checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Dy2N4@C81N

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: Dy2N4@C81N

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Bond precision:  C-C = 0.0123 A          Wavelength=0.71073

Cell:           a=25.3003(3)    b=15.2149(2)         c=19.8299(4)
                alpha=90        beta=95.6439(15)     gamma=90
Temperature:    173 K
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	Calculated	Reported
Volume	7596.4(2)	7596.4(2)
Space group	C 2/m	C 2/m
Hall group	-C 2y	-C 2y
Moiety formula	C82, C36 H44 N4 Ni, Dy2 N4, 2(C3 H3) [+ solvent]	C82 N4 Dy2, C36 H44 N4 Ni,C6 H6
Sum formula	C124 H50 Dy2 N8 Ni [+ solvent]	C124 H50 Dy2 N8 Ni
Mr	2035.35	2035.35
Dx,g cm-3	1.780	1.780
Z	4	4
Mu (mm-1)	2.263	2.262
F000	4039.9	4040.0
F000’	4040.89	
h,k,lmax	32,19,25	32,19,25
Nref	9048	9045
Tmin,Tmax	0.729,0.798	0.624,0.745
Tmin’	0.689	

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Correction method= # Reported T Limits: Tmin=0.624 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 1.000          Theta(max)= 27.484

R(reflections)= 0.1232( 7633)     wR2(reflections)= 0.2841( 9045)

S = 1.093                 Npar= 838
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The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT082_ALERT_2_C High R1 Value ..... 0.12 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.28 Report
PLAT215_ALERT_3_C Disordered C102 has ADP max/min Ratio ..... 3.3 Note
PLAT215_ALERT_3_C Disordered C104 has ADP max/min Ratio ..... 3.6 Note
PLAT215_ALERT_3_C Disordered C109 has ADP max/min Ratio ..... 3.1 Note
PLAT215_ALERT_3_C Disordered C112 has ADP max/min Ratio ..... 3.7 Note
PLAT215_ALERT_3_C Disordered C131 has ADP max/min Ratio ..... 3.2 Note
PLAT215_ALERT_3_C Disordered C147 has ADP max/min Ratio ..... 3.1 Note
PLAT215_ALERT_3_C Disordered C149 has ADP max/min Ratio ..... 3.8 Note
PLAT215_ALERT_3_C Disordered C157 has ADP max/min Ratio ..... 3.3 Note
PLAT215_ALERT_3_C Disordered C179 has ADP max/min Ratio ..... 3.4 Note
PLAT234_ALERT_4_C Large Hirshfeld Difference Dy7 --N202 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Dy10 --N201 . 0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Dy11 --N202 . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Dy11 --N201_b . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Dy12 --N201 . 0.18 Ang.
PLAT243_ALERT_4_C High Solvent Ueq as Compared to Neighbors of C304 Check
PLAT244_ALERT_4_C Low Solvent Ueq as Compared to Neighbors of N201 Check
PLAT244_ALERT_4_C Low Solvent Ueq as Compared to Neighbors of C305 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including C101 0.101 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01228 Ang.
PLAT368_ALERT_2_C Short C(sp2)-C(sp2) Bond C301 - C302 . 1.20 Ang.
PLAT374_ALERT_2_C Long N - N Bond N201 - N202 . 1.59 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 4.459 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 28 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H306 -0.41 eA-3

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 120 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 180.57 Why ?
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 4 Report
PLAT231_ALERT_4_G Hirshfeld Test (Solvent) N201 --N202 . 6.7 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent) Dy1 --N201 . 9.0 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent) Dy1 --N202 . 9.5 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent) Dy1 --N201_b . 12.0 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent) Dy2 --N201 . 6.3 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent) Dy2 --N202 . 5.7 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent) Dy2 --N201_b . 6.0 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent) Dy2 --N202_b . 11.0 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent) Dy4 --N201_b . 7.2 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent) Dy6 --N202 . 6.0 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent) Dy7 --N201 . 12.8 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent) Dy7 --N201_b . 10.2 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent) Dy8 --N201 . 8.3 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent) Dy8 --N201_b . 9.3 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent) Dy11 --N201 . 8.3 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of C101 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C102 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C103 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C104 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C105 Constrained at 0.5 Check

