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: COF-300-123-triazole

```
Bond precision:   C-C = 0.0055 A          Wavelength=1.54178

Cell:             a=26.0064(13)      b=26.0064(13)      c=7.7568(7)
                  alpha=90           beta=90            gamma=90
Temperature:      293 K

                 Calculated                  Reported
Volume           5246.2(7)                   5246.2(7)
Space group      I 41/a                      I 41/a
Hall group       -I 4ad                      -I 4ad
Moiety formula   C98 H80 N32, 8(C2 H3 N3)    C49 H40 N16, 4(C2 H3 N3)
Sum formula      C114 H104 N56               C57 H52 N28
Mr               2258.53                     1129.26
Dx,g cm-3        1.430                       1.430
Z                2                           4
Mu (mm-1)        0.763                       0.763
F000             2360.0                      2360.0
F000'            2366.82
h,k,lmax         30,30,9                     25,30,9
Nref             2181                        2139
Tmin,Tmax        0.872,0.906                 0.594,0.752
Tmin'            0.858

Correction method= # Reported T Limits: Tmin=0.594 Tmax=0.752
AbsCorr = MULTI-SCAN

Data completeness= 0.981           Theta(max)= 64.055

R(reflections)= 0.0914( 1739)                    wR2(reflections)=
                                                 0.2793( 2139)
S = 1.102                  Npar= 185
```

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

```
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
           Calculated sin(theta_max)/wavelength =    0.5832
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
             Calc: C114 H104 N56
             Rep.: C57 H52 N28
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C98 H80 N32, 8(C2 H3 N3)
             Rep.: C49 H40 N16, 4(C2 H3 N3)
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.28 Report
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        N5      0.256 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0055 Ang.
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          5 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms          5 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
             H1    H5
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.500 Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.15 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      12.13 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0300 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT793_ALERT_4_G Model has Chirality at C8          (Centro SpGr)          R Verify
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON           1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         97 Note
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ          5 Units
```

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

   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   5 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
   5 ALERT type 4 Improvement, methodology, query or suggestion
   3 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

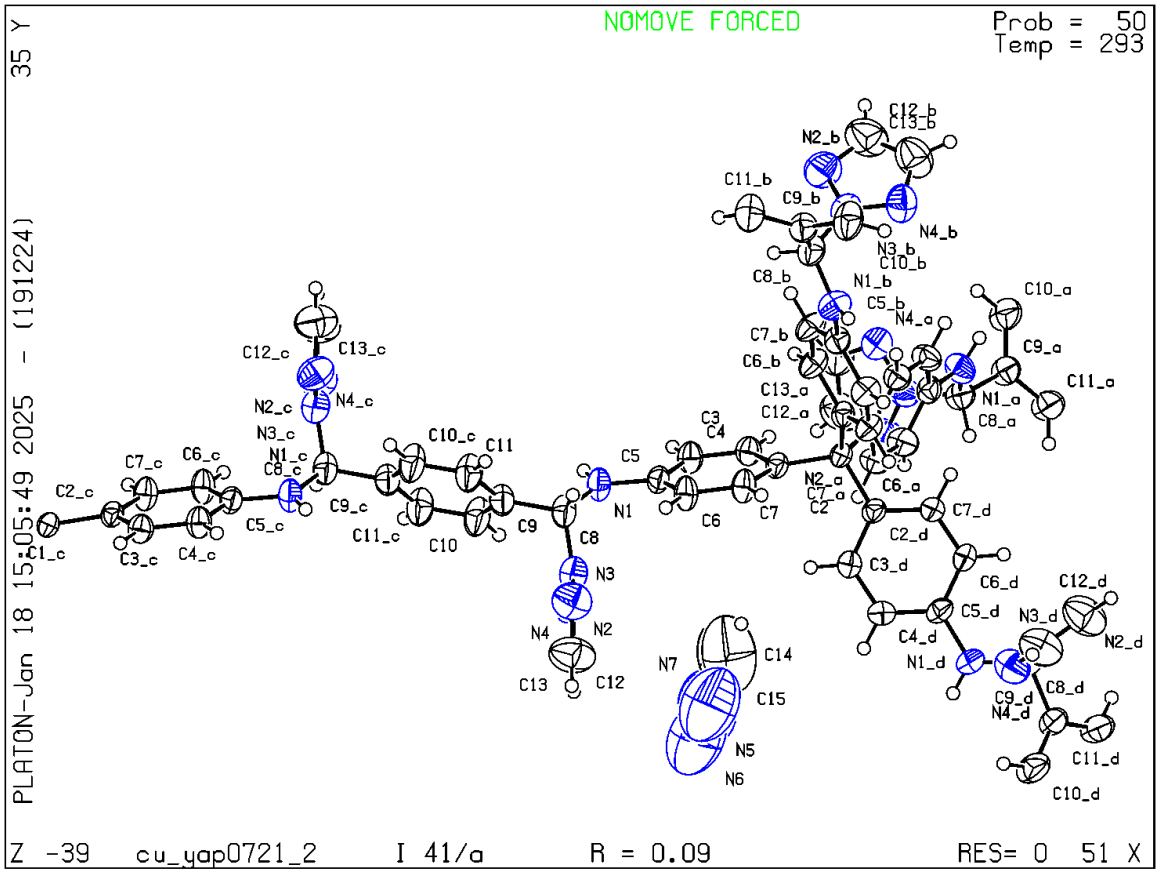
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* 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 19/12/2024; check.def file version of 19/12/2024

Datablock cu_yap0721_2 - ellipsoid plot



checkCIF/PLATON report

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: COF-300-124-triazole

Bond precision: C-C = 0.0077 A Wavelength=1.54178

Cell: a=25.844(9) b=25.844(9) c=7.879(6)
alpha=90 beta=90 gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	5263(5)	5263(6)
Space group	I 41/a	I 41/a
Hall group	-I 4ad	-I 4ad
Moiety formula	C98 H80 N32, 8(C2 H3 N3)	C49 H40 N16, C8 H12 N12, 4[C2N3H3]
Sum formula	C114 H104 N56	C57 H52 N28
Mr	2258.53	1129.26
Dx,g cm-3	1.425	1.425
Z	2	4
Mu (mm-1)	0.760	0.760
F000	2360.0	2360.0
F000'	2366.82	
h,k,lmax	25,25,7	25,25,7
Nref	1342	1330
Tmin,Tmax	0.872,0.906	0.445,0.752
Tmin'	0.859	

