd1 39.2(3) . . . . ?
O53 Zn2 O51 Gd1 -94.97(13) . . . . ?
O73 Zn2 O51 Gd1 94.89(13) . . . . ?
O71 Gd1 O51 C56 170.2(3) . . . . ?
O31 Gd1 O51 C56 -49.0(3) . . . . ?
O11 Gd1 O51 C56 -113.6(17) . . . . ?
O94 Gd1 O51 C56 76.4(3) . . . . ?
O93 Gd1 O51 C56 43.8(3) . . . . ?
O12 Gd1 O51 C56 128.9(3) . . . . ?

O32 Gd1 O51 C56 -89.9(3) . . . . ?
O52 Gd1 O51 C56 -5.3(3) . . . . ?
O72 Gd1 O51 C56 -149.6(3) . . . . ?
N91 Gd1 O51 C56 60.7(3) . . . . ?
O71 Gd1 O51 Zn2 13.31(11) . . . . ?
O31 Gd1 O51 Zn2 154.05(11) . . . . ?
O11 Gd1 O51 Zn2 89.5(18) . . . . ?
O94 Gd1 O51 Zn2 -80.49(13) . . . . ?
O93 Gd1 O51 Zn2 -113.15(13) . . . . ?
O12 Gd1 O51 Zn2 -28.00(16) . . . . ?
O32 Gd1 O51 Zn2 113.21(14) . . . . ?
O52 Gd1 O51 Zn2 -162.22(16) . . . . ?
O72 Gd1 O51 Zn2 53.48(14) . . . . ?
N91 Gd1 O51 Zn2 -96.23(15) . . . . ?
O31 Zn3 O13 C24 -167.0(3) . . . . ?
N11 Zn3 O13 C24 -8.5(3) . . . . ?
O11 Zn3 O13 C24 -94.6(3) . . . . ?
N31 Zn3 O13 C24 106.4(3) . . . . ?
O33 Zn3 O13 C24 51.0(6) . . . . ?
O71 Gd1 O12 C15 130.7(3) . . . . ?
O31 Gd1 O12 C15 -13.1(3) . . . . ?
O11 Gd1 O12 C15 -7.8(3) . . . . ?
O94 Gd1 O12 C15 -138.4(3) . . . . ?
O93 Gd1 O12 C15 -83.2(3) . . . . ?
O51 Gd1 O12 C15 169.1(3) . . . . ?
O32 Gd1 O12 C15 72.2(3) . . . . ?
O52 Gd1 O12 C15 -111.3(3) . . . . ?
O72 Gd1 O12 C15 65.7(3) . . . . ?
N91 Gd1 O12 C15 -110.5(3) . . . . ?
O71 Gd1 O12 C25 -48.0(3) . . . . ?
O31 Gd1 O12 C25 168.2(3) . . . . ?
O11 Gd1 O12 C25 173.6(3) . . . . ?
O94 Gd1 O12 C25 42.9(3) . . . . ?
O93 Gd1 O12 C25 98.1(3) . . . . ?
O51 Gd1 O12 C25 -9.6(3) . . . . ?
O32 Gd1 O12 C25 -106.5(3) . . . . ?
O52 Gd1 O12 C25 70.0(4) . . . . ?
O72 Gd1 O12 C25 -113.0(3) . . . . ?
N91 Gd1 O12 C25 70.9(3) . . . . ?
O71 Gd1 O32 C35 174.8(3) . . . . ?
O31 Gd1 O32 C35 -23.9(3) . . . . ?
O11 Gd1 O32 C35 -67.3(3) . . . . ?
O94 Gd1 O32 C35 94.4(3) . . . . ?
O93 Gd1 O32 C35 12.2(3) . . . . ?
O51 Gd1 O32 C35 114.0(3) . . . . ?
O12 Gd1 O32 C35 -131.8(3) . . . . ?
O52 Gd1 O32 C35 50.5(3) . . . . ?

O72 Gd1 O32 C35 -125.3(3) . . . . ?
N91 Gd1 O32 C35 52.7(4) . . . . ?
O71 Gd1 O32 C45 7.2(4) . . . . ?
O31 Gd1 O32 C45 168.4(4) . . . . ?
O11 Gd1 O32 C45 125.0(3) . . . . ?
O94 Gd1 O32 C45 -73.3(4) . . . . ?
O93 Gd1 O32 C45 -155.5(3) . . . . ?
O51 Gd1 O32 C45 -53.7(3) . . . . ?
O12 Gd1 O32 C45 60.5(4) . . . . ?
O52 Gd1 O32 C45 -117.2(4) . . . . ?
O72 Gd1 O32 C45 67.0(3) . . . . ?
N91 Gd1 O32 C45 -115.0(4) . . . . ?
O71 Zn2 O53 C64 -170.4(3) . . . . ?
N51 Zn2 O53 C64 -8.9(3) . . . . ?
O51 Zn2 O53 C64 -96.7(3) . . . . ?
N71 Zn2 O53 C64 102.2(3) . . . . ?
O73 Zn2 O53 C64 46.9(5) . . . . ?
N51 Zn2 O71 C76 -106.9(4) . . . . ?
O51 Zn2 O71 C76 -159.5(3) . . . . ?
N71 Zn2 O71 C76 41.8(3) . . . . ?
O53 Zn2 O71 C76 -47.1(3) . . . . ?
O73 Zn2 O71 C76 122.5(3) . . . . ?
N51 Zn2 O71 Gd1 68.2(4) . . . . ?
O51 Zn2 O71 Gd1 15.64(13) . . . . ?
N71 Zn2 O71 Gd1 -143.09(15) . . . . ?
O53 Zn2 O71 Gd1 128.02(14) . . . . ?
O73 Zn2 O71 Gd1 -62.42(15) . . . . ?
O31 Gd1 O71 C76 63.8(4) . . . . ?
O11 Gd1 O71 C76 -15.9(3) . . . . ?
O94 Gd1 O71 C76 -128.1(3) . . . . ?
O93 Gd1 O71 C76 -102.5(3) . . . . ?
O51 Gd1 O71 C76 160.7(3) . . . . ?
O12 Gd1 O71 C76 -56.4(3) . . . . ?
O32 Gd1 O71 C76 93.3(3) . . . . ?
O52 Gd1 O71 C76 165.4(3) . . . . ?
O72 Gd1 O71 C76 24.5(3) . . . . ?
N91 Gd1 O71 C76 -116.7(3) . . . . ?
O31 Gd1 O71 Zn2 -111.01(18) . . . . ?
O11 Gd1 O71 Zn2 169.33(12) . . . . ?
O94 Gd1 O71 Zn2 57.15(14) . . . . ?
O93 Gd1 O71 Zn2 82.72(18) . . . . ?
O51 Gd1 O71 Zn2 -14.03(12) . . . . ?
O12 Gd1 O71 Zn2 128.79(16) . . . . ?
O32 Gd1 O71 Zn2 -81.50(14) . . . . ?
O52 Gd1 O71 Zn2 -9.39(19) . . . . ?
O72 Gd1 O71 Zn2 -150.25(18) . . . . ?
N91 Gd1 O71 Zn2 68.57(17) . . . . ?

O71 Gd1 O72 C71 -21.6(3) . . . . ?
O31 Gd1 O72 C71 179.6(3) . . . . ?
O11 Gd1 O72 C71 119.6(3) . . . . ?
O94 Gd1 O72 C71 20.3(3) . . . . ?
O93 Gd1 O72 C71 99.9(3) . . . . ?
O51 Gd1 O72 C71 -62.3(3) . . . . ?
O12 Gd1 O72 C71 54.7(3) . . . . ?
O32 Gd1 O72 C71 -121.3(3) . . . . ?
O52 Gd1 O72 C71 -128.7(3) . . . . ?
N91 Gd1 O72 C71 60.7(4) . . . . ?
O71 Gd1 O72 C85 177.3(4) . . . . ?
O31 Gd1 O72 C85 18.5(3) . . . . ?
O11 Gd1 O72 C85 -41.4(3) . . . . ?
O94 Gd1 O72 C85 -140.7(3) . . . . ?
O93 Gd1 O72 C85 -61.1(4) . . . . ?
O51 Gd1 O72 C85 136.6(3) . . . . ?
O12 Gd1 O72 C85 -106.4(3) . . . . ?
O32 Gd1 O72 C85 77.7(3) . . . . ?
O52 Gd1 O72 C85 70.2(4) . . . . ?
N91 Gd1 O72 C85 -100.4(4) . . . . ?
O71 Gd1 O93 N91 -31.6(3) . . . . ?
O31 Gd1 O93 N91 156.3(3) . . . . ?
O11 Gd1 O93 N91 -140.3(3) . . . . ?
O94 Gd1 O93 N91 1.1(2) . . . . ?
O51 Gd1 O93 N91 41.0(3) . . . . ?
O12 Gd1 O93 N91 -76.2(3) . . . . ?
O32 Gd1 O93 N91 124.9(3) . . . . ?
O52 Gd1 O93 N91 85.3(3) . . . . ?
O72 Gd1 O93 N91 -120.9(3) . . . . ?
O71 Zn2 N51 C57 -69.4(5) . . . . ?
O51 Zn2 N51 C57 -19.1(4) . . . . ?
N71 Zn2 N51 C57 144.2(3) . . . . ?
O53 Zn2 N51 C57 -130.0(4) . . . . ?
O73 Zn2 N51 C57 63.8(4) . . . . ?
O71 Zn2 N51 C58 120.5(4) . . . . ?
O51 Zn2 N51 C58 170.9(3) . . . . ?
N71 Zn2 N51 C58 -25.8(3) . . . . ?
O53 Zn2 N51 C58 60.0(3) . . . . ?
O73 Zn2 N51 C58 -106.3(3) . . . . ?
O71 Zn2 N71 C77 -34.5(3) . . . . ?
N51 Zn2 N71 C77 133.8(3) . . . . ?
O51 Zn2 N71 C77 -85.6(4) . . . . ?
O53 Zn2 N71 C77 52.2(3) . . . . ?
O73 Zn2 N71 C77 -141.5(4) . . . . ?
O71 Zn2 N71 C78 157.7(3) . . . . ?
N51 Zn2 N71 C78 -34.0(4) . . . . ?
O51 Zn2 N71 C78 106.6(4) . . . . ?