PLAT300_ALERT_4_G Atom Site Occupancy of C106 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C107 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C108 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C109 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C110 Constrained at 0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of C118 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C119 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C120 Constrained at 0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of C122 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C123 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C124 Constrained at 0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of C131 Constrained at 0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of C133 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C134 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C135 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C136 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C137 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C138 Constrained at 0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of C140 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C141 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C142 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C143 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C144 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C145 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C146 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C147 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C148 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C149 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C150 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C151 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C152 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C153 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C154 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C155 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C156 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C157 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C158 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C159 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C160 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C161 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C162 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C163 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C164 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C165 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C166 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C167 Constrained at 0.5 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of C168       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C169       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C170       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C171       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C172       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C173       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C174       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C175       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C176       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C177       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C178       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C179       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C180       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C181       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C182       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Dy1        Constrained at     0.2647 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Dy2        Constrained at     0.1848 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Dy3        Constrained at     0.1572 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Dy4        Constrained at     0.0838 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Dy5        Constrained at     0.0792 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Dy6        Constrained at     0.0739 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Dy7        Constrained at     0.0737 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Dy8        Constrained at      0.064 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Dy9        Constrained at     0.0568 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Dy10       Constrained at     0.0483 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Dy11       Constrained at     0.0432 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Dy12       Constrained at     0.0251 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )        37% Note
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C101     -C149     .       1.43 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C102     -C104     .       1.43 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C105     -C120     .       1.45 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C108     -C112     .       1.43 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C109     -C111     .       1.44 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C113     -C130     .       1.43 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C122     -C126     .       1.43 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C123     -C125     .       1.43 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C118     -C182           0.21 Ang.
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        327 A**3
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.10 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        815 Check
              DY8  -N201 -DY3     1.555   1.555   1.555             39.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        823 Check
              DY1  -N201 -DY4     1.555   1.555   1.555             15.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        831 Check
              DY1  -N201 -DY6     1.555   1.555   1.555             27.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        833 Check
              N202 -N201 -DY6     1.555   1.555   1.555             40.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        837 Check
              DY4  -N201 -DY6     1.555   1.555   1.555             18.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        841 Check
              N201 -N201 -DY8     6.555   1.555   6.555             31.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        845 Check
              DY3  -N201 -DY8     1.555   1.555   6.555             32.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        854 Check
              DY11 -N201 -DY10    1.555   1.555   1.555             34.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        855 Check
              DY3  -N201 -DY10    1.555   1.555   1.555             34.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        867 Check
              N201 -N202 -DY7     1.555   1.555   1.555             40.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        874 Check
              DY9  -N202 -DY2     1.555   1.555   1.555             16.80 Deg.
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PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        877 Check
             DY11 -N202 -DY2     1.555   1.555   1.555             40.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        881 Check
             DY6  -N202 -DY4     1.555   1.555   1.555             21.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        888 Check
             DY6  -N202 -DY5     1.555   1.555   1.555             43.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        896 Check
             DY6  -N202 -DY1     1.555   1.555   1.555             37.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        902 Check
             DY4  -N202 -DY1     1.555   1.555   1.555             19.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        909 Check
             N202 -N202 -DY9     6.555   1.555   6.555             39.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        910 Check
             DY2  -N202 -DY9     1.555   1.555   6.555             41.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        914 Check
             DY9  -N202 -DY2     1.555   1.555   6.555             39.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        920 Check
             DY2  -N202 -DY2     1.555   1.555   6.555             28.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        924 Check
             DY9  -N202 -DY2     6.555   1.555   6.555             15.40 Deg.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         82 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       1014 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed            ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          5 Info
PLAT982_ALERT_1_G The Dy-f'=   -0.1318 Deviates from  IT-value =      -0.1892 Check
PLAT982_ALERT_1_G The Ni-f'=    0.3437 Deviates from  IT-value =       0.3393 Check
PLAT983_ALERT_1_G The Dy-f"=    4.4580 Deviates from  IT-Value =       4.4098 Check
PLAT983_ALERT_1_G The Ni-f"=    1.1214 Deviates from  IT-Value =       1.1124 Check
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  27 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 159 ALERT level G = General information/check it is not something unexpected

   7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  17 ALERT type 2 Indicator that the structure model may be wrong or deficient
  17 ALERT type 3 Indicator that the structure quality may be low
 144 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 22/12/2019; check.def file version of 13/12/2019

Datablock Dy2N4@C81N - ellipsoid plot