Correction method= # Reported T Limits: Tmin=0.445 Tmax=0.752
AbsCorr = MULTI-SCAN

Data completeness= 0.991 Theta(max)= 49.720

R(reflections)= 0.1121(1066) wR2(reflections)= 0.3318(1330)

S = 1.063 Npar= 193

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

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.4948

Author Response: The value of sine(theta_max)/wavelength is less than 0.550 RESPONSE: The value of sine(theta_max)/wavelength is less than 0.550 The value of sine(theta_max)/wavelength is less than 0.550 due to the weak diffraction ability of the crystal. Despite the lower resolution, the data quality is sufficient to support the structural determination and the conclusions drawn in the manuscript. The key features of the structure, such as the molecular packing and framework, are clearly resolved and consistent with the chemical context of the study.

Alert level B

PLAT088_ALERT_3_B Poor Data / Parameter Ratio ..... 6.95 Note

Author Response: The poor data-to-parameter ratio is due to the relatively weak diffraction data obtained from the crystal. Despite efforts to optimize data collection, the crystal quality was not ideal, resulting in a limited number of observed reflections. However, the structural model is consistent with the chemical expectations, and the key features of the structure are well-supported by the data. We have applied appropriate constraints and restraints to ensure the reliability of the refinement.

PLAT260_ALERT_2_B Large Average Ueq of Residue Including N5 0.347 Check

Author Response: The large average Ueq value for the N5 is attributed to partial disorder or incomplete occupancy in the crystal lattice. This disorder was modeled appropriately during refinement, and the final structural model is consistent with the electron density map. The refinement parameters confirm the reliability of the structure.

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
Calc: C114 H104 N56
Rep.: C57 H52 N28
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C98 H80 N32, 8(C2 H3 N3)
Rep.: C49 H40 N16, C8 H12 N12, 4[C2N3H3]
PLAT082_ALERT_2_C High R1 Value ..... 0.11 Report

```
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..................       0.33 Report
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference N3       --C13      .       0.18 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         N4 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N2 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00771 Ang.
```

Alert level G

```
FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C57 H52 N28
           Atom count from _chemical_formula_moiety:C65 H64 N40
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         10 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms          6 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
             H1    H5
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.500 Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.20 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      25.00 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          6 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          2 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0200 Report
PLAT793_ALERT_4_G Model has Chirality at C8          (Centro SpGr)          R Verify
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON          13 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        108 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          7 Note
               0  2  0,   0  3  1,   1  4  1,   2  7  1,   2  8  0,   2 10  2,
               4  5  1,
```

```
   1 ALERT level A = Most likely a serious problem - resolve or explain
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   6 ALERT type 3 Indicator that the structure quality may be low
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   2 ALERT type 5 Informative message, check
```

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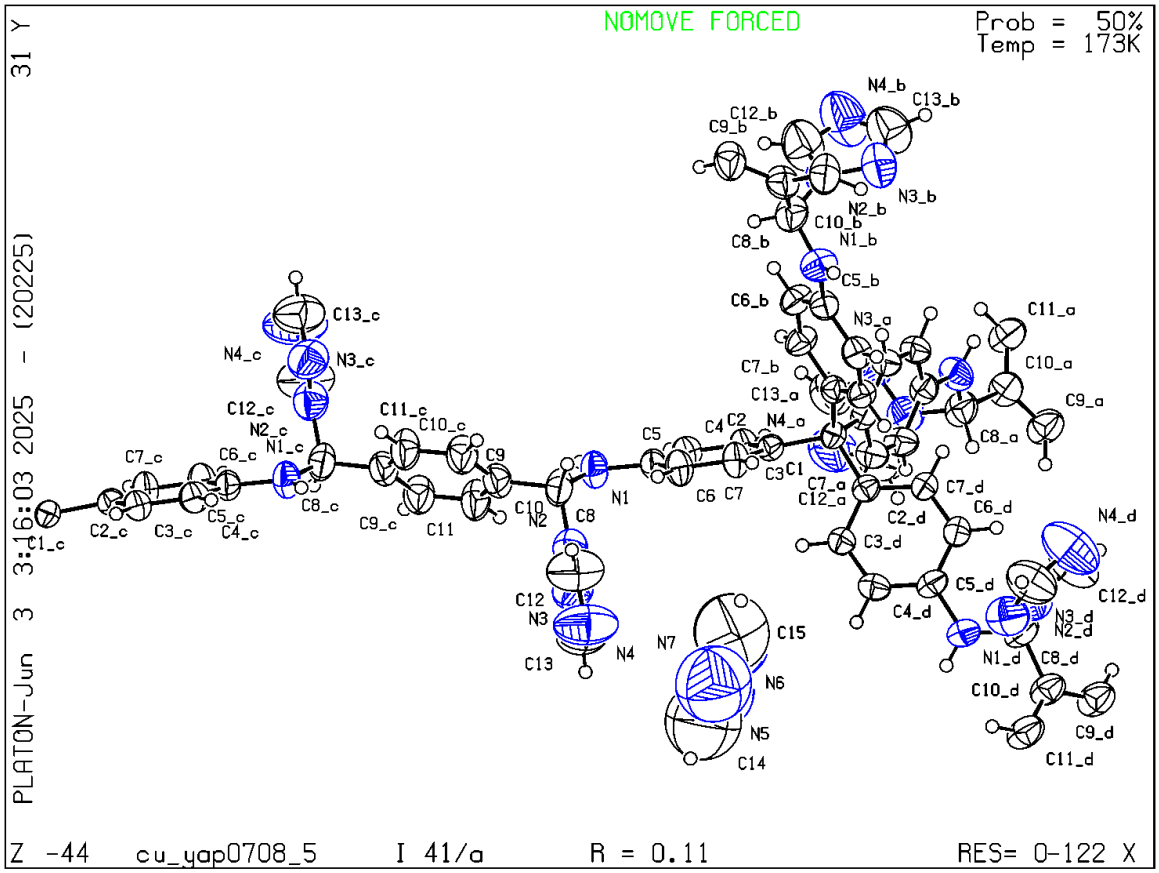
PLATON version of 02/02/2025; check.def file version of 02/02/2025