O53 Zn2 N71 C78 -115.6(3) . . . . ?
O73 Zn2 N71 C78 50.6(3) . . . . ?
O31 Zn3 N11 C17 -65.2(5) . . . . ?
O11 Zn3 N11 C17 -10.8(4) . . . . ?
N31 Zn3 N11 C17 154.2(3) . . . . ?
O33 Zn3 N11 C17 70.7(4) . . . . ?
O13 Zn3 N11 C17 -123.9(4) . . . . ?
O31 Zn3 N11 C18 118.3(4) . . . . ?
O11 Zn3 N11 C18 172.7(3) . . . . ?
N31 Zn3 N11 C18 -22.3(3) . . . . ?
O33 Zn3 N11 C18 -105.8(3) . . . . ?
O13 Zn3 N11 C18 59.6(3) . . . . ?
O31 Zn3 N31 C37 -30.5(4) . . . . ?
N11 Zn3 N31 C37 133.6(3) . . . . ?
O11 Zn3 N31 C37 -79.7(5) . . . . ?
O33 Zn3 N31 C37 -138.1(4) . . . . ?
O13 Zn3 N31 C37 55.9(4) . . . . ?
O31 Zn3 N31 C38 157.2(3) . . . . ?
N11 Zn3 N31 C38 -38.6(4) . . . . ?
O11 Zn3 N31 C38 108.1(4) . . . . ?
O33 Zn3 N31 C38 49.7(3) . . . . ?
O13 Zn3 N31 C38 -116.3(3) . . . . ?
Gd1 O93 N91 O94 -2.0(4) . . . . ?
Gd1 O93 N91 O92 177.3(4) . . . . ?
Gd1 O94 N91 O93 2.0(4) . . . . ?
Gd1 O94 N91 O92 -177.3(4) . . . . ?
O71 Gd1 N91 O93 155.7(2) . . . . ?
O31 Gd1 N91 O93 -24.6(3) . . . . ?
O11 Gd1 N91 O93 37.0(3) . . . . ?
O94 Gd1 N91 O93 -178.0(4) . . . . ?
O51 Gd1 N91 O93 -142.7(3) . . . . ?
O12 Gd1 N91 O93 95.5(3) . . . . ?
O32 Gd1 N91 O93 -87.3(3) . . . . ?
O52 Gd1 N91 O93 -85.1(3) . . . . ?
O72 Gd1 N91 O93 89.4(3) . . . . ?
O71 Gd1 N91 O94 -26.4(3) . . . . ?
O31 Gd1 N91 O94 153.4(2) . . . . ?
O11 Gd1 N91 O94 -145.1(3) . . . . ?
O93 Gd1 N91 O94 178.0(4) . . . . ?
O51 Gd1 N91 O94 35.2(3) . . . . ?
O12 Gd1 N91 O94 -86.5(3) . . . . ?
O32 Gd1 N91 O94 90.6(3) . . . . ?
O52 Gd1 N91 O94 92.9(3) . . . . ?
O72 Gd1 N91 O94 -92.6(3) . . . . ?
O71 Gd1 N91 O92 50(9) . . . . ?
O31 Gd1 N91 O92 -130(9) . . . . ?
O11 Gd1 N91 O92 -69(9) . . . . ?

O94 Gd1 N91 O92 77(9) . . . . ?
O93 Gd1 N91 O92 -106(9) . . . . ?
O51 Gd1 N91 O92 112(9) . . . . ?
O12 Gd1 N91 O92 -10(9) . . . . ?
O32 Gd1 N91 O92 167(9) . . . . ?
O52 Gd1 N91 O92 169(9) . . . . ?
O72 Gd1 N91 O92 -16(9) . . . . ?
C45 O32 C35 C34 8.8(6) . . . . ?
Gd1 O32 C35 C34 -159.8(3) . . . . ?
C45 O32 C35 C36 -170.2(4) . . . . ?
Gd1 O32 C35 C36 21.1(4) . . . . ?
Zn3 O13 C24 C23 -40.7(5) . . . . ?
C53 C54 C55 O52 178.7(4) . . . . ?
C53 C54 C55 C56 -1.7(7) . . . . ?
C65 O52 C55 C54 5.5(6) . . . . ?
Gd1 O52 C55 C54 175.3(3) . . . . ?
C65 O52 C55 C56 -174.1(4) . . . . ?
Gd1 O52 C55 C56 -4.4(5) . . . . ?
C21 C20 C19 C18 0.4(7) . . . . ?
C85 O72 C71 C72 2.7(6) . . . . ?
Gd1 O72 C71 C72 -160.1(4) . . . . ?
C85 O72 C71 C76 -178.0(4) . . . . ?
Gd1 O72 C71 C76 19.2(5) . . . . ?
C19 C20 C21 C22 -0.4(7) . . . . ?
Zn2 O51 C56 C55 158.5(3) . . . . ?
Gd1 O51 C56 C55 5.3(5) . . . . ?
Zn2 O51 C56 C51 -21.0(6) . . . . ?
Gd1 O51 C56 C51 -174.2(3) . . . . ?
C54 C55 C56 O51 -179.9(4) . . . . ?
O52 C55 C56 O51 -0.2(5) . . . . ?
C54 C55 C56 C51 -0.3(6) . . . . ?
O52 C55 C56 C51 179.3(4) . . . . ?
C52 C51 C56 O51 -178.0(4) . . . . ?
C57 C51 C56 O51 2.4(7) . . . . ?
C52 C51 C56 C55 2.5(6) . . . . ?
C57 C51 C56 C55 -177.1(4) . . . . ?
C56 C51 C52 C53 -2.8(6) . . . . ?
C57 C51 C52 C53 176.9(4) . . . . ?
C72 C73 C74 C75 0.2(7) . . . . ?
C76 C75 C74 C73 -0.1(7) . . . . ?
C77 C75 C74 C73 -176.0(4) . . . . ?
C77 N71 C78 C79 -47.3(6) . . . . ?
Zn2 N71 C78 C79 121.0(4) . . . . ?
C77 N71 C78 C83 133.2(4) . . . . ?
Zn2 N71 C78 C83 -58.5(5) . . . . ?
O13 C24 C23 C22 -124.9(4) . . . . ?
O13 C24 C23 C18 58.4(6) . . . . ?

