checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 1

```
Bond precision:  C-C = 0.0104 A          Wavelength=0.71073

Cell:             a=14.538(4)     b=19.804(4)        c=13.695(3)
                  alpha=90        beta=97.69(3)      gamma=90
Temperature:      293 K

                 Calculated                Reported
Volume           3907.5(16)                3907.4(16)
Space group      I 2/a                     I 2/a
Hall group       -I 2ya                    ?
Moiety formula   C19 H18 Cl2 N2 Ni S2      C19 H18 Cl2 N2 Ni S2
Sum formula      C19 H18 Cl2 N2 Ni S2      C19 H18 Cl2 N2 Ni S2
Mr               468.06                    468.08
Dx,g cm-3        1.591                     1.591
Z                8                         8
Mu (mm-1)        1.486                     1.486
F000             1920.0                    1920.0
F000'            1927.42
h,k,lmax         17,23,16                  17,22,16
Nref             3321                      3084
Tmin,Tmax        0.647,0.690               0.561,0.625
Tmin'            0.634

Correction method= # Reported T Limits: Tmin=0.561 Tmax=0.625
AbsCorr = REFDELF

Data completeness= 0.929          Theta(max)= 24.710

R(reflections)= 0.0401( 1136)     wR2(reflections)= 0.0905( 3084)

S = 0.972                 Npar= 235
```

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 A

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low ..... 0.926 Note

Author Response: the crystal was low diffracting

Alert level B

PLAT026_ALERT_3_B Ratio Observed / Unique Reflections too Low .... 37 %

Author Response: the crystal was low diffracting

Alert level C

```
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
           Calculated sin(theta_max)/wavelength =    0.5882
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C13    --  C14     ..        6.5 su
PLAT234_ALERT_4_C Large Hirshfeld Difference C10    --  C19     ..       0.16 Ang.
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.0104 Ang.
```

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT128_ALERT_4_G Alternate Setting for Input Space Group  I2/a       I2/c    Note
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C19 Check
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #          4 Do !
           CL1 -NI  -S1  -C7     -6.80  0.80   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #          9 Do !
           CL1 -NI  -S1  -C6   -110.90  0.70   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         13 Do !
           CL2 -NI  -S2  -C12    -8.30  0.70   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         18 Do !
           CL2 -NI  -S2  -C13  -114.40  0.70   1.555   1.555   1.555   1.555
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
```

```
   1 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   4 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  10 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   1 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
   8 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Datablock: 2

Bond precision: C-C = 0.0080 A Wavelength=0.71073

Cell: a=14.640(3) b=20.671(4) c=14.070(3)
       alpha=90 beta=95.43(3) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	4238.8(15)	4238.8(15)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	?
Moiety formula	C19 H18 N8 Ni S2	?
Sum formula	C19 H18 N8 Ni S2	C19 H18 N8 Ni S2
Mr	481.22	481.24
Dx,g cm-3	1.508	1.508
Z	8	8
Mu (mm-1)	1.136	1.136
F000	1984.0	1984.0
F000’	1989.05	
h,k,lmax	17,24,16	17,24,16
Nref	6969	6918
Tmin,Tmax	0.656,0.815	0.592,0.692
Tmin’	0.643	

Correction method= # Reported T Limits: Tmin=0.592 Tmax=0.692
AbsCorr = REFDELF

Data completeness= 0.993 Theta(max)= 24.400

R(reflections)= 0.0395(3199) wR2(reflections)= 0.0961(6918)

S = 0.974 Npar= 544

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 B

PLAT242_ALERT_2_B Low Ueq as Compared to Neighbors for ..... N15 Check

Author Response: this is due to libration of the azide ligands

PLAT242_ALERT_2_B Low Ueq as Compared to Neighbors for ..... N17 Check

Author Response: this is due to libration of the azide ligands

Alert level C

```
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
           Calculated sin(theta_max)/wavelength =    0.5812
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections too Low ....         46 %
PLAT165_ALERT_3_C Nr. of Status R Flagged Non-Hydrogen Atoms .....          1
PLAT220_ALERT_2_C Large Non-Solvent  N     Ueq(max)/Ueq(min) Range        3.2 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N14    --  N15     ..        5.8 su
PLAT234_ALERT_4_C Large Hirshfeld Difference N17    --  N18     ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C29    --  C30     ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C10    --  C19     ..       0.17 Ang.
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        N13 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        N14 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C23 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....         N4 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....         C2 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....         C9 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        Ni2 Check
```

