Supplementary Information

Four monomeric copper(II) complexes of non-steroidal anti-inflammatory drug Ibuprofen and N-donor ligands: Syntheses, characterization, crystal structures and cytotoxicity studies.

Santosh Kuma, Shipra Garg, Raj Pal Sharma, Paloth Venugopalan, Lorenzo Tenti, Valeria Ferretti, Laetitia Nivelle, Michel Tarpin, Emmanuel Guillon

Table of Contents

Table S1. Hydrogen bonding parameters (Å, °) for complexes 1-4

Figure S1. FT-IR spectra of complexes 1-4

Figure S2. UV-Visible spectra of complexes 1-4 in DMSO and methanol solvent.

Figure S3. Diffuse Reflectance spectra of complexes 1-4

Figure S4: UV-Visible spectra of complexes 1-4 using DMSO and DMSO-H₂O (2:1) as solvent.

Figure S5. Combined TGA-DTA plots for complexes 1-4

Checkcif report of complex 1
Checkcif report of complex 2
Checkcif report of complex 3
Checkcif report of complex 4
Table S1. Hydrogen bonding parameters (Å, °) for complexes 1-4

<table>
<thead>
<tr>
<th>Complex</th>
<th>D-H</th>
<th>D....A</th>
<th>H....A</th>
<th>D-H...A</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Complex 1</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O1W-H...O4</td>
<td>0.85(4)</td>
<td>2.608(4)</td>
<td>1.78(4)</td>
<td>168(3)</td>
</tr>
<tr>
<td>O1W-H...O1&lt;sup&gt;i&lt;/sup&gt;</td>
<td>0.87(3)</td>
<td>2.768(3)</td>
<td>1.91(3)</td>
<td>164(3)</td>
</tr>
<tr>
<td>C11-H...O1&lt;sup&gt;i&lt;/sup&gt;</td>
<td>0.93</td>
<td>3.594(3)</td>
<td>2.67</td>
<td>170</td>
</tr>
</tbody>
</table>

Symmetry code: (i) 1-x,-y,-z

<table>
<thead>
<tr>
<th>Complex 2</th>
<th>D-H</th>
<th>D....A</th>
<th>H....A</th>
<th>D-H...A</th>
</tr>
</thead>
<tbody>
<tr>
<td>O1W-H...O2</td>
<td>0.87(3)</td>
<td>2.648(3)</td>
<td>1.83(4)</td>
<td>155(3)</td>
</tr>
<tr>
<td>C1-H...O2W</td>
<td>0.93</td>
<td>3.295(4)</td>
<td>2.44</td>
<td>152</td>
</tr>
<tr>
<td>O1W-H...O3&lt;sup&gt;i&lt;/sup&gt;</td>
<td>0.84(2)</td>
<td>2.807(2)</td>
<td>1.98(2)</td>
<td>170(2)</td>
</tr>
<tr>
<td>C5-H...O3&lt;sup&gt;i&lt;/sup&gt;</td>
<td>0.93</td>
<td>3.485(3)</td>
<td>2.56</td>
<td>170</td>
</tr>
<tr>
<td>C10-H...O2W&lt;sup&gt;ii&lt;/sup&gt;</td>
<td>0.93</td>
<td>3.386(4)</td>
<td>2.53</td>
<td>153</td>
</tr>
</tbody>
</table>

*Short contacts:*
<table>
<thead>
<tr>
<th></th>
<th>D-H</th>
<th>D....A</th>
</tr>
</thead>
<tbody>
<tr>
<td>O4 ...O2W</td>
<td>2.703(5)</td>
<td></td>
</tr>
<tr>
<td>O2W...O1&lt;sup&gt;iii&lt;/sup&gt;</td>
<td>3.014(3)</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry codes: (i) 1-x,-y,-z; (ii) x+1,y,z; (iii) 1-x,1-y,-z