C58 N51 C57 C51 178.3(4) . . . . ?
Zn2 N51 C57 C51 8.7(6) . . . . ?
C52 C51 C57 N51 -175.0(4) . . . . ?
C56 C51 C57 N51 4.6(7) . . . . ?
Zn3 O11 C16 C15 162.4(3) . . . . ?
Gd1 O11 C16 C15 -6.4(5) . . . . ?
Zn3 O11 C16 C11 -17.7(6) . . . . ?
Gd1 O11 C16 C11 173.6(3) . . . . ?
C12 C11 C16 O11 -177.9(4) . . . . ?
C17 C11 C16 O11 5.3(7) . . . . ?
C12 C11 C16 C15 2.1(6) . . . . ?
C17 C11 C16 C15 -174.8(4) . . . . ?
Zn2 O73 C84 C83 -46.6(5) . . . . ?
C61 C60 C59 C58 -0.4(7) . . . . ?
O32 C35 C34 C33 176.6(4) . . . . ?
C36 C35 C34 C33 -4.4(6) . . . . ?
C78 N71 C77 C75 -176.5(4) . . . . ?
Zn2 N71 C77 C75 15.4(6) . . . . ?
C76 C75 C77 N71 11.8(7) . . . . ?
C74 C75 C77 N71 -172.5(4) . . . . ?
C41 C40 C39 C38 0.3(7) . . . . ?
C31 C32 C33 C34 2.3(7) . . . . ?
C35 C34 C33 C32 2.4(7) . . . . ?
O72 C71 C72 C73 179.4(4) . . . . ?
C76 C71 C72 C73 0.2(7) . . . . ?
C74 C73 C72 C71 -0.3(7) . . . . ?
C39 C40 C41 C42 0.5(7) . . . . ?
C83 C82 C81 C80 -2.5(7) . . . . ?
Zn2 O53 C64 C63 -42.2(5) . . . . ?
C62 C63 C64 O53 -119.2(5) . . . . ?
C58 C63 C64 O53 62.9(6) . . . . ?
Zn2 O71 C76 C75 -30.9(6) . . . . ?
Gd1 O71 C76 C75 154.8(3) . . . . ?
Zn2 O71 C76 C71 150.0(3) . . . . ?
Gd1 O71 C76 C71 -24.4(5) . . . . ?
C74 C75 C76 O71 -179.1(4) . . . . ?
C77 C75 C76 O71 -3.5(7) . . . . ?
C74 C75 C76 C71 0.0(6) . . . . ?
C77 C75 C76 C71 175.6(4) . . . . ?
O72 C71 C76 O71 -0.2(6) . . . . ?
C72 C71 C76 O71 179.2(4) . . . . ?
O72 C71 C76 C75 -179.4(4) . . . . ?
C72 C71 C76 C75 0.0(7) . . . . ?
C20 C19 C18 C23 -0.8(7) . . . . ?
C20 C19 C18 N11 -177.3(4) . . . . ?
C22 C23 C18 C19 1.2(6) . . . . ?
C24 C23 C18 C19 178.1(4) . . . . ?

C22 C23 C18 N11 177.9(4) . . . . ?
C24 C23 C18 N11 -5.3(6) . . . . ?
C17 N11 C18 C19 -65.2(6) . . . . ?
Zn3 N11 C18 C19 111.6(4) . . . . ?
C17 N11 C18 C23 118.2(5) . . . . ?
Zn3 N11 C18 C23 -65.1(4) . . . . ?
C83 C78 C79 C80 -3.1(7) . . . . ?
N71 C78 C79 C80 177.5(4) . . . . ?
C40 C41 C42 C43 -0.7(7) . . . . ?
C41 C42 C43 C38 0.2(7) . . . . ?
C41 C42 C43 C44 -174.6(4) . . . . ?
C33 C32 C31 C36 -5.0(6) . . . . ?
C33 C32 C31 C37 178.3(4) . . . . ?
C12 C13 C14 C15 1.6(7) . . . . ?
Zn3 O33 C44 C43 -47.9(5) . . . . ?
C42 C43 C44 O33 -126.9(4) . . . . ?
C38 C43 C44 O33 58.5(6) . . . . ?
C60 C59 C58 C63 1.6(7) . . . . ?
C60 C59 C58 N51 -173.8(4) . . . . ?
C62 C63 C58 C59 -1.6(7) . . . . ?
C64 C63 C58 C59 176.4(4) . . . . ?
C62 C63 C58 N51 174.1(4) . . . . ?
C64 C63 C58 N51 -8.0(6) . . . . ?
C57 N51 C58 C59 -56.4(6) . . . . ?
Zn2 N51 C58 C59 114.2(4) . . . . ?
C57 N51 C58 C63 128.0(5) . . . . ?
Zn2 N51 C58 C63 -61.4(5) . . . . ?
C58 C63 C62 C61 0.4(7) . . . . ?
C64 C63 C62 C61 -177.6(4) . . . . ?
C13 C14 C15 O12 179.9(4) . . . . ?
C13 C14 C15 C16 -1.3(7) . . . . ?
C25 O12 C15 C14 5.7(6) . . . . ?
Gd1 O12 C15 C14 -173.1(3) . . . . ?
C25 O12 C15 C16 -173.2(4) . . . . ?
Gd1 O12 C15 C16 8.0(5) . . . . ?
O11 C16 C15 C14 179.4(4) . . . . ?
C11 C16 C15 C14 -0.5(6) . . . . ?
O11 C16 C15 O12 -1.6(6) . . . . ?
C11 C16 C15 O12 178.4(4) . . . . ?
C14 C13 C12 C11 0.0(7) . . . . ?
C16 C11 C12 C13 -1.8(6) . . . . ?
C17 C11 C12 C13 175.3(4) . . . . ?
Zn3 O31 C36 C31 -36.0(5) . . . . ?
Gd1 O31 C36 C31 152.7(3) . . . . ?
Zn3 O31 C36 C35 144.5(3) . . . . ?
Gd1 O31 C36 C35 -26.8(5) . . . . ?
C32 C31 C36 O31 -176.4(4) . . . . ?

C37 C31 C36 O31 0.1(7) . . . . ?
C32 C31 C36 C35 3.0(6) . . . . ?
C37 C31 C36 C35 179.6(4) . . . . ?
O32 C35 C36 O31 0.3(5) . . . . ?
C34 C35 C36 O31 -178.9(4) . . . . ?
O32 C35 C36 C31 -179.2(4) . . . . ?
C34 C35 C36 C31 1.6(6) . . . . ?
C78 C79 C80 C81 1.2(7) . . . . ?
C82 C81 C80 C79 1.6(7) . . . . ?
C38 N31 C37 C31 -178.5(4) . . . . ?
Zn3 N31 C37 C31 9.3(6) . . . . ?
C36 C31 C37 N31 14.1(7) . . . . ?
C32 C31 C37 N31 -169.3(4) . . . . ?
C20 C21 C22 C23 0.9(7) . . . . ?
C18 C23 C22 C21 -1.3(7) . . . . ?
C24 C23 C22 C21 -178.1(4) . . . . ?
C59 C60 C61 C62 -0.9(8) . . . . ?
C63 C62 C61 C60 0.8(7) . . . . ?
C51 C52 C53 C54 0.7(7) . . . . ?
C55 C54 C53 C52 1.5(7) . . . . ?
C40 C39 C38 C43 -0.9(7) . . . . ?
C40 C39 C38 N31 178.4(4) . . . . ?
C42 C43 C38 C39 0.6(7) . . . . ?
C44 C43 C38 C39 175.3(4) . . . . ?
C42 C43 C38 N31 -178.7(4) . . . . ?
C44 C43 C38 N31 -4.0(6) . . . . ?
C37 N31 C38 C39 -48.4(6) . . . . ?
Zn3 N31 C38 C39 124.1(4) . . . . ?
C37 N31 C38 C43 130.9(4) . . . . ?
Zn3 N31 C38 C43 -56.6(5) . . . . ?
C81 C82 C83 C78 0.7(7) . . . . ?
C81 C82 C83 C84 -174.7(4) . . . . ?
C79 C78 C83 C82 2.1(7) . . . . ?
N71 C78 C83 C82 -178.5(4) . . . . ?
C79 C78 C83 C84 177.5(4) . . . . ?
N71 C78 C83 C84 -3.1(6) . . . . ?
O73 C84 C83 C82 -128.3(4) . . . . ?
O73 C84 C83 C78 56.4(5) . . . . ?
C18 N11 C17 C11 -179.9(4) . . . . ?
Zn3 N11 C17 C11 3.7(6) . . . . ?
C16 C11 C17 N11 2.5(7) . . . . ?
C12 C11 C17 N11 -174.5(4) . . . . ?

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_diffrn_reflns_theta_full 25.00
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_refine_diff_density_max 1.161

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_refine_diff_density_rms    0.117
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Complex **5**:

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;
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 'C61.25 H61 N7 O22.25 Pr Zn2'
_chemical_formula_weight        1522.82

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 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'  'N'   0.0061   0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Pr'  'Pr'  -0.2180   2.8214
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Zn'  'Zn'   0.2839   1.4301
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_space_group_name_H-M    P-1

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-x, -y, -z'

_cell_length_a                12.809(7)
_cell_length_b                13.227(7)
_cell_length_c                21.704(10)
_cell_angle_alpha               92.342(4)
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_cell_angle_beta                91.904(6)
_cell_angle_gamma               118.684(7)
_cell_volume                    3217(3)
_cell_formula_units_Z           2
_cell_measurement_temperature     100(2)
_cell_measurement_reflns_used     6825
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_cell_measurement_theta_max       25.0

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_exptl_crystal_size_mid           0.09
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_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.572
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              1549
_exptl_absorpt_coefficient_mu     1.568
_exptl_absorpt_correction_type    Numerical
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_exptl_special_details
;
 CrystalClear-SM Expert 2.1 b24 (Rigaku, 2012) was used for absorption correction.
R(int) was 0.1509 before and 0.1088 after correction.
;

_diffrn_ambient_temperature       100(2)
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;
Rigaku Saturn724+ (4x4 bin mode)
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_diffrn_reflns_number             43900
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_diffrn_reflns_limit_k_min        -15
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_reflns_number_gt 9576
_reflns_threshold_expression >2sigma(I)

_computing_data_collection
;
CrystalClear-SM Expert 2.1 b24 (Rigaku, 2012)
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_computing_cell_refinement
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_computing_data_reduction
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_computing_structure_refinement 'SHELXL-97 (Sheldrick, 2008)'
_computing_molecular_graphics 'Bruker SHELXTL'
_computing_publication_material 'Bruker SHELXTL'

_refine_special_details
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Refinement of F^2^ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2^, conventional R-factors R are based on F, with F set to zero for negative F^2^. The threshold expression of F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2^ are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All the non-hydrogen atoms (except the disorded atoms and solvent molecule) were refined anisotropically.The hydrogen atoms were added in its calculated geometric position. The hydrogen atoms were refined as a riding model.