Datablock cu_yap0708_5 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_yap250610_1

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: COF-300-pyrazole

```
Bond precision:   C-C = 0.0171 A          Wavelength=1.54178

Cell:               a=25.946(3)      b=25.946(3)      c=7.6916(14)
                    alpha=90         beta=90          gamma=90
Temperature:        293 K

                 Calculated                  Reported
Volume           5178.0(15)                  5178.1(14)
Space group      I 41/a                      I 41/a
Hall group       -I 4ad                      -I 4ad
Moiety formula   C53 H44 N12 [+ solvent]     C53 H44 N12, 4[C3N2H4]
Sum formula      C53 H44 N12 [+ solvent]     C65 H60 N20
Mr               849.00                      1121.33
Dx,g cm-3        1.089                       1.438
Z                4                           4
Mu (mm-1)        0.531                       0.722
F000             1784.0                      2360.0
F000'            1788.89
h,k,lmax         23,23,6                     23,22,6
Nref             961                         939
Tmin,Tmax        0.878,0.910                 0.424,0.749
Tmin'            0.866

Correction method= # Reported T Limits: Tmin=0.424 Tmax=0.749
AbsCorr = MULTI-SCAN

Data completeness= 0.977           Theta(max)= 43.436

R(reflections)= 0.2502( 621)                    wR2(reflections)=
                                                0.6022( 939)
S = 1.039                  Npar= 127
```

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

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.4459

Author Response: The value of sine(theta_max)/wavelength is less than 0.550 due to the weak diffraction ability of the crystal. Despite the lower resolution, the data quality is sufficient to support the structural determination and the conclusions drawn in the manuscript. The key features of the structure, such as the molecular packing and framework, are clearly resolved and consistent with the chemical context of the study.

PLAT082_ALERT_2_A High R1 Value ..... 0.25 Report

Author Response: The high R1 value is likely due to the relatively weak diffraction data obtained from the crystal. Despite efforts to optimize data collection, the crystal quality was not ideal, resulting in higher uncertainties in the refinement. However, the structural model is consistent with the chemical expectations and other validation metrics (e.g., wR2, GooF) are within acceptable ranges. We believe the reported structure is reliable despite the elevated R1 value.

PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) ..... 0.60 Report

Author Response: The high R1 value is likely due to the relatively weak diffraction data obtained from the crystal. Despite efforts to optimize data collection, the crystal quality was not ideal, resulting in higher uncertainties in the refinement. However, the structural model is consistent with the chemical expectations and other validation metrics (e.g., wR2, GooF) are within acceptable ranges. We believe the reported structure is reliable despite the elevated R1 value.

Alert level B

DIFMN02_ALERT_2_B The minimum difference density is < -0.1*ZMAX*1.00
_refine_diff_density_min given = -0.802
Test value = -0.700

Author Response: The minimum difference density of < -0.1 is attributed to partial disorder or incomplete occupancy in the crystal lattice. This disorder was modeled appropriately during refinement, and the final structural model is consistent with the electron density map. The refinement parameters confirm the reliability of the structure.

PLAT088_ALERT_3_B Poor Data / Parameter Ratio ..... 7.39 Note

Author Response: The poor data-to-parameter ratio is due to the relatively weak diffraction data obtained from the crystal. Despite efforts to optimize data collection, the crystal quality was not ideal, resulting in a limited number of observed reflections. However, the structural model is consistent with the chemical expectations, and the key features of the structure are well-supported by the data. We have applied appropriate constraints and restraints to ensure the reliability of the refinement.

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 0.90 eA-3

Author Response: The large positive residual density is attributed to partial disorder or incomplete occupancy in the crystal lattice. This disorder was modeled appropriately during refinement, and the final structural model is consistent with the electron density map. The refinement parameters confirm the reliability of the structure.

PLAT098_ALERT_2_B Large Reported Min. (Negative) Residual Density -0.80 eA-3

Author Response: The large positive residual density is attributed to partial disorder or incomplete occupancy in the crystal lattice. This disorder was modeled appropriately during refinement, and the final structural model is consistent with the electron density map. The refinement parameters confirm the reliability of the structure.

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.01712 Ang.

Author Response: The low bond precision on C-C bonds is likely due to the relatively weak diffraction data obtained from the crystal. Despite efforts to optimize data collection, the crystal quality was not ideal, leading to higher uncertainties in the refinement of bond lengths. However, the structural model is consistent with the chemical expectations, and the key features of the structure are well-supported by the data.

Alert level C

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75

```
           The relevant atom site should be identified.
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.977 Why?
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range       3.8 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference N1       --C5       .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N1       --C8       .       0.18 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...    -0.184 Report
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     2.070 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.446        21 Report
                0  4  0,  -2  6  0,   0  6  0,  -2 20  0,  -6 22  0,  -4 22  0,
                9 20  1,  10 18  2,  12 18  2,   7 19  2,  11 19  2,   8 20  2,
                4 19  3,   3 20  3,   5 20  3, -11 15  4,  -1 17  4,   2 18  4,
               -9 12  5,  -8 13  5,   2 15  5,
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .         1 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H11       .     -0.40 eA-3
```

Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C65 H60 N20
           Atom count from the _atom_site data:  C53 H44 N12
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    4
          From the CIF: _chemical_formula_sum  C65 H60 N20
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        260.00    212.00   48.00
          H        240.00    176.00   64.00
          N         80.00     48.00   32.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         8 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms        17 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............         1 Report
             H1
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
             Calc: C53 H44 N12
             Rep.: C65 H60 N20
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C53 H44 N12
             Rep.: C53 H44 N12, 4[C3N2H4]
PLAT051_ALERT_1_G Mu(calc) and Mu(cif) Ratio Differs from 1.0 by .     26.50 %
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large      0.40 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large    200.00 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         5 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records         1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used    0.0300 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)       293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)       293 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure       363 A**3
PLAT793_ALERT_4_G Model has Chirality at C8          (Centro SpGr)         S Verify
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON         1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       399 Note
```

