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: alectinib_hydrochloride

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Bond precision:    C-C = 0.0088 A              Wavelength=1.54449

Cell:              a=20.3941(2)      b=10.4451(3)           c=12.6842(3)
                   alpha=90          beta=93.113(8)         gamma=90
Temperature:       298 K

                   Calculated                  Reported
Volume             2697.98(11)                 2698.00(10)
Space group        P 21/n                      P 1 21/n 1
Hall group         -P 2yn                      -P 2yn
Moiety formula     C30 H35 N4 O2, Cl           C30 H35 N4 O2, Cl
Sum formula        C30 H35 Cl N4 O2            C30 H35 Cl N4 O2
Mr                 519.07                      519.06
Dx,g cm-3          1.278                       1.278
Z                  4                           4
Mu (mm-1)          1.521                       0.000
F000               1104.0                      276.0
F000'              1108.34
h,k,lmax
Nref
Tmin,Tmax
Tmin'

Correction method= Not given

Data completeness=                 Theta(max)=

R(reflections)=                                   wR2(reflections)=
S =                          Npar=
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The following ALERTS were generated. Each ALERT has the format
        test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

🔴 **Alert level B**
PLAT362_ALERT_2_B Short C(sp3)-C(sp2) Bond C15   - C16   .   1.31 Ang.

🟡 **Alert level C**
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.00883 Ang.
PLAT351_ALERT_3_C Long   C-H (X0.96,N1.08A) C22   - H16A   .   1.11 Ang.
PLAT351_ALERT_3_C Long   C-H (X0.96,N1.08A) C24   - H4   .   1.11 Ang.
PLAT351_ALERT_3_C Long   C-H (X0.96,N1.08A) C26   - H20B   .   1.12 Ang.
PLAT351_ALERT_3_C Long   C-H (X0.96,N1.08A) C27   - H40A   .   1.11 Ang.
PLAT351_ALERT_3_C Long   C-H (X0.96,N1.08A) C28   - H80A   .   1.11 Ang.
PLAT351_ALERT_3_C Long   C-H (X0.96,N1.08A) C29   - H82B   .   1.11 Ang.
PLAT351_ALERT_3_C Long   C-H (X0.96,N1.08A) C30   - H42B   .   1.11 Ang.
PLAT353_ALERT_3_C Long   N-H (N0.87,N1.01A) N1   - H12   .   1.04 Ang.
PLAT360_ALERT_2_C Short   C(sp3)-C(sp3) Bond C15   - C21   .   1.37 Ang.
PLAT360_ALERT_2_C Short   C(sp3)-C(sp3) Bond C18   - C19   .   1.40 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond C25   - C26   .   1.65 Ang.
PLAT368_ALERT_2_C Short   C(sp2)-C(sp2) Bond C1   - C2   .   1.23 Ang.

⚪ **Alert level G**
RADNT01_ALERT_1_G Extra text has been found in the _diffrn_radiation_type field.
            Radiation given as Cu K\a~1~, K\a~2~
            Radiation identified as Cu K\a~1~
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   2 Report
             H8   H12
PLAT158_ALERT_4_G The Input Unitcell is NOT Standard/Reduced .....   Please Check
PLAT343_ALERT_2_G Unusual sp3   Angle Range in Main Residue for   C23 Check
PLAT343_ALERT_2_G Unusual sp3   Angle Range in Main Residue for   C24 Check
PLAT343_ALERT_2_G Unusual sp3   Angle Range in Main Residue for   C26 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   105 Note

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

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 ALERT type 2 Indicator that the structure model may be wrong or deficient
  10 ALERT type 3 Indicator that the structure quality may be low
   1 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 14/11/2023; check.def file version of 14/09/2023