For the better convergence of disordered solvents we have employed several restraints and constraints such as DFIX, DANG, SIMU etc.

Hydrogen atoms were not added on the disordered solvent molecules, but the corresponding number of hydrogens were inlcuded in the sum formula.
;

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_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type           full
_refine_ls_weighting_scheme      calc
_refine_ls_weighting_details
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_atom_sites_solution_primary     direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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_refine_ls_extinction_method      none
_refine_ls_extinction_coef       ?
_refine_ls_number_reflns         11297
_refine_ls_number_parameters      848
_refine_ls_number_restraints      6
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_refine_ls_R_factor_gt           0.0794
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Pr1 Pr -0.72468(4) 0.38767(4) 0.738409(19) 0.01555(16) Uani 1 1 d . . .
Zn1 Zn -0.40630(8) 0.52244(8) 0.78726(4) 0.0159(2) Uani 1 1 d . . .
Zn2 Zn -1.04128(8) 0.20907(8) 0.68820(4) 0.0167(2) Uani 1 1 d . . .
N11 N -0.3625(6) 0.5825(6) 0.8796(3) 0.0151(14) Uani 1 1 d . . .
N31 N -0.2568(6) 0.5834(6) 0.7372(3) 0.0193(15) Uani 1 1 d . . .
N51 N -1.1860(6) 0.1249(6) 0.7394(3) 0.0170(14) Uani 1 1 d . . .
N71 N -1.0840(6) 0.2093(6) 0.5940(3) 0.0174(14) Uani 1 1 d . . .
N91 N -0.7342(8) 0.6036(8) 0.7340(4) 0.036(2) Uani 1 1 d . . .
N101 N 0.1017(9) -0.1111(8) 0.6456(4) 0.046(2) Uani 1 1 d . . .
N111 N 0.6979(7) 0.3235(7) 0.9544(3) 0.0261(17) Uani 1 1 d . . .
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O11 O -0.5723(5) 0.4137(5) 0.8144(2) 0.0161(11) Uani 1 1 d . . .
O12 O -0.7619(5) 0.2161(5) 0.8117(2) 0.0192(12) Uani 1 1 d . . .
O13 O -0.4009(5) 0.6965(5) 0.7791(2) 0.0192(12) Uani 1 1 d . . .
H13 H -0.4172 0.7168 0.7398 0.023 Uiso 1 1 calc R . .
O31 O -0.5115(5) 0.4827(5) 0.7063(2) 0.0156(11) Uani 1 1 d . . .
O32 O -0.6743(5) 0.4697(5) 0.6263(2) 0.0180(12) Uani 1 1 d . . .
O33 O -0.3600(5) 0.3813(5) 0.8063(3) 0.0196(12) Uani 1 1 d . . .
H33 H -0.4134 0.3144 0.8260 0.023 Uiso 1 1 calc R . .
O51 O -0.9356(5) 0.2843(5) 0.7689(2) 0.0168(12) Uani 1 1 d . . .
O52 O -0.7792(5) 0.4383(5) 0.8483(2) 0.0194(12) Uani 1 1 d . . .
O53 O -1.0809(5) 0.0182(5) 0.6686(3) 0.0230(13) Uani 1 1 d . . .
H53 H -1.0262 0.0033 0.6468 0.028 Uiso 1 1 calc R . .
O71 O -0.8748(5) 0.2546(5) 0.6631(2) 0.0155(11) Uani 1 1 d . . .
O72 O -0.6882(5) 0.2327(5) 0.6740(2) 0.0193(12) Uani 1 1 d . . .
O73 O -1.0581(5) 0.3695(5) 0.6948(3) 0.0220(13) Uani 1 1 d . . .
H73 H -1.0460 0.4093 0.7340 0.026 Uiso 1 1 calc R . .
O91 O -0.8246(5) 0.5101(5) 0.7180(3) 0.0225(13) Uani 1 1 d . . .
O92 O -0.6360(5) 0.6055(5) 0.7518(3) 0.0234(13) Uani 1 1 d . . .
O93 O -0.7363(10) 0.7181(9) 0.7319(5) 0.082(3) Uani 1 1 d . . .
O101 O 0.1926(10) -0.1173(12) 0.6336(7) 0.107(4) Uani 1 1 d . . .
O102 O 0.1023(10) -0.0354(9) 0.6824(5) 0.077(3) Uani 1 1 d . . .
O103 O 0.0034(8) -0.1730(13) 0.6216(5) 0.111(5) Uani 1 1 d . . .
O111 O 0.7017(6) 0.2736(6) 1.0013(3) 0.0357(16) Uani 1 1 d . . .
O112 O 0.6381(6) 0.2637(6) 0.9059(3) 0.0294(14) Uani 1 1 d . . .
O113 O 0.7526(6) 0.4304(5) 0.9529(3) 0.0306(15) Uani 1 1 d . . .
C11 C -0.5111(7) 0.4007(8) 0.9183(4) 0.0184(17) Uani 1 1 d . . .
C12 C -0.5879(7) 0.3578(7) 0.8657(3) 0.0144(16) Uani 1 1 d . . .
C13 C -0.6899(7) 0.2509(7) 0.8665(4) 0.0178(17) Uani 1 1 d . . .
C14 C -0.7163(7) 0.1842(7) 0.9177(4) 0.0210(18) Uani 1 1 d . . .
H14A H -0.7859 0.1109 0.9169 0.025 Uiso 1 1 calc R . .
C15 C -0.6380(8) 0.2278(8) 0.9702(4) 0.0224(18) Uani 1 1 d . . .
H15A H -0.6543 0.1841 1.0057 0.027 Uiso 1 1 calc R . .
C16 C -0.5382(7) 0.3329(7) 0.9706(4) 0.0178(17) Uani 1 1 d . . .
H16A H -0.4857 0.3614 1.0066 0.021 Uiso 1 1 calc R . .
C17 C -0.4067(7) 0.5148(7) 0.9240(4) 0.0164(16) Uani 1 1 d . . .
H17A H -0.3675 0.5420 0.9638 0.020 Uiso 1 1 calc R . .
C18 C -0.2621(7) 0.6959(7) 0.8950(3) 0.0160(16) Uani 1 1 d . . .
C19 C -0.1667(7) 0.7096(8) 0.9323(4) 0.0213(18) Uani 1 1 d . . .
H19A H -0.1640 0.6442 0.9471 0.026 Uiso 1 1 calc R . .
C20 C -0.0739(8) 0.8209(8) 0.9483(4) 0.0235(19) Uani 1 1 d . . .
H20A H -0.0083 0.8315 0.9747 0.028 Uiso 1 1 calc R . .
C21 C -0.0772(8) 0.9167(7) 0.9254(4) 0.0248(19) Uani 1 1 d . . .
H21A H -0.0151 0.9925 0.9370 0.030 Uiso 1 1 calc R . .
C22 C -0.1715(7) 0.9004(7) 0.8858(4) 0.0222(18) Uani 1 1 d . . .
H22A H -0.1715 0.9655 0.8689 0.027 Uiso 1 1 calc R . .
C23 C -0.2665(7) 0.7908(8) 0.8701(4) 0.0205(18) Uani 1 1 d . . .
C24 C -0.3734(7) 0.7762(7) 0.8320(4) 0.0208(18) Uani 1 1 d . . .