```
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still         52% Note
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min)[Deg]=        4.82 Note
                  0  2  0,
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....           2 Note
                  0  2  0,   0  4  0,
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law ( 1 1 0)         Est.d BASF        0.07 Check
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........         4.3 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       9.744 Note
               Predicted wR2: Based on SigI**2  6.18 or SHELX Weight 57.95
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.           0 Info
```

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

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

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Publication of your CIF in IUCr journals

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Publication of your CIF in other journals

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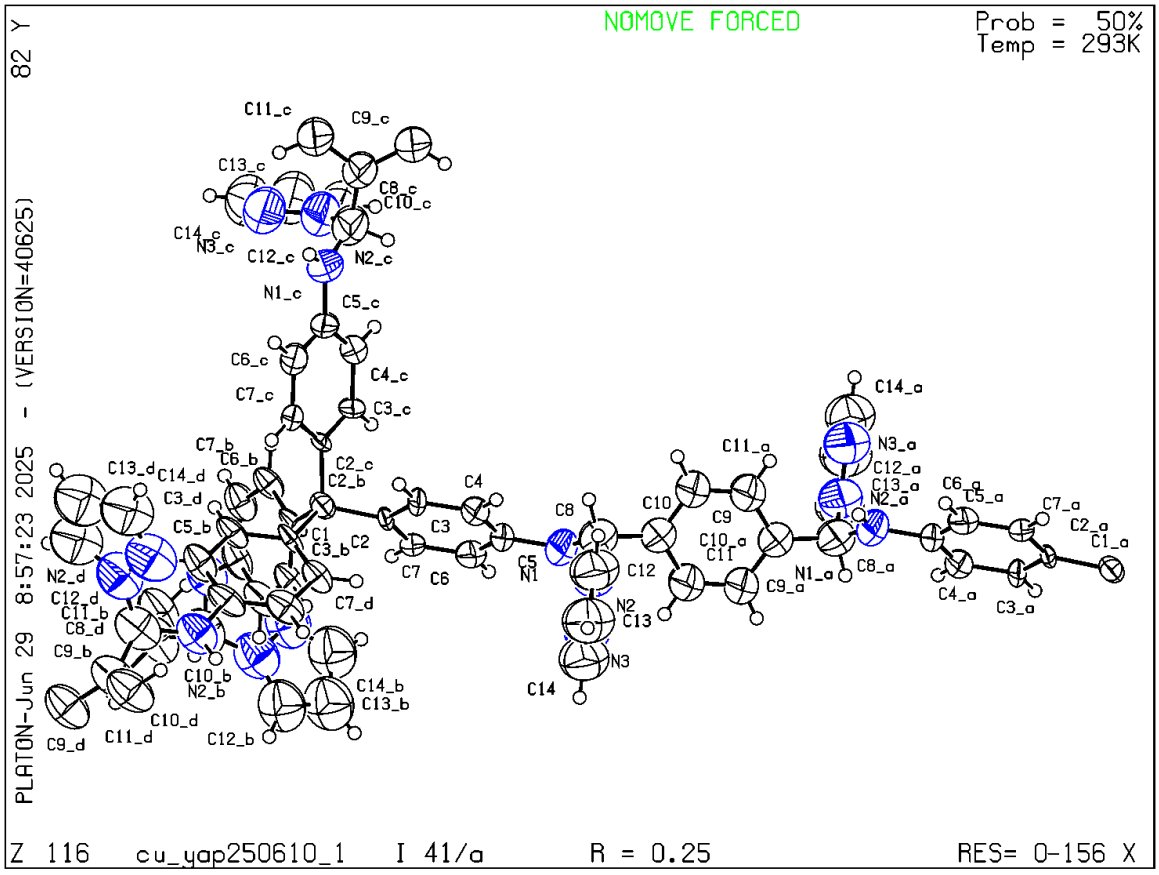
PLATON version of 04/06/2025; check.def file version of 30/05/2025

Datablock cu_yap250610_1 - ellipsoid plot



checkCIF/PLATON report

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: imidazole@COF-300

Bond precision: C-C = 0.0057 A Wavelength=1.54178

Cell: a=26.166(4) b=26.166(4) c=7.6048(19)
alpha=90 beta=90 gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	5207(2)	5206.6(19)
Space group	I 41/a	I 41/a
Hall group	-I 4ad	-I 4ad
Moiety formula	C41 H28 N4 [+ solvent]	C41 H28 N4, 4[C3N2H4]
Sum formula	C41 H28 N4 [+ solvent]	C53 H44 N12
Mr	576.67	849.00
Dx,g cm-3	0.736	1.083
Z	4	4
Mu (mm-1)	0.338	0.528
F000	1208.0	1784.0
F000'	1211.24	
h,k,lmax	25,25,7	25,25,7
Nref	1242	1219
Tmin,Tmax	0.909,0.934	0.840,0.860
Tmin'	0.900	

Correction method= # Reported T Limits: Tmin=0.840 Tmax=0.860
AbsCorr = MULTI-SCAN

Data completeness= 0.981 Theta(max)= 48.229

R(reflections)= 0.0966(973) wR2(reflections)= 0.2867(1219)

S = 1.006 Npar= 102

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.

[IMAGE] **Alert level A**

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.4837

Author Response: The value of sine(theta_max)/wavelength is less than 0.550 due to the weak diffraction ability of the crystal. Despite the lower resolution, the data quality is sufficient to support the structural determination and the conclusions drawn in the manuscript. The key features of the structure, such as the molecular packing and framework, are clearly resolved and consistent with the chemical context of the study.

[IMAGE] **Alert level C**

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.29 Report
PLAT230_ALERT_2_C Hirshfeld Test Diff for C3 --C4 . 6.2 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C10 --C11 . 5.3 s.u.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C8 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C10 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 2.3 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including N1 0.102 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00571 Ang.

[IMAGE] **Alert level G**

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C53 H44 N12
Atom count from the _atom_site data: C41 H28 N4
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum C53 H44 N12
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	212.00	164.00	48.00
H	176.00	112.00	64.00
N	48.00	16.00	32.00

PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms 6 Report
PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check
Calc: C41 H28 N4
Rep.: C53 H44 N12
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C41 H28 N4
Rep.: C41 H28 N4, 4[C3N2H4]
PLAT051_ALERT_1_G Mu(calc) and Mu(cif) Ratio Differs from 1.0 by . 36.04 %
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.20 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report