Author Response: this is due to libration of the azide ligands

```
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....         N5 Check
```

Author Response: this is due to libration of the azide ligands

```
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....         N7 Check
```

Author Response: this is due to libration of the azide ligands

```
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C10 Check
```

Author Response: this is due to libration of the azide ligands

```
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0080 Ang.
```

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as .      mixed Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT301_ALERT_3_G Main Residue  Disorder ............ Percentage =          2 Note
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #          1 Do !
            N4  -NI1 -S1  -C7     59.10  1.30   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #          6 Do !
            N4  -NI1 -S1  -C6    -46.50  1.30   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         12 Do !
            N3  -NI1 -S2  -C12     7.30  1.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         17 Do !
            N3  -NI1 -S2  -C13   -98.70  1.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         44 Do !
            S2  -NI1 -N3  -N7    144.60  0.80   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         50 Do !
            S1  -NI1 -N4  -N5   -148.20  1.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         51 Do !
```

```
            NI1 -N4  -N5  -N6   -163.00 12.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         52 Do !
            NI1 -N3  -N7  -N8   -139.00  7.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        104 Do !
            N13 -NI2 -S4  -C32    41.90  1.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        109 Do !
            N13 -NI2 -S4  -C33   -63.00  1.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        115 Do !
            N14 -NI2 -S3  -C27    76.00  2.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        120 Do !
            N14 -NI2 -S3  -C26   -29.00  2.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        148 Do !
            S4  -NI2 -N13 -N17  -137.90  0.80   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        152 Do !
            S3  -NI2 -N14 -N15   -99.00  2.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        154 Do !
            NI2 -N14 -N15 -N16  -167.00 16.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        155 Do !
            NI2 -N13 -N17 -N18   117.00  6.00   1.555   1.555   1.555   1.555
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        161 Check
              C39  -C29  -H29     1.555   1.555   1.555              6.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        168 Check
              C29  -C39  -H29     1.555   1.555   1.555             11.50 Deg.
```

---

  0 **ALERT level A** = Most likely a serious problem - resolve or explain
  2 **ALERT level B** = A potentially serious problem, consider carefully
 19 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 23 **ALERT level G** = General information/check it is not something unexpected

  3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 14 ALERT type 2 Indicator that the structure model may be wrong or deficient
  5 ALERT type 3 Indicator that the structure quality may be low
 21 ALERT type 4 Improvement, methodology, query or suggestion
  1 ALERT type 5 Informative message, check

Datablock: 3

Bond precision: C-C = 0.0119 A Wavelength=0.71073

Cell:	a=14.473(4)	b=20.889(5)	c=14.151(3)
	alpha=90	beta=95.18(3)	gamma=90
Temperature:	293 K		

	Calculated	Reported
Volume	4260.8(18)	4260.7(18)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	?
Moiety formula	C21 H18 N4 Ni O2 S2	?
Sum formula	C21 H18 N4 Ni O2 S2	C21 H18 N4 Ni O2 S2
Mr	481.20	481.22
Dx,g cm-3	1.500	1.500
Z	8	8
Mu (mm-1)	1.132	1.132
F000	1984.0	1984.0
F000'	1989.23	
h,k,lmax	16,24,16	16,23,16
Nref	6768	5983
Tmin,Tmax	0.687,0.893	0.661,0.824
Tmin'	0.674	

Correction method= # Reported T Limits: Tmin=0.661 Tmax=0.824
AbsCorr = REFDELF

Data completeness= 0.884 Theta(max)= 24.100

R(reflections)= 0.0397(1953) wR2(reflections)= 0.0817(5983)

S = 0.851 Npar= 546

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 A

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low ..... 0.884 Note

---

Alert level B

THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575
Calculated sin(theta_max)/wavelength = 0.5745

Author Response: this is due to low diffracting crystal

PLAT026_ALERT_3_B Ratio Observed / Unique Reflections too Low .... 33 %

Author Response: this is due to low diffracting crystal

PLAT242_ALERT_2_B Low Ueq as Compared to Neighbors for ..... C41 Check

Author Response: this is due to libration of the isothiocyanate ligands

```
PLAT242_ALERT_2_B Low       Ueq as Compared to Neighbors for .....        C42 Check
```

Author Response: this is due to libration of the isothiocyanate ligands

---

Alert level C

