

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_hku_mcp_tph_0m

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: cu_hku_mcp_tph_0m

Bond precision: C-C = 0.0055 Å Wavelength=1.54178

Cell: a=19.8177(5) b=20.7758(5) c=26.2065(6)
 alpha=94.329(2) beta=102.462(2) gamma=116.553(1)
Temperature: 223 K

| | Calculated | Reported |
|------------------------|----------------------------|----------------|
| Volume | 9240.0(4) | 9240.0(4) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C92 H88 Cl4 N4 [+ solvent] | C92 H88 Cl4 N4 |
| Sum formula | C92 H88 Cl4 N4 [+ solvent] | C92 H88 Cl4 N4 |
| Mr | 1391.47 | 1391.46 |
| Dx, g cm ⁻³ | 1.000 | 1.000 |
| Z | 4 | 4 |
| Mu (mm ⁻¹) | 1.471 | 1.471 |
| F000 | 2944.0 | 2944.0 |
| F000' | 2956.63 | |
| h,k,lmax | 23,25,31 | 23,25,31 |
| Nref | 34056 | 33887 |
| Tmin,Tmax | 0.826,0.851 | 0.656,0.753 |
| Tmin' | 0.826 | |

Correction method= # Reported T Limits: Tmin=0.656 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 68.560

| | |
|--------------------------------|----------------------------------|
| R(reflections)= 0.0664(22236) | wR2(reflections)= 0.2174(33887) |
| S = 1.026 | Npar= 1928 |

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

| | | | | | |
|-------------------|----------------|-------------------------------------|--|---------|-----------|
| PLAT213_ALERT_2_C | Atom C1B | has ADP max/min Ratio | | 3.2 | oblate |
| PLAT220_ALERT_2_C | NonSolvent | Resd 1 | C Ueq(max)/Ueq(min) Range | 4.3 | Ratio |
| PLAT220_ALERT_2_C | NonSolvent | Resd 2 | C Ueq(max)/Ueq(min) Range | 4.2 | Ratio |
| PLAT222_ALERT_3_C | NonSolvent | Resd 1 | H Uiso(max)/Uiso(min) Range | 5.4 | Ratio |
| PLAT222_ALERT_3_C | NonSolvent | Resd 2 | H Uiso(max)/Uiso(min) Range | 5.0 | Ratio |
| PLAT230_ALERT_2_C | Hirshfeld Test | Diff for | C37 --C40 | . | 5.2 s.u. |
| PLAT234_ALERT_4_C | Large | Hirshfeld Difference | C27 --C28A | . | 0.20 Ang. |
| PLAT234_ALERT_4_C | Large | Hirshfeld Difference | C27 --C30A | . | 0.18 Ang. |
| PLAT234_ALERT_4_C | Large | Hirshfeld Difference | C69 --C71 | . | 0.16 Ang. |
| PLAT234_ALERT_4_C | Large | Hirshfeld Difference | C69 --C72 | . | 0.16 Ang. |
| PLAT234_ALERT_4_C | Large | Hirshfeld Difference | C69 --C70A | . | 0.17 Ang. |
| PLAT234_ALERT_4_C | Large | Hirshfeld Difference | C69 --C71A | . | 0.16 Ang. |