```
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par     0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0010 Report
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........           ! Info
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON            1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         21 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed           ! Info
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File           9 Note
               -4  8  0,  -1  2  1,   0  1  1,   0  2  2,   1  2  1,   2  2  0,
                2  4  0,   4 10  0,   6 12  0,
```

```
  1 ALERT level A = Most likely a serious problem - resolve or explain
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  8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 17 ALERT level G = General information/check it is not something unexpected

  5 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
  4 ALERT type 4 Improvement, methodology, query or suggestion
  1 ALERT type 5 Informative message, check
```

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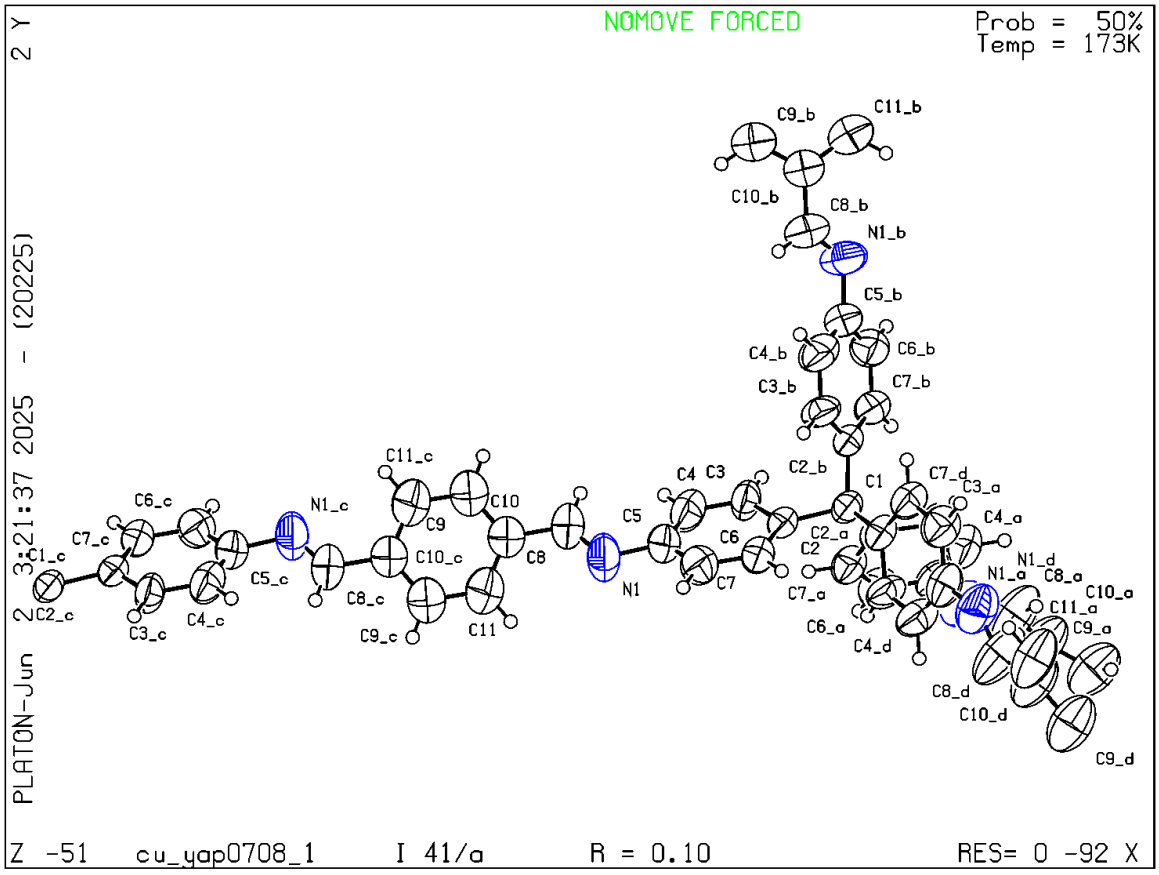
PLATON version of 02/02/2025; check.def file version of 02/02/2025

Datablock cu_yap0708_1 - ellipsoid plot



checkCIF/PLATON report

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 2-Methylimidazole@COF-300

Bond precision: C-C = 0.0057 A Wavelength=1.54178

Cell: a=26.166(4) b=26.166(4) c=7.6048(19)
alpha=90 beta=90 gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	5207(2)	5206.6(19)
Space group	I 41/a	I 41/a
Hall group	-I 4ad	-I 4ad
Moiety formula	C41 H28 N4 [+ solvent]	C41 H28 N4, 4[C3N2H4]
Sum formula	C41 H28 N4 [+ solvent]	C53 H44 N12
Mr	576.67	849.00
Dx,g cm-3	0.736	1.083
Z	4	4
Mu (mm-1)	0.338	0.528
F000	1208.0	1784.0
F000'	1211.24	
h,k,lmax	25,25,7	25,25,7
Nref	1242	1219
Tmin,Tmax	0.909,0.934	0.840,0.860
Tmin'	0.900	

Correction method= # Reported T Limits: Tmin=0.840 Tmax=0.860
AbsCorr = MULTI-SCAN

Data completeness= 0.981 Theta(max)= 48.229

R(reflections)= 0.0966(973) wR2(reflections)= 0.2867(1219)

S = 1.006 Npar= 102

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
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[IMAGE] **Alert level A**

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Calculated sin(theta_max)/wavelength = 0.4837

Author Response: The value of sine(theta_max)/wavelength is less than 0.550 due to the weak diffraction ability of the crystal. Despite the lower resolution, the data quality is sufficient to support the structural determination and the conclusions drawn in the manuscript. The key features of the structure, such as the molecular packing and framework, are clearly resolved and consistent with the chemical context of the study.

[IMAGE] **Alert level C**

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PLAT230_ALERT_2_C Hirshfeld Test Diff for C10 --C11 . 5.3 s.u.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C8 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C10 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 2.3 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including N1 0.102 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00571 Ang.

[IMAGE] **Alert level G**

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C53 H44 N12
Atom count from the _atom_site data: C41 H28 N4
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum C53 H44 N12
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	212.00	164.00	48.00
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PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms 6 Report
PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check
Calc: C41 H28 N4
Rep.: C53 H44 N12
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C41 H28 N4
Rep.: C41 H28 N4, 4[C3N2H4]
PLAT051_ALERT_1_G Mu(calc) and Mu(cif) Ratio Differs from 1.0 by . 36.04 %
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.20 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report