```
PLAT165_ALERT_3_C Nr. of Status R Flagged Non-Hydrogen Atoms .....          2
PLAT234_ALERT_4_C Large Hirshfeld Difference N12    --  C34     ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N13    --  C53     ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C37    --  C38     ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C8     --  C9      ..       0.18 Ang.
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C37 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....         N3 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C10 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C16 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C17 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C53 Check
```

Author Response: this is due to libration of the isothiocyanate ligands

```
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C54 Check
```

Author Response: this is due to libration of the isothiocyanate ligands

```
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....         C9 Check
```

Author Response: this is due to libration of the isothiocyanate ligands

```
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0119 Ang.
```

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as .      mixed Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT301_ALERT_3_G Main Residue  Disorder ............ Percentage =          2 Note
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #          2 Do !
            N4  -NI1 -S1  -C7     14.00  2.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #          7 Do !
            N4  -NI1 -S1  -C6    -91.00  2.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         11 Do !
            N3  -NI1 -S2  -C12    17.00  2.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         16 Do !
            N3  -NI1 -S2  -C13   -89.00  2.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         44 Do !
            S1  -NI1 -N4  -C42   151.80  1.60   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         50 Do !
            S2  -NI1 -N3  -C41  -117.00  2.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         51 Do !
            NI1 -N3  -C41 -O1    -67.00 15.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         52 Do !
            NI1 -N4  -C42 -O2    154.00  8.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        104 Do !
            N13 -NI2 -S4  -C32    17.80  1.90   1.555   1.555   1.555   1.555
```

```
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        109 Do !
            N13 -NI2 -S4  -C33   -86.80  1.90   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        115 Do !
            N14 -NI2 -S3  -C27    17.70  1.60   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        120 Do !
            N14 -NI2 -S3  -C26   -88.60  1.60   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        148 Do !
            S3  -NI2 -N14 -C54   -50.00  3.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        152 Do !
            S4  -NI2 -N13 -C53  -100.00  2.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        154 Do !
            NI2 -N13 -C53 -O3     83.00 15.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        155 Do !
            NI2 -N14 -C54 -O4    141.00 23.00   1.555   1.555   1.555   1.555
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        161 Check
              C39  -C29  -H29     1.555   1.555   1.555              7.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        168 Check
              C29  -C39  -H29     1.555   1.555   1.555             11.20 Deg.
```

```
  1 ALERT level A = Most likely a serious problem - resolve or explain
  4 ALERT level B = A potentially serious problem, consider carefully
 14 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 23 ALERT level G = General information/check it is not something unexpected

  3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 10 ALERT type 2 Indicator that the structure model may be wrong or deficient
  6 ALERT type 3 Indicator that the structure quality may be low
 22 ALERT type 4 Improvement, methodology, query or suggestion
  1 ALERT type 5 Informative message, check
```

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

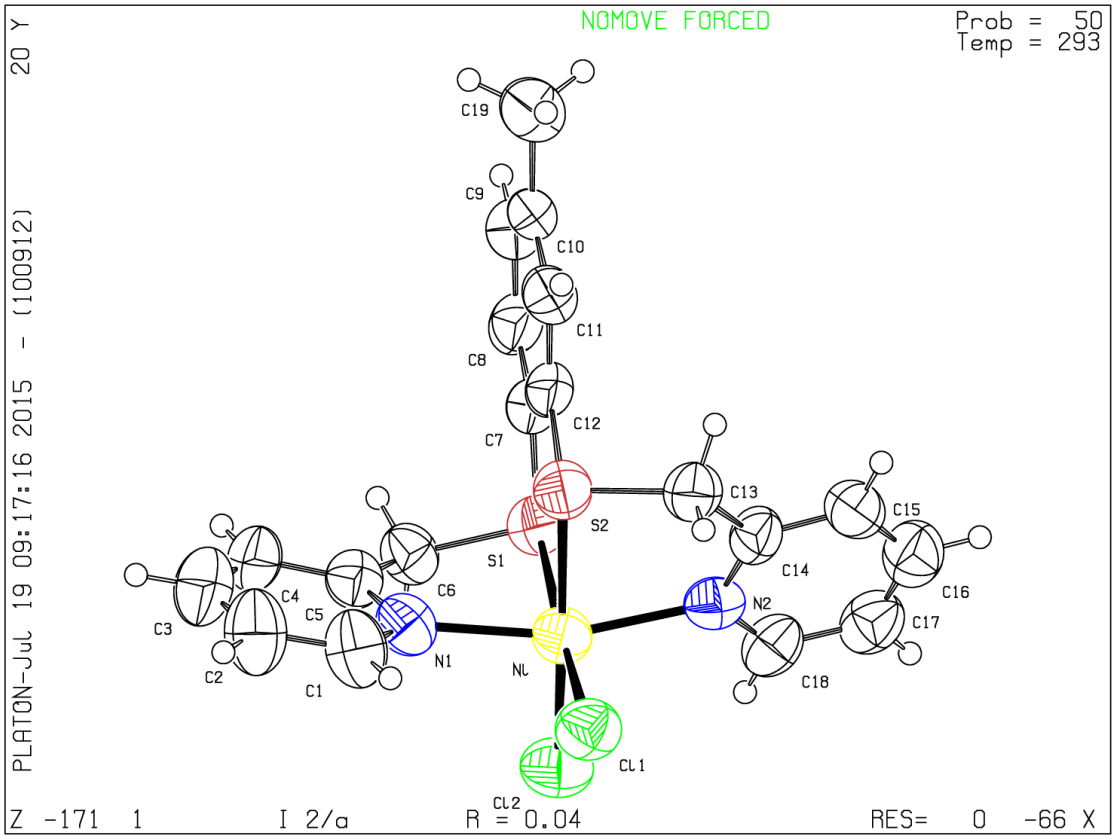
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, 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