<table>
<thead>
<tr>
<th>Complex 3</th>
<th>D-H</th>
<th>D....A</th>
<th>H....A</th>
<th>D-H...A</th>
</tr>
</thead>
<tbody>
<tr>
<td>O1W-H...O2</td>
<td>0.87(3)</td>
<td>2.967(5)</td>
<td>2.10(4)</td>
<td>174(3)</td>
</tr>
<tr>
<td>N1-H...O1W&lt;sup&gt;i&lt;/sup&gt;</td>
<td>0.86(3)</td>
<td>3.102(5)</td>
<td>2.27(3)</td>
<td>162(3)</td>
</tr>
<tr>
<td>O1W-H...O2&lt;sup&gt;ii&lt;/sup&gt;</td>
<td>0.85(3)</td>
<td>3.030(5)</td>
<td>2.19(4)</td>
<td>168(3)</td>
</tr>
<tr>
<td>C1-H...O1&lt;sup&gt;iii&lt;/sup&gt;</td>
<td>0.97</td>
<td>3.442(4)</td>
<td>2.61</td>
<td>143</td>
</tr>
</tbody>
</table>

Symmetry codes: (i) x,y+1,z; (ii) -x,y-1/2,1/2-z; (iii) -x,1-y,-z

<table>
<thead>
<tr>
<th>Complex 4</th>
<th>D-H</th>
<th>D....A</th>
<th>H....A</th>
<th>D-H...A</th>
</tr>
</thead>
<tbody>
<tr>
<td>C3-H...O2</td>
<td>0.96</td>
<td>3.417(7)</td>
<td>2.64</td>
<td>138</td>
</tr>
<tr>
<td>O1W-H...O2&lt;sup&gt;i&lt;/sup&gt;</td>
<td>0.83(6)</td>
<td>2.714(4)</td>
<td>1.91(6)</td>
<td>163(6)</td>
</tr>
<tr>
<td>N1-H...O3&lt;sup&gt;i&lt;/sup&gt;</td>
<td>0.86(4)</td>
<td>2.768(6)</td>
<td>1.94(4)</td>
<td>163(4)</td>
</tr>
<tr>
<td>N1-H...O2&lt;sup&gt;ii&lt;/sup&gt;</td>
<td>0.91(6)</td>
<td>2.886(6)</td>
<td>2.07(6)</td>
<td>148(6)</td>
</tr>
</tbody>
</table>

Symmetry codes: (i) 1-x,y+1,1/2-z; (ii) 1-x,y,1/2-z
Figure S1. FT-IR spectra of complexes 1-4
Figure S2. UV-Visible spectra of complexes 1-4 in DMSO and methanol solvent.

Figure S3. Diffuse Reflectance spectra of complexes 1-4.
Fig. S4: UV-Visible spectra of complexes 1-4 using DMSO and DMSO-H$_2$O (2:1) as solvent.
Fig. S5. Combined TGA-DTA plots for complexes 1-4
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**
PLAT413_ALERT_2_B Short Inter XH3 .. XHn H24B .. H38C 1.96 Ang.

**Alert level C**
PLAT019_ALERT_1_C_diffrn_measured_fraction_theta_full/*_max < 1.0 0.998 Report
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 5.3 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 6.7 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C23 -- C25 6.9 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C36 -- C37 6.1 s.u.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C22 Check
And 2 other PLAT242 Alerts
More...
PLAT314_ALERT_2_C Check Small Angle for H2O: Metal-O1W -H1W 78.11 Degree
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ............... 0.00628 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C36 - C37 1.41 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn H24A .. H25A 1.83 Ang.