```
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par     0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0010 Report
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........           ! Info
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON            1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         21 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed           ! Info
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File           9 Note
               -4  8  0,  -1  2  1,   0  1  1,   0  2  2,   1  2  1,   2  2  0,
                2  4  0,   4 10  0,   6 12  0,
```

```
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```

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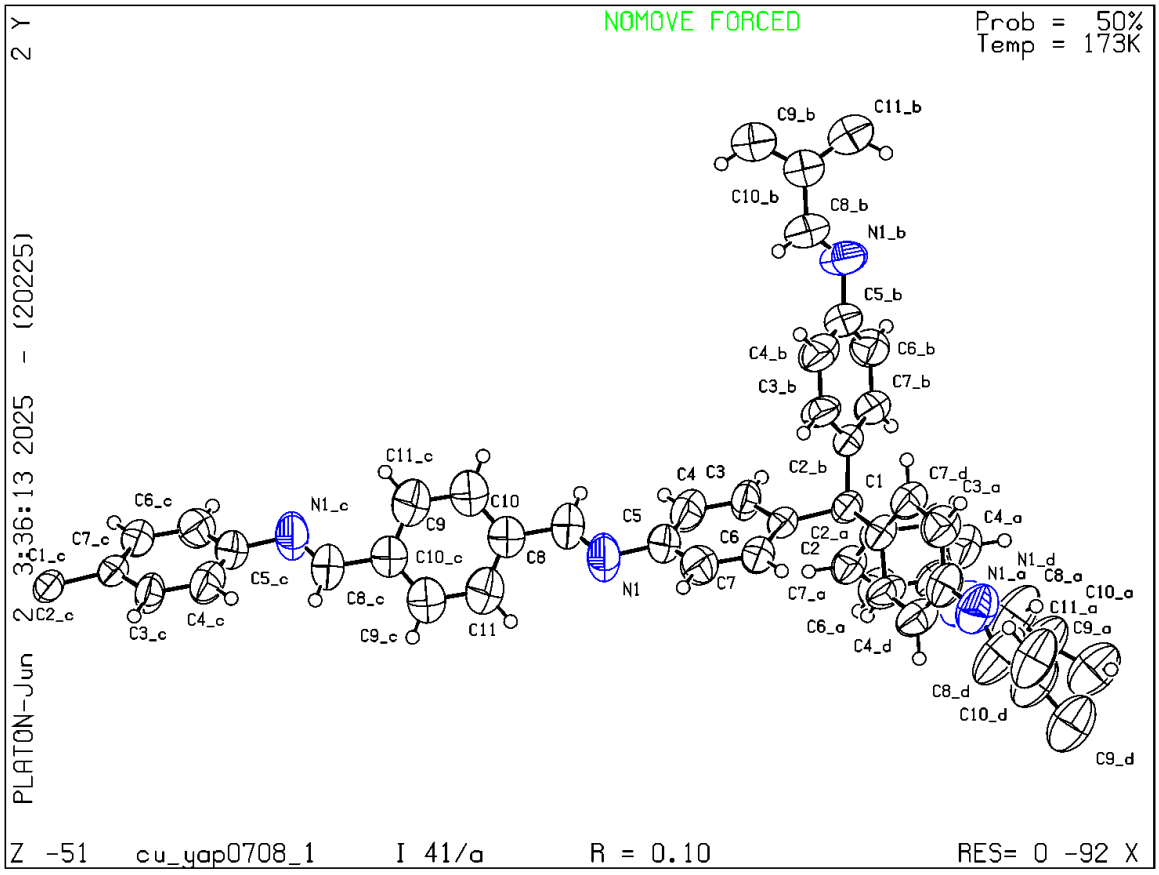
PLATON version of 02/02/2025; check.def file version of 02/02/2025

Datablock cu_yap0708_1 - ellipsoid plot



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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 2-Ethylimidazole@COF-300

```
Bond precision:   C-C = 0.0049 A          Wavelength=1.54178

Cell:             a=26.5843(17)      b=26.5843(17)      c=7.4767(8)
                  alpha=90           beta=90            gamma=90
Temperature:      293 K

                 Calculated                  Reported
Volume           5284.0(9)                   5284.0(9)
Space group      I -4                        I -4
Hall group       I -4                        I -4
Moiety formula   C41 H26 N4 [+ solvent]      C41 H26 N4
Sum formula      C41 H26 N4 [+ solvent]      C41 H26 N4
Mr               574.66                      574.66
Dx,g cm-3        0.722                       0.722
Z                4                           4
Mu (mm-1)        0.333                       0.333
F000             1200.0                      1200.0
F000'            1203.24
h,k,lmax         30,30,8                     30,26,8
Nref             4408[ 2392]                 4239
Tmin,Tmax        0.942,0.958                 0.512,0.752
Tmin'            0.936

Correction method= # Reported T Limits: Tmin=0.512 Tmax=0.752
AbsCorr = MULTI-SCAN

Data completeness= 1.77/0.96        Theta(max)= 64.058

                                                    wR2(reflections)=
R(reflections)= 0.0512( 2527)                       0.1493( 4239)
S = 0.934                  Npar= 204
```

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.

[IMAGE] **Alert level C**

```
STRVA01_ALERT_2_C           Chirality of atom sites is inverted?
          From the CIF: _refine_ls_abs_structure_Flack    0.800
          From the CIF: _refine_ls_abs_structure_Flack_su    0.700
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
           Calculated sin(theta_max)/wavelength =    0.5832
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.977 Why?
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C4       --C5       .        6.0 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C9       --C14      .        6.4 s.u.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C13 Check
PLAT334_ALERT_2_C Small <C-C> Benzene Dist.   C2       -C7       .       1.37 Ang.
PLAT334_ALERT_2_C Small <C-C> Benzene Dist.   C17      -C22      .       1.36 Ang.
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00493 Ang.
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4     Please Check
PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? .       0.80 Check
```