H24A H -0.4429 0.7477 0.8579 0.025 Uiso 1 1 calc R . .
H24B H -0.3580 0.8521 0.8179 0.025 Uiso 1 1 calc R . .
C25 C -0.8660(8) 0.1054(7) 0.8076(4) 0.0254(19) Uani 1 1 d . . .
H25A H -0.8434 0.0460 0.8159 0.038 Uiso 1 1 calc R . .
H25B H -0.9049 0.0900 0.7661 0.038 Uiso 1 1 calc R . .
H25C H -0.9212 0.1043 0.8382 0.038 Uiso 1 1 calc R . .
C31 C -0.3511(7) 0.5934(7) 0.6405(4) 0.0183(17) Uani 1 1 d . . .
C32 C -0.4726(7) 0.5337(7) 0.6548(3) 0.0156(16) Uani 1 1 d . . .
C33 C -0.5564(7) 0.5305(7) 0.6097(4) 0.0179(17) Uani 1 1 d . . .
C34 C -0.5251(8) 0.5799(8) 0.5547(4) 0.0235(19) Uani 1 1 d . . .
H34A H -0.5848 0.5760 0.5260 0.028 Uiso 1 1 calc R . .
C35 C -0.4050(8) 0.6367(7) 0.5404(4) 0.0232(19) Uani 1 1 d . . .
H35A H -0.3837 0.6708 0.5020 0.028 Uiso 1 1 calc R . .
C36 C -0.3187(8) 0.6432(7) 0.5816(4) 0.0220(18) Uani 1 1 d . . .
H36A H -0.2376 0.6803 0.5715 0.026 Uiso 1 1 calc R . .
C37 C -0.2508(7) 0.6119(7) 0.6815(4) 0.0195(17) Uani 1 1 d . . .
H37A H -0.1740 0.6485 0.6654 0.023 Uiso 1 1 calc R . .
C38 C -0.1500(7) 0.6083(7) 0.7725(3) 0.0180(17) Uani 1 1 d . . .
C39 C -0.1457(7) 0.5174(7) 0.8020(4) 0.0198(18) Uani 1 1 d . . .
C40 C -0.0490(8) 0.5410(8) 0.8406(4) 0.028(2) Uani 1 1 d . . .
H40A H -0.0458 0.4798 0.8605 0.034 Uiso 1 1 calc R . .
C41 C 0.0450(9) 0.6531(10) 0.8511(4) 0.036(2) Uani 1 1 d . . .
H41A H 0.1107 0.6688 0.8789 0.044 Uiso 1 1 calc R . .
C42 C 0.0414(8) 0.7426(8) 0.8202(4) 0.029(2) Uani 1 1 d . . .
H42A H 0.1068 0.8187 0.8258 0.034 Uiso 1 1 calc R . .
C43 C -0.0556(7) 0.7218(8) 0.7818(4) 0.0226(18) Uani 1 1 d . . .
H43A H -0.0586 0.7831 0.7619 0.027 Uiso 1 1 calc R . .
C44 C -0.2454(8) 0.3962(8) 0.7874(4) 0.0248(19) Uani 1 1 d . . .
H44A H -0.2514 0.3772 0.7424 0.030 Uiso 1 1 calc R . .
H44B H -0.2266 0.3417 0.8087 0.030 Uiso 1 1 calc R . .
C45 C -0.7628(8) 0.4719(8) 0.5841(4) 0.0244(19) Uani 1 1 d . . .
H45A H -0.7416 0.5522 0.5774 0.037 Uiso 1 1 calc R . .
H45B H -0.8411 0.4333 0.6017 0.037 Uiso 1 1 calc R . .
H45C H -0.7658 0.4318 0.5446 0.037 Uiso 1 1 calc R . .
C51 C -1.0935(7) 0.2251(7) 0.8399(4) 0.0168(17) Uani 1 1 d . . .
C52 C -1.1233(8) 0.2378(8) 0.9009(4) 0.0225(18) Uani 1 1 d . . .
H52A H -1.2022 0.1900 0.9126 0.027 Uiso 1 1 calc R . .
C53 C -1.0390(8) 0.3190(8) 0.9439(4) 0.0235(19) Uani 1 1 d . . .
H53A H -1.0606 0.3276 0.9844 0.028 Uiso 1 1 calc R . .
C54 C -0.9242(7) 0.3869(8) 0.9275(4) 0.0210(18) Uani 1 1 d . . .
H54A H -0.8667 0.4424 0.9570 0.025 Uiso 1 1 calc R . .
C55 C -0.8912(7) 0.3757(7) 0.8691(4) 0.0176(17) Uani 1 1 d . . .
C56 C -0.9748(7) 0.2930(7) 0.8237(3) 0.0162(16) Uani 1 1 d . . .
C57 C -1.1897(7) 0.1449(7) 0.7975(4) 0.0177(17) Uani 1 1 d . . .
H57A H -1.2649 0.1018 0.8145 0.021 Uiso 1 1 calc R . .
C58 C -1.2926(7) 0.0402(7) 0.7059(3) 0.0166(16) Uani 1 1 d . . .
C59 C -1.2908(7) -0.0566(7) 0.6788(4) 0.0189(17) Uani 1 1 d . . .

C60 C -1.3935(8) -0.1388(7) 0.6444(4) 0.0220(18) Uani 1 1 d . . .
H60A H -1.3949 -0.2058 0.6259 0.026 Uiso 1 1 calc R . .
C61 C -1.4931(8) -0.1239(8) 0.6368(4) 0.026(2) Uani 1 1 d . . .
H61A H -1.5619 -0.1801 0.6131 0.031 Uiso 1 1 calc R . .
C62 C -1.4918(8) -0.0247(8) 0.6644(4) 0.027(2) Uani 1 1 d . . .
H62A H -1.5602 -0.0146 0.6598 0.033 Uiso 1 1 calc R . .
C63 C -1.3920(8) 0.0569(8) 0.6978(4) 0.026(2) Uani 1 1 d . . .
H63A H -1.3902 0.1246 0.7155 0.031 Uiso 1 1 calc R . .
C64 C -1.1856(7) -0.0759(7) 0.6888(4) 0.0208(18) Uani 1 1 d . . .
H64A H -1.1740 -0.0842 0.7333 0.025 Uiso 1 1 calc R . .
H64B H -1.2008 -0.1482 0.6657 0.025 Uiso 1 1 calc R . .
C65 C -0.6948(7) 0.5318(8) 0.8897(4) 0.0245(19) Uani 1 1 d . . .
H65A H -0.7258 0.5851 0.8994 0.037 Uiso 1 1 calc R . .
H65B H -0.6190 0.5730 0.8700 0.037 Uiso 1 1 calc R . .
H65C H -0.6821 0.5009 0.9278 0.037 Uiso 1 1 calc R . .
C71 C -0.9257(7) 0.1715(7) 0.5580(4) 0.0190(17) Uani 1 1 d . . .
C72 C -0.8928(8) 0.1262(8) 0.5078(4) 0.0260(19) Uani 1 1 d . . .
H72A H -0.9382 0.1068 0.4695 0.031 Uiso 1 1 calc R . .
C73 C -0.7952(8) 0.1094(7) 0.5132(4) 0.0239(19) Uani 1 1 d . . .
H73A H -0.7751 0.0766 0.4789 0.029 Uiso 1 1 calc R . .
C74 C -0.7246(7) 0.1399(7) 0.5690(4) 0.0210(18) Uani 1 1 d . . .
H74A H -0.6585 0.1261 0.5728 0.025 Uiso 1 1 calc R . .
C75 C -0.7525(7) 0.1900(7) 0.6178(4) 0.0183(17) Uani 1 1 d . . .
C76 C -0.8530(7) 0.2066(7) 0.6135(4) 0.0186(17) Uani 1 1 d . . .
C77 C -1.0328(7) 0.1842(7) 0.5505(4) 0.0207(18) Uani 1 1 d . . .
H77A H -1.0677 0.1728 0.5098 0.025 Uiso 1 1 calc R . .
C78 C -1.1873(7) 0.2207(8) 0.5774(4) 0.0212(18) Uani 1 1 d . . .
C79 C -1.1902(8) 0.3186(8) 0.6037(4) 0.0232(19) Uani 1 1 d . . .
C80 C -1.2902(8) 0.3313(8) 0.5874(4) 0.027(2) Uani 1 1 d . . .
H80A H -1.2945 0.3966 0.6042 0.032 Uiso 1 1 calc R . .
C81 C -1.3821(8) 0.2521(9) 0.5480(5) 0.033(2) Uani 1 1 d . . .
H81A H -1.4487 0.2627 0.5378 0.040 Uiso 1 1 calc R . .
C82 C -1.3766(8) 0.1563(9) 0.5233(4) 0.033(2) Uani 1 1 d . . .
H82A H -1.4394 0.1015 0.4958 0.040 Uiso 1 1 calc R . .
C83 C -1.2791(9) 0.1402(9) 0.5388(4) 0.033(2) Uani 1 1 d . . .
H83A H -1.2765 0.0737 0.5227 0.039 Uiso 1 1 calc R . .
C84 C -1.0866(8) 0.4138(8) 0.6418(4) 0.026(2) Uani 1 1 d . . .
H84A H -1.0164 0.4493 0.6164 0.031 Uiso 1 1 calc R . .
H84B H -1.1070 0.4744 0.6550 0.031 Uiso 1 1 calc R . .
C85 C -0.5936(9) 0.2066(10) 0.6862(5) 0.037(2) Uani 1 1 d . . .
H85A H -0.6250 0.1228 0.6819 0.055 Uiso 1 1 calc R . .
H85B H -0.5591 0.2354 0.7284 0.055 Uiso 1 1 calc R . .
H85C H -0.5320 0.2438 0.6568 0.055 Uiso 1 1 calc R . .
O1S O 0.0110(14) 0.3670(19) 0.4464(10) 0.082(6) Uiso 0.50 1 d PDU . .
C1S C -0.1030(15) 0.342(2) 0.4368(11) 0.049(5) Uiso 0.50 1 d PDU . .
O2S O 0.5954(17) 0.982(2) 0.1703(10) 0.092(6) Uiso 0.50 1 d PDU A 1
C2S C 0.6919(18) 1.033(2) 0.1372(10) 0.053(6) Uiso 0.50 1 d PDU A 1