**Alert level G**
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 6 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms 4 Report
<table>
<thead>
<tr>
<th>ALERT level</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Most likely a serious problem - resolve or explain</td>
</tr>
<tr>
<td>B</td>
<td>A potentially serious problem, consider carefully</td>
</tr>
<tr>
<td>C</td>
<td>Check. Ensure it is not caused by an omission or oversight</td>
</tr>
<tr>
<td>G</td>
<td>General information/check it is not something unexpected</td>
</tr>
</tbody>
</table>

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
15 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 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.
Datablock betapic - ellipsoid plot

Prob = 50
Temp = 295
Complex 2- checkcif

Datablock: Cuibufgmapic

Bond precision: C-C = 0.0047 Å  Wavelength=0.7107 Å

Cell: 
\[a=10.2706(2) \quad b=11.8221(3) \quad c=17.2366(3)\]  
\[\alpha=104.3850(14) \quad \beta=95.6170(14) \quad \gamma=109.5680(13)\]

Temperature: 295 K

<table>
<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>1872.20(7)</td>
</tr>
<tr>
<td>Space group</td>
<td>P -1</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 1</td>
</tr>
</tbody>
</table>

Moiety formula: C38 H50 Cu N2 O5, O  C38 H50 Cu N2 O5, H2 O

Sum formula: C38 H50 Cu N2 O6  C38 H52 Cu N2 O6

Mr: 694.35  696.35

Dx, g cm\(^{-3}\): 1.232  1.235

Z: 2  2

Mu (mm\(^{-1}\)): 0.628  0.629

F000: 738.0  742.0

F000': 738.92

h,k,lmax: 13,15,22  13,15,22

Nref: 9057  8977

Tmin, Tmax: 0.773, 0.865  0.646, 0.892

Tmin': 0.773

Correction method= # Reported T Limits: Tmin=0.646  Tmax=0.892  AbsCorr = MULTI-SCAN

Data completeness= 0.991  Theta(max)= 27.998

R(reflections)= 0.0490( 7084)  wR2(reflections)= 0.1452( 8977)

S = 1.042  Npar= 432

---

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**

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......  O2W Check

PLAT430_ALERT_2_B Short Inter D...A Contact  O2W .. O4 .. 2.70 Ang.

**Alert level C**

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ  Please Check

PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..  2.00 Check

PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...  Please Check

PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range  5.0 Ratio

PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range  5.7 Ratio

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O4 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C23 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C36 Check

PLAT314_ALERT_2_C Check Small Angle for H2O: Metal-O1W -H2W  94.81 Degree

PLAT413_ALERT_2_C Short Inter XH3 .. XHn H24A .. H24A .. 2.09 Ang.

**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:C38 H52 Cu1 N2 O6
Atom count from the _atom_site data: C38 H50 Cu1 N2 O6

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected. CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?

From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_sum C38 H52 Cu1 N2 O6

TEST: Compare cell contents of formula and atom_site data

<table>
<thead>
<tr>
<th>atom</th>
<th>Z*formula</th>
<th>cif sites</th>
<th>diff</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>76.00</td>
<td>76.00</td>
<td>0.00</td>
</tr>
<tr>
<td>H</td>
<td>104.00</td>
<td>100.00</td>
<td>4.00</td>
</tr>
<tr>
<td>Cu</td>
<td>2.00</td>
<td>2.00</td>
<td>0.00</td>
</tr>
<tr>
<td>N</td>
<td>4.00</td>
<td>4.00</td>
<td>0.00</td>
</tr>
<tr>
<td>O</td>
<td>12.00</td>
<td>12.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 3 Note
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 = 3 Note
PLAT793_ALERT_4_G The Model has Chirality at C14 (Centro SPGR) S Verify
PLAT793_ALERT_4_G The Model has Chirality at C27 (Centro SPGR) R Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (II) ...... 2.03 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ................. 2 Note
PLAT933_ALERT_2_G Number of OMIT records in Embedded RES ............ 5 Note

0 ALERT level A = Most likely a serious problem - resolve or explain
2 ALERT level B = A potentially serious problem, consider carefully
10 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

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
11 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 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.
**Complex 3- checkcif**

**Datablock: pyrrolidine**

Bond precision:  C-C = 0.0056 Å  Wavelength=0.71073 Å

Cell:  
  \[ a=16.5388(4) \hspace{1cm} b=6.1918(1) \hspace{1cm} c=17.4653(4) \]  
  \[ \alpha=90 \hspace{1cm} \beta=94.8030(14) \hspace{1cm} \gamma=90 \]  