[IMAGE] **Alert level G**

```
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms         14 Report
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High .      0.700 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          2 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par     0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0010 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C14 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON           7 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         45 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          6 Note
               -1  3  0,   0 10  0,   1  1  0,   1  3  0,   2  4  0,   4  8  0,
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ           4 Units
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
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  11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
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   2 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
   6 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
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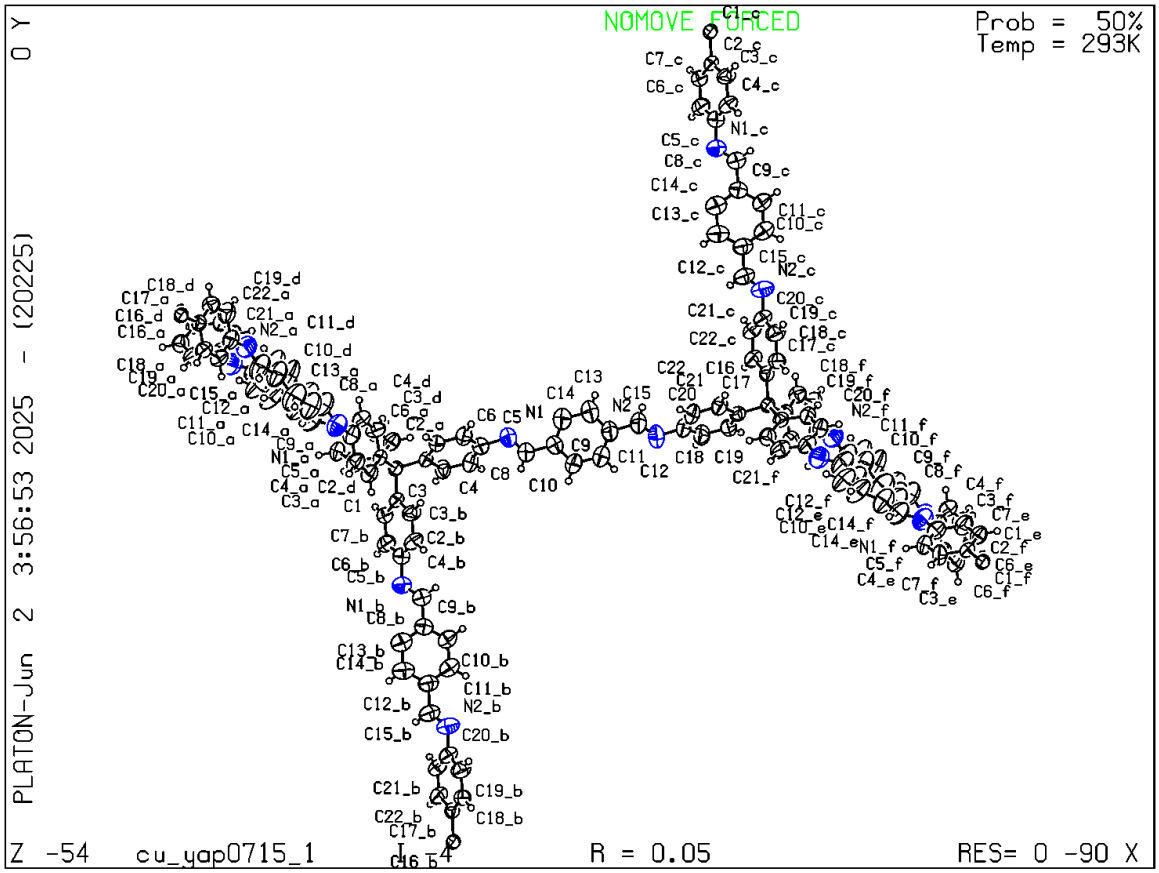
PLATON version of 02/02/2025; check.def file version of 02/02/2025

Datablock cu_yap0715_1 - ellipsoid plot



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No syntax errors found. CIF dictionary Interpreting this report

Datablock: benzimidazole@COF-300

Bond precision: C-C = 0.0051 A Wavelength=1.54178

Cell: a=27.031(5) b=27.031(5) c=7.394(2)
alpha=90 beta=90 gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	5403(2)	5402(3)
Space group	I 41/a	I 41/a
Hall group	-I 4ad	-I 4ad
Moiety formula	C41 H28 N4 [+ solvent]	C41 H28 N4, 4[C7N2H6]
Sum formula	C41 H28 N4 [+ solvent]	C41 H28 N4
Mr	576.67	576.67
Dx,g cm-3	0.709	0.709
Z	4	4
Mu (mm-1)	0.325	0.326
F000	1208.0	1208.0
F000'	1211.24	
h,k,lmax	27,27,7	26,27,7
Nref	1522	1501
Tmin,Tmax	0.943,0.959	0.840,0.860
Tmin'	0.937	

Correction method= # Reported T Limits: Tmin=0.840 Tmax=0.860
AbsCorr = MULTI-SCAN

Data completeness= 0.986 Theta(max)= 52.212

R(reflections)= 0.0901(1235) wR2(reflections)= 0.2705(1501)

S = 1.106 Npar= 102

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.

[IMAGE] **Alert level A**

```
THETM01_ALERT_3_A  The value of sine(theta_max)/wavelength is less than 0.550
           Calculated sin(theta_max)/wavelength =    0.5126
```

Author Response: The value of sine(theta_max)/wavelength is less than 0.550 due to the weak diffraction ability of the crystal. Despite the lower resolution, the data quality is sufficient to support the structural determination and the conclusions drawn in the manuscript. The key features of the structure, such as the molecular packing and framework, are clearly resolved and consistent with the chemical context of the study.

[IMAGE] **Alert level C**

```
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..................       0.27 Report
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C9       --C10      .        5.7 s.u.
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd    1)        2.5 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        N1      0.102 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00507 Ang.
```

[IMAGE] **Alert level G**