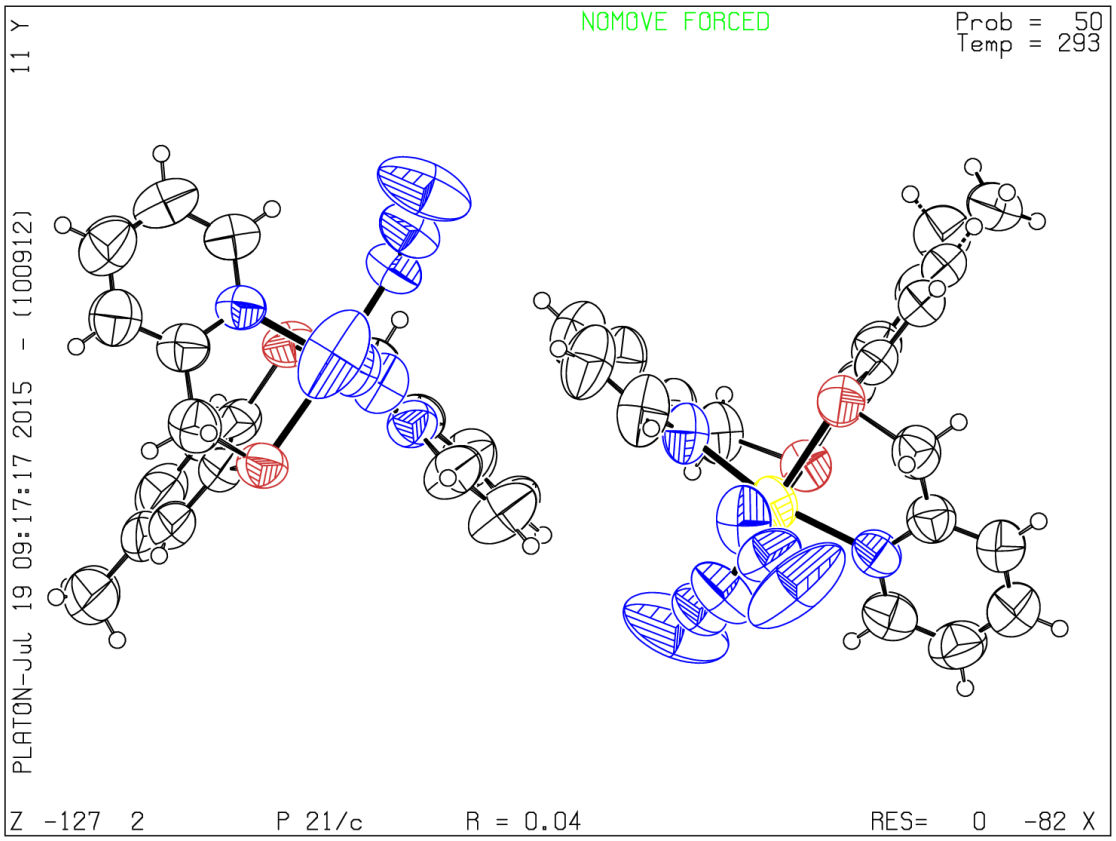
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 21/06/2015; check.def file version of 21/06/2015

Datablock 1 - ellipsoid plot



Datablock 2 - ellipsoid plot



Datablock 3 - ellipsoid plot