Temperature: 295 K

<table>
<thead>
<tr>
<th></th>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>1782.25(7)</td>
<td>1782.25(7)</td>
</tr>
<tr>
<td>Space group</td>
<td>P 21/c</td>
<td>P 21/c</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 2ybC</td>
<td>-P 2ybC</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C34 H52 Cu N2 O4, 2(H2 O)</td>
<td>C34 H52 Cu N2 O4, 2(H2 O)</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C34 H56 Cu N2 O6</td>
<td>C34 H56 Cu N2 O6</td>
</tr>
<tr>
<td>Mr</td>
<td>652.36</td>
<td>652.34</td>
</tr>
<tr>
<td>Dx, g cm⁻³</td>
<td>1.216</td>
<td>1.216</td>
</tr>
<tr>
<td>Z</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>Mu (mm⁻¹)</td>
<td>0.655</td>
<td>0.655</td>
</tr>
<tr>
<td>F000</td>
<td>702.0</td>
<td>702.0</td>
</tr>
<tr>
<td>F000'</td>
<td>702.90</td>
<td></td>
</tr>
<tr>
<td>h,k,lmax</td>
<td>21,8,23</td>
<td>21,8,23</td>
</tr>
<tr>
<td>Nref</td>
<td>4303</td>
<td>4282</td>
</tr>
<tr>
<td>Tmin,Tmax</td>
<td>0.855,0.943</td>
<td>0.848,0.945</td>
</tr>
<tr>
<td>Tmin'</td>
<td>0.735</td>
<td></td>
</tr>
</tbody>
</table>

Correction method= # Reported T Limits: Tmin=0.848  
Tmax=0.945 AbsCorr = MULTI-SCAN

Data completeness= 0.995  
Theta(max)= 28.000

R(reflections)= 0.0548(3371)  
wR2(reflections)= 0.1572(4282)

S = 1.064  
Npar= 235

The following ALERTS were generated. Each ALERT has the format

\[ \text{test-name\_ALERT\_alert\_type\_alert-level} \]

Click on the hyperlinks for more details of the test.

### Alert level B

**PLAT230_ALERT_2_B** Hirshfeld Test Diff for  C8 -- C9 .. 8.0 s.u.

### Alert level C

**PLAT213_ALERT_2_C** Atom C16A  has ADP max/min Ratio ...... 3.4 prolat

**PLAT222_ALERT_3_C** Non-Solvent Resid 1  H Uiso(max)/Uiso(min) Range  4.3 Ratio

**PLAT234_ALERT_4_C** Large Hirshfeld Difference C15 -- C17 .. 0.21 Ang.

**PLAT241_ALERT_2_C** 'MainMol' Ueq as Compared to Neighbors of C3 Check

**PLAT242_ALERT_2_C** Low 'MainMol' Ueq as Compared to Neighbors of C5 Check

And 2 other PLAT242 Alerts

More ...

**PLAT250_ALERT_2_C** Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.6 Note

**PLAT334_ALERT_2_C** Small Average Benzene C-C Dist. C8 -- C13  1.37 Ang.

**PLAT360_ALERT_2_C** Short (sp3)-(sp3) Bond C6 -- C7 .. 1.38 Ang.

### Alert level G

**PLAT002_ALERT_2_G** Number of Distance or Angle Restraints on AtSite  11 Note

**PLAT066_ALERT_1_G** Predicted and Reported Tmin&Tmax Range Identical  ? Check

**PLAT172_ALERT_4_G** The CIF-Embedded .res File Contains DFIX Records  3 Report
The CIF-Embedded .res File Contains SADI Records

Atom Site Occupancy of >C15 is Constrained at 0.6 Check

And 23 other PLAT300 Alerts

More ...