| PLAT234_ALERT_4_C | Large | Hirshfeld Difference | C69 --C72A | . | 0.18 Ang. |
| PLAT234_ALERT_4_C | Large | Hirshfeld Difference | C170 --C1A | . | 0.23 Ang. |
| PLAT234_ALERT_4_C | Large | Hirshfeld Difference | C170 --C1B | . | 0.19 Ang. |
| PLAT242_ALERT_2_C | Low | 'MainMol' | Ueq as Compared to Neighbors of | C17 | Check |
| PLAT242_ALERT_2_C | Low | 'MainMol' | Ueq as Compared to Neighbors of | C27 | Check |
| PLAT242_ALERT_2_C | Low | 'MainMol' | Ueq as Compared to Neighbors of | C37 | Check |
| PLAT242_ALERT_2_C | Low | 'MainMol' | Ueq as Compared to Neighbors of | C53 | Check |
| PLAT242_ALERT_2_C | Low | 'MainMol' | Ueq as Compared to Neighbors of | C69 | Check |
| PLAT242_ALERT_2_C | Low | 'MainMol' | Ueq as Compared to Neighbors of | C89 | Check |
| PLAT242_ALERT_2_C | Low | 'MainMol' | Ueq as Compared to Neighbors of | C113 | Check |
| PLAT242_ALERT_2_C | Low | 'MainMol' | Ueq as Compared to Neighbors of | C123 | Check |
| PLAT242_ALERT_2_C | Low | 'MainMol' | Ueq as Compared to Neighbors of | C139 | Check |
| PLAT242_ALERT_2_C | Low | 'MainMol' | Ueq as Compared to Neighbors of | C170 | Check |
| PLAT242_ALERT_2_C | Low | 'MainMol' | Ueq as Compared to Neighbors of | C182 | Check |
| PLAT340_ALERT_3_C | Low | Bond Precision on | C-C Bonds | 0.00545 | Ang. |
| PLAT906_ALERT_3_C | Large | K Value in the Analysis of Variance | | 3.590 | Check |
| PLAT911_ALERT_3_C | Missing | FCF Refl Between Thmin & STh/L= | 0.600 | 63 | Report |
| | 4 | -4 | 1, -1 0 1, -9 24 1, 1 -2 2, -1 1 2, -10 10 2, | | |
| | 1 | -3 | 3, 0 -1 3, 1 -1 3, 1 0 3, -7 6 3, -4 7 3, | | |
| | -8 | 24 | 3, 1 0 4, 4 4 4, 2 -1 5, 2 1 5, 2 2 5, | | |
| | -2 | -11 | 6, 0 -4 6, 2 -1 6, 3 -1 6, 2 0 6, 2 2 6, | | |
| | 3 | -2 | 7, -4 -1 7, -3 -1 7, 2 -1 7, 4 0 7, -1 -4 8, | | |
| | -2 | -2 | 8, 1 -1 8, 3 -2 9, 4 -6 10, -1 0 10, 11 -4 12, | | |
| | 6 | -20 | 13, 17-19 13, 11 -4 13, 16-19 14, 10-16 14, 12-14 15, | | |
| | -8 | 17 | 15, 9-20 16, -8 17 16, 4 10 17, 13-19 18, 9 -7 19, | | |
| | 2 | -9 | 20, 7 -5 20, -2 -3 23, 10 -2 23, 10 -1 23, 3 2 23, | | |
| | 9 | -1 | 24, 8 -1 25, -15 2 25, -14 5 26, -13 -3 28, -12 -3 28, | | |
| | -11 | -3 | 28, -12 -1 28, -14 1 28, | | |
| PLAT918_ALERT_3_C | Reflection(s) | with I(obs) much Smaller I(calc) | . | 1 | Check |