O2A O 0.510(2) 1.009(2) 0.1533(11) 0.034(6) Uiso 0.25 1 d PDU B 2
C2A C 0.431(4) 1.016(5) 0.114(2) 0.058(11) Uiso 0.25 1 d PDU B 2

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N31 0.024(4) 0.019(4) 0.022(4) 0.001(3) 0.002(3) 0.016(3)
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N101 0.059(7) 0.022(5) 0.049(6) 0.007(4) 0.009(5) 0.013(5)
N111 0.028(4) 0.025(4) 0.030(4) 0.007(3) 0.005(3) 0.017(4)
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O12 0.021(3) 0.014(3) 0.021(3) 0.006(2) 0.001(2) 0.006(3)
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O32 0.017(3) 0.013(3) 0.019(3) 0.011(2) 0.001(2) 0.002(2)
O33 0.021(3) 0.017(3) 0.027(3) 0.008(2) 0.007(2) 0.013(3)
O51 0.017(3) 0.022(3) 0.013(3) 0.001(2) 0.001(2) 0.011(3)
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O53 0.019(3) 0.021(3) 0.032(3) 0.007(3) 0.008(2) 0.012(3)
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O91 0.021(3) 0.011(3) 0.032(3) 0.001(3) -0.005(3) 0.005(3)
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C21 0.022(4) 0.011(4) 0.032(5) 0.000(4) -0.005(4) 0.001(4)
C22 0.020(4) 0.013(4) 0.026(4) 0.000(4) -0.003(3) 0.002(4)
C23 0.025(4) 0.030(5) 0.018(4) 0.003(4) 0.002(3) 0.022(4)
C24 0.020(4) 0.018(4) 0.024(4) 0.003(4) 0.002(3) 0.009(4)
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C31 0.028(5) 0.012(4) 0.016(4) 0.002(3) 0.004(3) 0.010(4)
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C41 0.027(5) 0.054(7) 0.033(5) 0.012(5) 0.005(4) 0.023(5)
C42 0.014(4) 0.026(5) 0.037(5) 0.010(4) 0.011(4) 0.002(4)
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C45 0.033(5) 0.023(5) 0.023(4) 0.003(4) -0.004(4) 0.018(4)
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C59 0.023(4) 0.011(4) 0.018(4) 0.005(3) 0.000(3) 0.005(4)
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C61 0.023(4) 0.019(5) 0.023(4) 0.006(4) -0.003(4) 0.000(4)
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C73 0.026(5) 0.017(4) 0.027(4) 0.002(4) 0.011(4) 0.008(4)
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C77 0.025(4) 0.018(4) 0.019(4) 0.001(3) -0.003(3) 0.010(4)

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C79 0.028(5) 0.025(5) 0.019(4) 0.010(4) 0.002(4) 0.014(4)
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C83 0.037(5) 0.033(6) 0.028(5) -0.005(4) -0.016(4) 0.019(5)
C84 0.020(4) 0.025(5) 0.038(5) 0.011(4) 0.004(4) 0.013(4)
C85 0.034(5) 0.044(6) 0.045(6) -0.012(5) -0.010(5) 0.030(5)

_geom_special_details
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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.
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Zn2 O71 2.019(5) . ?
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O11 Zn1 O13 105.5(2) . . ?
N31 Zn1 O13 88.0(2) . . ?
O31 Zn1 O13 81.8(2) . . ?
N11 Zn1 O13 81.8(2) . . ?
O33 Zn1 O13 164.2(2) . . ?
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O71 Zn2 O51 76.2(2) . . ?
N51 Zn2 O51 89.6(2) . . ?
O71 Zn2 N71 86.1(2) . . ?
N51 Zn2 N71 114.1(3) . . ?
O51 Zn2 N71 152.3(3) . . ?
O71 Zn2 O73 107.3(2) . . ?

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O73 Zn2 O53 163.1(2) . . ?
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C17 N11 Zn1 121.9(5) . . ?
C18 N11 Zn1 119.1(5) . . ?
C37 N31 C38 119.6(7) . . ?
C37 N31 Zn1 125.6(6) . . ?
C38 N31 Zn1 114.3(5) . . ?
C57 N51 C58 118.6(7) . . ?
C57 N51 Zn2 125.7(6) . . ?
C58 N51 Zn2 115.7(5) . . ?
C77 N71 C78 118.1(7) . . ?
C77 N71 Zn2 123.2(5) . . ?
C78 N71 Zn2 118.0(5) . . ?
O91 N91 O92 120.3(8) . . ?
O91 N91 O93 121.0(8) . . ?
O92 N91 O93 118.7(8) . . ?
O91 N91 Pr1 60.2(4) . . ?
O92 N91 Pr1 60.1(4) . . ?
O93 N91 Pr1 178.8(7) . . ?
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O103 N101 O102 111.6(12) . . ?
O101 N101 O102 123.5(12) . . ?
O113 N111 O111 122.3(8) . . ?
O113 N111 O112 118.3(7) . . ?
O111 N111 O112 119.4(8) . . ?
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Zn1 O11 Pr1 111.7(2) . . ?
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C13 O12 Pr1 114.7(5) . . ?
C25 O12 Pr1 124.8(4) . . ?
C24 O13 Zn1 121.6(4) . . ?
C24 O13 H13 119.2 . . ?
Zn1 O13 H13 119.2 . . ?
C32 O31 Zn1 123.6(5) . . ?
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Zn1 O31 Pr1 105.6(2) . . ?
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C45 O32 Pr1 122.6(5) . . ?

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Zn1 O33 H33 121.1 . . ?
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C56 O51 Pr1 126.7(5) . . ?
Zn2 O51 Pr1 106.6(2) . . ?
C55 O52 C65 115.7(6) . . ?
C55 O52 Pr1 121.5(5) . . ?
C65 O52 Pr1 122.9(5) . . ?
C64 O53 Zn2 121.1(5) . . ?
C64 O53 H53 119.5 . . ?
Zn2 O53 H53 119.5 . . ?
C76 O71 Zn2 123.0(5) . . ?
C76 O71 Pr1 124.5(5) . . ?
Zn2 O71 Pr1 112.2(2) . . ?
C75 O72 C85 116.7(6) . . ?
C75 O72 Pr1 116.4(4) . . ?
C85 O72 Pr1 125.8(5) . . ?
C84 O73 Zn2 121.8(5) . . ?
C84 O73 H73 119.1 . . ?
Zn2 O73 H73 119.1 . . ?
N91 O91 Pr1 94.6(5) . . ?
N91 O92 Pr1 93.7(5) . . ?
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C12 C11 C17 123.2(7) . . ?
C16 C11 C17 117.8(7) . . ?
O11 C12 C11 124.2(7) . . ?
O11 C12 C13 117.0(7) . . ?
C11 C12 C13 118.7(7) . . ?
C12 C13 C14 122.4(7) . . ?
C12 C13 O12 114.3(7) . . ?
C14 C13 O12 123.3(7) . . ?
C13 C14 C15 118.3(8) . . ?
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C15 C16 C11 121.3(8) . . ?
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N11 C17 C11 125.8(7) . . ?
N11 C17 H17A 117.1 . . ?
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C23 C18 N11 117.2(7) . . ?