Main Residue Disorder Percentage = 15 Note

Centre of Gravity not Within Unit Cell: Resd. # 2 Note

The Model has Chirality at C6 (Centro SPGR) S Verify

Number of Least-Squares Restraints .......... 5 Note

Number of OMIT records in Embedded RES ........ 4 Note

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

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.
**Datablock pyrrolidine - ellipsoid plot**
## Complex 4- checkcif

### Datablock: ibu7

<table>
<thead>
<tr>
<th>Bond precision:</th>
<th>C-C = 0.0081 Å</th>
<th>Wavelength=0.71073</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Cell:</strong></td>
<td>a=9.6804(8)</td>
<td>b=6.7371(4)</td>
</tr>
<tr>
<td></td>
<td>alpha=90</td>
<td>beta=92.188(3)</td>
</tr>
<tr>
<td><strong>Temperature:</strong></td>
<td>295 K</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>1919.5(3)</td>
</tr>
<tr>
<td>Space group</td>
<td>P 2/c</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 2yc</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>2(C13 H17 O2), C8 H26 Cu N4 O</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C34 H60 Cu N4 O5</td>
</tr>
<tr>
<td>Mr</td>
<td>668.41</td>
</tr>
<tr>
<td>Dx, g cm⁻³</td>
<td>1.156</td>
</tr>
<tr>
<td>Z</td>
<td>2</td>
</tr>
<tr>
<td>Mu (mm⁻¹)</td>
<td>0.609</td>
</tr>
<tr>
<td>F₀₀₀</td>
<td>722.0</td>
</tr>
<tr>
<td>F₀₀₀'</td>
<td>722.89</td>
</tr>
<tr>
<td>h, k, lmax</td>
<td>11,8,34</td>
</tr>
<tr>
<td>Nref</td>
<td>3372</td>
</tr>
<tr>
<td>Tmin, Tmax</td>
<td>0.903, 0.941</td>
</tr>
<tr>
<td>Tmin'</td>
<td>0.808</td>
</tr>
</tbody>
</table>

Correction method= # Reported T Limits: Tmin=0.621
Tmax=0.947 AbsCorr = MULTI-SCAN

Data completeness= 0.822   Theta(max)= 24.992
R(reflections)= 0.0640( 2162)   wR2(reflections)= 0.1489( 2773)
S = 1.058   Npar= 230

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 value Low_.  0.822 Note

### Alert level B

**PLAT241_ALERT_2_B** High 'MainMol' Ueq as Compared to Neighbors of C17 Check

### Alert level C

**PLAT220_ALERT_2_C** Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 4.9 Ratio
**PLAT222_ALERT_3_C** Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 6.1 Ratio
**PLAT234_ALERT_4_C** Large Hirshfeld Difference C14 -- C15A ... 0.16 Ang.
**PLAT241_ALERT_2_C** High 'MainMol' Ueq as Compared to Neighbors of C10 Check
**PLAT241_ALERT_2_C** High 'MainMol' Ueq as Compared to Neighbors of C14 Check
**PLAT242_ALERT_2_C** Low 'MainMol' Ueq as Compared to Neighbors of C5 Check

**And 2 other PLAT242 Alerts**

More...
**PLAT341_ALERT_3_C** Low Bond Precision on C-C Bonds ......... 0.00809 Ang.
**PLATT1_ALERT_1_C** BOND Unknown or Inconsistent Label ....... O1
**CU1** O1
**PLAT712_ALERT_1_C** ANGLE Unknown or Inconsistent Label ....... O1
**Alert level G**

- PLAT02_ALERT_2_G Number of Distance or Angle Restraints on AtSite
- PLAT03_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms
- PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records
- PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records
- PLAT300_ALERT_4_G Atom Site Occupancy of >C15A is Constrained at 0.6

**And 15 other PLAT300 Alerts**

More ...

- PLAT301_ALERT_3_G Main Residue Disorder Percentage =
- PLAT773_ALERT_2_G Check long C-C Bond in CIF: C15 -- C16 . 1.72 Ang.
- PLAT793_ALERT_4_G The Model has Chirality at C6 (Centro SPGR)
- PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (II) ..... 2.12
- PLAT860_ALERT_3_G Number of Least-Squares Restraints
- PLAT933_ALERT_2_G Number of OMIT records in Embedded RES

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

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.

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.