Alert level G

| | | | |
|-------------------|--|------|--------|
| PLAT002_ALERT_2_G | Number of Distance or Angle Restraints on AtSite | 21 | Note |
| PLAT003_ALERT_2_G | Number of Uiso or U(i,j) Restrained non-H Atoms | 18 | Report |
| PLAT072_ALERT_2_G | SHELXL First Parameter in WGHT Unusually Large | 0.12 | Report |
| PLAT176_ALERT_4_G | The CIF-Embedded .res File Contains SADI Records | 9 | Report |
| PLAT178_ALERT_4_G | The CIF-Embedded .res File Contains SIMU Records | 3 | Report |
| PLAT187_ALERT_4_G | The CIF-Embedded .res File Contains RIGU Records | 6 | Report |

| | | | |
|-------------------|--|--------|--------|
| PLAT188_ALERT_3_G | A Non-default SIMU Restraint Value has been used | 0.0100 | Report |
| PLAT188_ALERT_3_G | A Non-default SIMU Restraint Value has been used | 0.0100 | Report |
| PLAT188_ALERT_3_G | A Non-default SIMU Restraint Value has been used | 0.0100 | Report |
| PLAT190_ALERT_3_G | A Non-default RIGU Restraint Value for First Par | 0.0100 | Report |
| PLAT190_ALERT_3_G | A Non-default RIGU Restraint Value for SecondPar | 0.0200 | Report |
| PLAT190_ALERT_3_G | A Non-default RIGU Restraint Value for First Par | 0.0100 | Report |
| PLAT190_ALERT_3_G | A Non-default RIGU Restraint Value for SecondPar | 0.0200 | Report |
| PLAT190_ALERT_3_G | A Non-default RIGU Restraint Value for First Par | 0.0100 | Report |
| PLAT190_ALERT_3_G | A Non-default RIGU Restraint Value for SecondPar | 0.0200 | Report |
| PLAT190_ALERT_3_G | A Non-default RIGU Restraint Value for First Par | 0.0100 | Report |
| PLAT190_ALERT_3_G | A Non-default RIGU Restraint Value for SecondPar | 0.0200 | Report |
| PLAT190_ALERT_3_G | A Non-default RIGU Restraint Value for First Par | 0.0100 | Report |
| PLAT190_ALERT_3_G | A Non-default RIGU Restraint Value for SecondPar | 0.0200 | Report |
| PLAT301_ALERT_3_G | Main Residue Disorder(Resd 1) | 6% | Note |
| PLAT301_ALERT_3_G | Main Residue Disorder(Resd 2) | 3% | Note |
| PLAT333_ALERT_2_G | Large Aver C6-Ring C-C Dist C75 -C84 . | 1.42 | Ang. |
| PLAT412_ALERT_2_G | Short Intra XH3 .. XHn H23 ..H29F . | 1.86 | Ang. |
| | x,y,z = | 1_555 | Check |
| PLAT412_ALERT_2_G | Short Intra XH3 .. XHn H25 ..H30D . | 2.14 | Ang. |
| | x,y,z = | 1_555 | Check |
| PLAT412_ALERT_2_G | Short Intra XH3 .. XHn H16L ..H164 . | 2.05 | Ang. |
| | x,y,z = | 1_555 | Check |
| PLAT412_ALERT_2_G | Short Intra XH3 .. XHn H164 ..H18J . | 1.71 | Ang. |
| | x,y,z = | 1_555 | Check |
| PLAT434_ALERT_2_G | Short Inter HL..HL Contact Cl3 ..Cl8 . | 3.38 | Ang. |
| | x,y,z = | 1_555 | Check |
| PLAT606_ALERT_4_G | Solvent Accessible VOID(S) in Structure | ! | Info |
| PLAT720_ALERT_4_G | Number of Unusual/Non-Standard Labels | 6 | Note |
| | H1AA H1AB H1AC H1BA H1BB H1BC | | |
| PLAT721_ALERT_1_G | Bond Calc 0.96000, Rep 0.97000 Dev... | 0.01 | Ang. |
| | C71A -H71D 1_555 1_555 | # 414 | Check |
| PLAT721_ALERT_1_G | Bond Calc 0.96000, Rep 0.97000 Dev... | 0.01 | Ang. |
| | C70A -H70D 1_555 1_555 | # 420 | Check |
| PLAT721_ALERT_1_G | Bond Calc 0.96000, Rep 0.97000 Dev... | 0.01 | Ang. |
| | C30A -H30D 1_555 1_555 | # 426 | Check |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints | 219 | Note |
| PLAT868_ALERT_4_G | ALERTS Due to the Use of _smtbx_masks Suppressed | ! | Info |
| PLAT910_ALERT_3_G | Missing # of FCF Reflection(s) Below Theta(Min). | 1 | Note |
| | 0 0 1, | | |
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L= 0.600 | 105 | Note |
| PLAT913_ALERT_3_G | Missing # of Very Strong Reflections in FCF | 1 | Note |
| | -1 0 1, | | |
| PLAT933_ALERT_2_G | Number of HKL-OMIT Records in Embedded .res File | 16 | Note |
| | -1 -4 8, 1 -3 3, -7 6 3, -2 -2 8, -4 -1 7, 0 -1 3, | | |
| | 2 2 5, 1 -1 3, -1 0 10, 4 4 4, 4 -6 10, 1 -2 2, | | |
| | -3 -1 7, 1 -1 8, 0 -4 6, -4 7 3, | | |
| PLAT941_ALERT_3_G | Average HKL Measurement Multiplicity | 3.5 | Low |
| PLAT969_ALERT_5_G | The 'Henn et al.' R-Factor-gap value | 3.870 | Note |
| | Predicted wR2: Based on SigI**2 5.62 or SHELX Weight 21.18 | | |
| PLAT978_ALERT_2_G | Number C-C Bonds with Positive Residual Density. | 1 | Info |

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 30 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

43 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
26 ALERT type 2 Indicator that the structure model may be wrong or deficient
27 ALERT type 3 Indicator that the structure quality may be low
16 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.

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