```
FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C41 H28 N4
           Atom count from _chemical_formula_moiety:C69 H52 N12
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms          5 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C41 H28 N4
             Rep.: C41 H28 N4, 4[C7N2H6]
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.15 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par     0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0010 Report
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON          1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        19 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
```

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

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
```

```
  5 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
  4 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

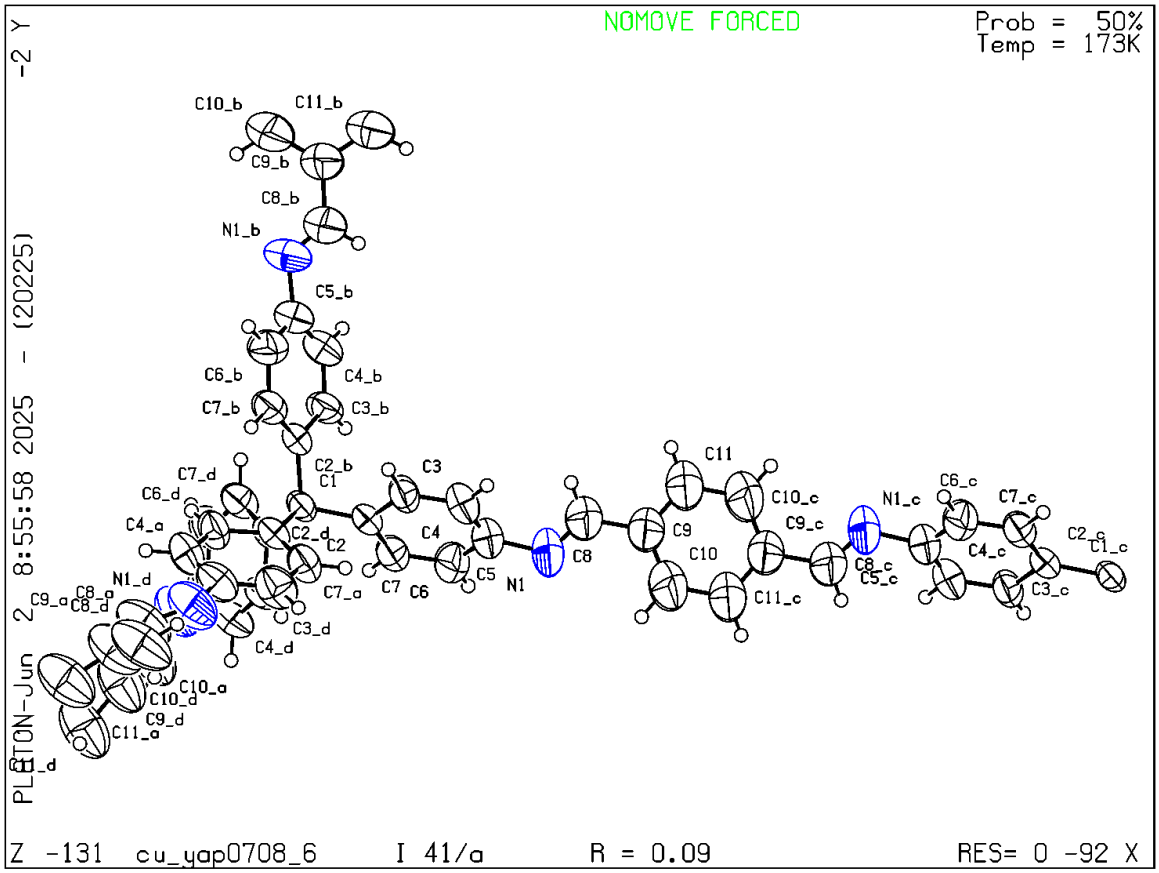
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* 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 02/02/2025; check.def file version of 02/02/2025

Datablock cu_yap0708_6 - ellipsoid plot



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: benzotriazole@COF-300

```
Bond precision:   C-C = 0.0094 A           Wavelength=1.54178

Cell:               a=26.659(2)      b=26.659(2)      c=7.4645(8)
                    alpha=90         beta=90          gamma=90
Temperature:        173 K

                 Calculated                  Reported
Volume           5305.0(10)                  5304.9(10)
Space group      I 41/a                      I 41/a
Hall group       -I 4ad                      -I 4ad
Moiety formula   C41 H28 N4 [+ solvent]      C41 H28 N4
Sum formula      C41 H28 N4 [+ solvent]      C41 H28 N4
Mr               576.67                      576.67
Dx,g cm-3        0.722                       0.722
Z                4                           4
Mu (mm-1)        0.331                       0.331
F000             1208.0                      1208.0
F000'            1211.24
h,k,lmax         25,25,7                     25,25,7
Nref             1237                        1226
Tmin,Tmax        0.942,0.958                 0.490,0.752
Tmin'            0.936

Correction method= # Reported T Limits: Tmin=0.490 Tmax=0.752
AbsCorr = MULTI-SCAN

Data completeness= 0.991            Theta(max)= 47.790

                                                    wR2(reflections)=
R(reflections)= 0.1417( 913)                        0.3662( 1226)
S = 1.058                  Npar= 103
```

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.

[IMAGE] **Alert level A**

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.4804

Author Response: The value of sine(theta_max)/wavelength is less than 0.550 RESPONSE: The value of sine(theta_max)/wavelength is less than 0.550 The value of sine(theta_max)/wavelength is less than 0.550 due to the weak diffraction ability of the crystal. Despite the lower resolution, the data quality is sufficient to support the structural determination and the conclusions drawn in the manuscript. The key features of the structure, such as the molecular packing and framework, are clearly resolved and consistent with the chemical context of the study.

[IMAGE] **Alert level B**

PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ..... 0.37 Report

Author Response: The high wR2 value is likely due to the relatively weak diffraction data obtained from the crystal. Despite efforts to optimize data collection, the crystal quality was not ideal, resulting in higher uncertainties in the refinement. However, the structural model is consistent with the chemical expectations and other validation metrics (e.g., R1, GooF) are within acceptable ranges. We believe the reported structure is reliable despite the elevated wR2 value.

[IMAGE] **Alert level C**

PLAT082_ALERT_2_C High R1 Value ..... 0.14 Report
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.5 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference N1 --C5 . 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N1 --C8 . 0.20 Ang.
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 3.5 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including N1 0.121 Check
PLAT334_ALERT_2_C Small <C-C> Benzene Dist. C2 -C7 . 1.37 Ang.
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00943 Ang.

[IMAGE] **Alert level G**

PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms 11 Report
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.20 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 16.00 Why ?
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par 0.0010 Report

```
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0010 Report
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON           1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         45 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
```

```
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   1 ALERT type 5 Informative message, check
```

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PLATON version of 02/02/2025; check.def file version of 02/02/2025

Datablock cu_yap0708_2 - ellipsoid plot