C18 C19 C20 119.1(8) . . ?
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C22 C21 C20 119.6(8) . . ?
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C21 C22 C23 121.6(8) . . ?
C21 C22 H22A 119.2 . . ?
C23 C22 H22A 119.2 . . ?
C22 C23 C18 117.6(7) . . ?
C22 C23 C24 120.5(8) . . ?
C18 C23 C24 121.7(8) . . ?
O13 C24 C23 111.8(7) . . ?
O13 C24 H24A 109.2 . . ?
C23 C24 H24A 109.2 . . ?
O13 C24 H24B 109.2 . . ?
C23 C24 H24B 109.2 . . ?
H24A C24 H24B 107.9 . . ?
O12 C25 H25A 109.5 . . ?
O12 C25 H25B 109.5 . . ?
H25A C25 H25B 109.5 . . ?
O12 C25 H25C 109.5 . . ?
H25A C25 H25C 109.5 . . ?
H25B C25 H25C 109.5 . . ?
C32 C31 C36 120.4(7) . . ?
C32 C31 C37 125.2(7) . . ?
C36 C31 C37 114.5(7) . . ?
O31 C32 C33 118.6(7) . . ?
O31 C32 C31 125.1(7) . . ?
C33 C32 C31 116.3(7) . . ?
C34 C33 O32 123.4(7) . . ?
C34 C33 C32 123.1(8) . . ?
O32 C33 C32 113.5(7) . . ?
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C35 C34 H34A 119.9 . . ?
C36 C35 C34 120.3(8) . . ?
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C35 C36 C31 119.8(8) . . ?
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N31 C37 C31 125.7(8) . . ?
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C43 C42 C41 121.0(9) . . ?
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C41 C42 H42A 119.5 . . ?
C42 C43 C38 118.8(8) . . ?
C42 C43 H43A 120.6 . . ?
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O33 C44 C39 112.4(7) . . ?
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C39 C44 H44A 109.1 . . ?
O33 C44 H44B 109.1 . . ?
C39 C44 H44B 109.1 . . ?
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O32 C45 H45B 109.5 . . ?
H45A C45 H45B 109.5 . . ?
O32 C45 H45C 109.5 . . ?
H45A C45 H45C 109.5 . . ?
H45B C45 H45C 109.5 . . ?
C56 C51 C52 119.1(7) . . ?
C56 C51 C57 124.2(7) . . ?
C52 C51 C57 116.7(7) . . ?
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C53 C52 H52A 119.5 . . ?
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C54 C53 C52 119.7(8) . . ?
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O52 C55 C56 113.3(7) . . ?
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O51 C56 C55 117.8(7) . . ?
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C62 C63 C58 119.8(8) . . ?
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O52 C65 H65A 109.5 . . ?
O52 C65 H65B 109.5 . . ?
H65A C65 H65B 109.5 . . ?
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H65A C65 H65C 109.5 . . ?
H65B C65 H65C 109.5 . . ?
C72 C71 C76 119.0(7) . . ?
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C76 C71 C77 122.4(7) . . ?
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O71 C76 C75 117.3(7) . . ?
O71 C76 C71 123.4(7) . . ?
C75 C76 C71 119.3(7) . . ?
N71 C77 C71 126.1(7) . . ?
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C81 C82 C83 120.2(9) . . ?
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O73 C84 H84B 109.6 . . ?
C79 C84 H84B 109.6 . . ?
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O72 C85 H85B 109.5 . . ?
H85A C85 H85B 109.5 . . ?
O72 C85 H85C 109.5 . . ?
H85A C85 H85C 109.5 . . ?
H85B C85 H85C 109.5 . . ?

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N31 Zn1 N11 C17 -133.8(6) . . . . ?
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O33 Zn1 N11 C17 -51.6(6) . . . . ?
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N31 Zn1 N11 C18 32.8(6) . . . . ?
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O33 Zn1 N11 C18 115.1(5) . . . . ?
O13 Zn1 N11 C18 -51.8(5) . . . . ?
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N11 Zn1 N31 C37 -144.0(7) . . . . ?
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O13 Zn1 N31 C37 -63.6(7) . . . . ?
O11 Zn1 N31 C38 -119.8(7) . . . . ?
O31 Zn1 N31 C38 -170.3(6) . . . . ?
N11 Zn1 N31 C38 27.5(6) . . . . ?
O33 Zn1 N31 C38 -59.1(6) . . . . ?
O13 Zn1 N31 C38 107.9(6) . . . . ?
O71 Zn2 N51 C57 66.5(9) . . . . ?
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N71 Zn2 N51 C57 -154.0(6) . . . . ?
O73 Zn2 N51 C57 -70.8(7) . . . . ?
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O51 Zn2 N51 C58 -171.7(5) . . . . ?
N71 Zn2 N51 C58 23.2(6) . . . . ?
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O53 Zn2 N51 C58 -59.2(5) . . . . ?
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O71 Pr1 N91 O92 -153.4(4) . . . . ?
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O71 Pr1 O11 C12 -63.0(7) . . . . ?
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O92 Pr1 O12 C13 -21.5(6) . . . . ?
O91 Pr1 O12 C13 -98.7(5) . . . . ?
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O51 Pr1 O32 C33 178.1(5) . . . . ?
O31 Pr1 O32 C33 -5.2(5) . . . . ?
O92 Pr1 O32 C33 72.2(5) . . . . ?
O91 Pr1 O32 C33 126.5(5) . . . . ?
O52 Pr1 O32 C33 99.0(5) . . . . ?
O72 Pr1 O32 C33 -81.1(5) . . . . ?
O12 Pr1 O32 C33 -84.7(6) . . . . ?
N91 Pr1 O32 C33 99.7(6) . . . . ?
O11 Pr1 O32 C45 -169.2(5) . . . . ?
O71 Pr1 O32 C45 46.9(5) . . . . ?
O51 Pr1 O32 C45 9.0(6) . . . . ?
O31 Pr1 O32 C45 -174.2(6) . . . . ?
O92 Pr1 O32 C45 -96.9(6) . . . . ?
O91 Pr1 O32 C45 -42.6(5) . . . . ?
O52 Pr1 O32 C45 -70.0(6) . . . . ?
O72 Pr1 O32 C45 109.8(6) . . . . ?
O12 Pr1 O32 C45 106.2(6) . . . . ?
N91 Pr1 O32 C45 -69.4(6) . . . . ?
O11 Zn1 O33 C44 171.6(6) . . . . ?
N31 Zn1 O33 C44 9.4(6) . . . . ?
O31 Zn1 O33 C44 96.6(6) . . . . ?
N11 Zn1 O33 C44 -102.1(6) . . . . ?
O13 Zn1 O33 C44 -46.5(10) . . . . ?
O71 Zn2 O51 C56 -177.2(6) . . . . ?
N51 Zn2 O51 C56 -18.7(6) . . . . ?
N71 Zn2 O51 C56 131.1(6) . . . . ?
O73 Zn2 O51 C56 72.7(6) . . . . ?
O53 Zn2 O51 C56 -97.5(6) . . . . ?
O71 Zn2 O51 Pr1 13.8(2) . . . . ?

N51 Zn2 O51 Pr1 172.4(3) . . . . ?
N71 Zn2 O51 Pr1 -37.9(6) . . . . ?
O73 Zn2 O51 Pr1 -96.3(2) . . . . ?
O53 Zn2 O51 Pr1 93.6(2) . . . . ?
O11 Pr1 O51 C56 37.8(6) . . . . ?
O71 Pr1 O51 C56 178.5(6) . . . . ?
O31 Pr1 O51 C56 121(3) . . . . ?
O92 Pr1 O51 C56 -58.2(6) . . . . ?
O91 Pr1 O51 C56 -88.9(6) . . . . ?
O52 Pr1 O51 C56 -6.1(5) . . . . ?
O72 Pr1 O51 C56 136.9(6) . . . . ?
O32 Pr1 O51 C56 -140.6(5) . . . . ?
O12 Pr1 O51 C56 74.5(6) . . . . ?
N91 Pr1 O51 C56 -73.8(6) . . . . ?
O11 Pr1 O51 Zn2 -153.5(2) . . . . ?
O71 Pr1 O51 Zn2 -12.8(2) . . . . ?
O31 Pr1 O51 Zn2 -70(3) . . . . ?
O92 Pr1 O51 Zn2 110.5(2) . . . . ?
O91 Pr1 O51 Zn2 79.9(2) . . . . ?
O52 Pr1 O51 Zn2 162.7(3) . . . . ?
O72 Pr1 O51 Zn2 -54.4(3) . . . . ?
O32 Pr1 O51 Zn2 28.2(3) . . . . ?
O12 Pr1 O51 Zn2 -116.7(3) . . . . ?
N91 Pr1 O51 Zn2 95.0(3) . . . . ?
O11 Pr1 O52 C55 -132.6(5) . . . . ?
O71 Pr1 O52 C55 11.4(6) . . . . ?
O51 Pr1 O52 C55 6.7(5) . . . . ?
O31 Pr1 O52 C55 -170.7(5) . . . . ?
O92 Pr1 O52 C55 136.5(5) . . . . ?
O91 Pr1 O52 C55 82.7(5) . . . . ?
O72 Pr1 O52 C55 -70.2(6) . . . . ?
O32 Pr1 O52 C55 109.6(5) . . . . ?
O12 Pr1 O52 C55 -68.3(5) . . . . ?
N91 Pr1 O52 C55 108.9(5) . . . . ?
O11 Pr1 O52 C65 47.3(6) . . . . ?
O71 Pr1 O52 C65 -168.7(5) . . . . ?
O51 Pr1 O52 C65 -173.5(6) . . . . ?
O31 Pr1 O52 C65 9.2(6) . . . . ?
O92 Pr1 O52 C65 -43.6(6) . . . . ?
O91 Pr1 O52 C65 -97.4(6) . . . . ?
O72 Pr1 O52 C65 109.6(6) . . . . ?
O32 Pr1 O52 C65 -70.5(6) . . . . ?
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N91 Pr1 O52 C65 -71.2(6) . . . . ?
O71 Zn2 O53 C64 166.7(6) . . . . ?
N51 Zn2 O53 C64 8.0(6) . . . . ?
O51 Zn2 O53 C64 93.3(6) . . . . ?

N71 Zn2 O53 C64 -107.1(6) . . . . ?
O73 Zn2 O53 C64 -51.0(10) . . . . ?
N51 Zn2 O71 C76 100.9(7) . . . . ?
O51 Zn2 O71 C76 158.8(6) . . . . ?
N71 Zn2 O71 C76 -42.7(6) . . . . ?
O73 Zn2 O71 C76 -124.3(6) . . . . ?
O53 Zn2 O71 C76 45.0(6) . . . . ?
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O53 Zn2 O71 Pr1 -128.7(2) . . . . ?
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O51 Pr1 O71 C76 -160.0(6) . . . . ?
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O92 Pr1 O71 C76 103.1(6) . . . . ?
O91 Pr1 O71 C76 128.5(6) . . . . ?
O52 Pr1 O71 C76 -164.7(5) . . . . ?
O72 Pr1 O71 C76 -27.3(5) . . . . ?
O32 Pr1 O71 C76 56.8(6) . . . . ?
O12 Pr1 O71 C76 -95.6(6) . . . . ?
N91 Pr1 O71 C76 117.8(6) . . . . ?
O11 Pr1 O71 Zn2 111.6(3) . . . . ?
O51 Pr1 O71 Zn2 13.6(2) . . . . ?
O31 Pr1 O71 Zn2 -169.1(2) . . . . ?
O92 Pr1 O71 Zn2 -83.3(3) . . . . ?
O91 Pr1 O71 Zn2 -57.9(2) . . . . ?
O52 Pr1 O71 Zn2 8.9(3) . . . . ?
O72 Pr1 O71 Zn2 146.3(3) . . . . ?
O32 Pr1 O71 Zn2 -129.6(3) . . . . ?
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N91 Pr1 O71 Zn2 -68.6(3) . . . . ?
O11 Pr1 O72 C75 -175.4(5) . . . . ?
O71 Pr1 O72 C75 23.5(5) . . . . ?
O51 Pr1 O72 C75 66.0(5) . . . . ?
O31 Pr1 O72 C75 -114.8(5) . . . . ?
O92 Pr1 O72 C75 -92.6(5) . . . . ?
O91 Pr1 O72 C75 -12.7(6) . . . . ?
O52 Pr1 O72 C75 127.8(5) . . . . ?
O32 Pr1 O72 C75 -52.1(5) . . . . ?
O12 Pr1 O72 C75 125.9(5) . . . . ?
N91 Pr1 O72 C75 -50.8(7) . . . . ?
O11 Pr1 O72 C85 -8.2(7) . . . . ?
O71 Pr1 O72 C85 -169.3(8) . . . . ?
O51 Pr1 O72 C85 -126.8(7) . . . . ?
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O92 Pr1 O72 C85 74.6(8) . . . . ?

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O91 N91 O92 Pr1 -0.8(8) . . . . ?
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O91 Pr1 O92 N91 0.4(4) . . . . ?
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O72 Pr1 O92 N91 120.3(5) . . . . ?
O32 Pr1 O92 N91 79.1(5) . . . . ?
O12 Pr1 O92 N91 -118.7(5) . . . . ?
Zn1 O11 C12 C11 31.8(10) . . . . ?
Pr1 O11 C12 C11 -155.1(6) . . . . ?
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O11 C12 C13 C14 -179.8(7) . . . . ?
C11 C12 C13 C14 -1.6(12) . . . . ?
O11 C12 C13 O12 1.0(10) . . . . ?
C11 C12 C13 O12 179.2(6) . . . . ?
C25 O12 C13 C12 177.6(7) . . . . ?
Pr1 O12 C13 C12 -19.4(8) . . . . ?
C25 O12 C13 C14 -1.6(11) . . . . ?

Pr1 O12 C13 C14 161.4(6) . . . . ?
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O12 C13 C14 C15 -179.8(7) . . . . ?
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Zn1 N11 C17 C11 -16.8(11) . . . . ?
C12 C11 C17 N11 -10.7(12) . . . . ?
C16 C11 C17 N11 172.5(7) . . . . ?
C17 N11 C18 C19 46.8(10) . . . . ?
Zn1 N11 C18 C19 -120.4(7) . . . . ?
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C19 C18 C23 C24 -176.9(7) . . . . ?
N11 C18 C23 C24 3.3(11) . . . . ?
Zn1 O13 C24 C23 46.5(8) . . . . ?
C22 C23 C24 O13 127.5(8) . . . . ?
C18 C23 C24 O13 -57.2(10) . . . . ?
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Pr1 O31 C32 C33 -4.6(10) . . . . ?
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Pr1 O31 C32 C31 175.1(6) . . . . ?
C36 C31 C32 O31 178.0(7) . . . . ?
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C36 C31 C32 C33 -2.2(11) . . . . ?
C37 C31 C32 C33 176.7(8) . . . . ?
C45 O32 C33 C34 -6.2(11) . . . . ?
Pr1 O32 C33 C34 -176.0(6) . . . . ?
C45 O32 C33 C32 175.0(7) . . . . ?
Pr1 O32 C33 C32 5.2(9) . . . . ?
O31 C32 C33 C34 -179.5(7) . . . . ?
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O31 C32 C33 O32 -0.7(10) . . . . ?
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C32 C33 C34 C35 0.6(13) . . . . ?

C33 C34 C35 C36 -0.3(13) . . . . ?
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C37 C31 C36 C35 -176.5(8) . . . . ?
C38 N31 C37 C31 -179.3(8) . . . . ?
Zn1 N31 C37 C31 -8.2(12) . . . . ?
C32 C31 C37 N31 -4.4(14) . . . . ?
C36 C31 C37 N31 174.7(8) . . . . ?
C37 N31 C38 C43 57.5(11) . . . . ?
Zn1 N31 C38 C43 -114.5(7) . . . . ?
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Zn1 N31 C38 C39 60.3(8) . . . . ?
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C43 C38 C39 C44 -176.2(7) . . . . ?
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Zn1 O33 C44 C39 42.6(8) . . . . ?
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C56 C51 C52 C53 2.7(12) . . . . ?
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C57 C51 C56 O51 -5.8(12) . . . . ?
C52 C51 C56 C55 -2.9(11) . . . . ?
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C54 C55 C56 O51 -177.8(7) . . . . ?
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C54 C55 C56 C51 1.8(11) . . . . ?
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C56 C51 C57 N51 -2.7(13) . . . . ?
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C60 C61 C62 C63 0.8(14) . . . . ?
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C76 C71 C72 C73 3.9(13) . . . . ?
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C71 C72 C73 C74 -1.5(13) . . . . ?
C72 C73 C74 C75 -1.7(13) . . . . ?
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C73 C74 C75 C76 2.6(12) . . . . ?
C85 O72 C75 C74 -10.2(12) . . . . ?
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C85 O72 C75 C76 172.0(8) . . . . ?
Pr1 O72 C75 C76 -19.6(8) . . . . ?
Zn2 O71 C76 C75 -144.1(6) . . . . ?
Pr1 O71 C76 C75 28.9(9) . . . . ?
Zn2 O71 C76 C71 35.4(10) . . . . ?
Pr1 O71 C76 C71 -151.7(6) . . . . ?
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O72 C75 C76 C71 177.7(7) . . . . ?
C72 C71 C76 O71 177.5(8) . . . . ?
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C72 C71 C76 C75 -3.0(12) . . . . ?
C77 C71 C76 C75 178.9(8) . . . . ?
C78 N71 C77 C71 178.6(8) . . . . ?
Zn2 N71 C77 C71 -11.2(12) . . . . ?

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C77 N71 C78 C83 47.6(12) . . . . ?
Zn2 N71 C78 C83 -123.1(8) . . . . ?
C77 N71 C78 C79 -133.1(8) . . . . ?
Zn2 N71 C78 C79 56.1(9) . . . . ?
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N71 C78 C79 C80 179.4(7) . . . . ?
C83 C78 C79 C84 -174.6(8) . . . . ?
N71 C78 C79 C84 6.2(12) . . . . ?
C78 C79 C80 C81 0.4(13) . . . . ?
C84 C79 C80 C81 173.8(8) . . . . ?
C79 C80 C81 C82 0.0(14) . . . . ?
C80 C81 C82 C83 0.6(15) . . . . ?
C79 C78 C83 C82 2.0(14) . . . . ?
N71 C78 C83 C82 -178.9(8) . . . . ?
C81 C82 C83 C78 -1.6(15) . . . . ?
Zn2 O73 C84 C79 47.1(8) . . . . ?
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C78 C79 C84 O73 -60.2(11) . . . . ?

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