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: d520-sr_sq

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Bond precision:   C-C = 0.0084 A           Wavelength=0.71073

Cell:          a=13.3496(7)     b=13.6078(5)         c=15.8972(6)
               alpha=90         beta=106.944(5)      gamma=90
Temperature:   294 K

                   Calculated              Reported
Volume         2762.5(2)               2762.5(2)
Space group    P 21/n                  P 1 21/n 1
Hall group     -P 2yn                  -P 2yn
                C42 H36 Cl2 Co3 N6 O18 [+
Moiety formula                          C42 H36 Cl2 Co3 N6 O18
                solvent]
                C42 H36 Cl2 Co3 N6 O18 [+
Sum formula                             C42 H36 Cl2 Co3 N6 O18
                solvent]
Mr             1160.46                 1160.46
Dx,g cm-3      1.395                   1.395
Z              2                       2
Mu (mm-1)      1.057                   1.057
F000           1178.0                  1178.0
F000'          1181.22
h,k,lmax       16,16,19                16,16,19
Nref           5442                    5416
Tmin,Tmax      0.806,0.862             0.952,1.000
Tmin'          0.801

Correction method= # Reported T Limits: Tmin=0.952 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.995          Theta(max)= 26.019

R(reflections)= 0.0642( 2957)     wR2(reflections)= 0.1620( 5416)

S = 0.992                   Npar= 363
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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 C

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PLAT220_ALERT_2_C Non-Solvent Resd 1  O   Ueq(max)/Ueq(min) Range        4.3 Ratio
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C19 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............   0.00839 Ang.
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⚪ Alert level G

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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 ...       8 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records       2 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records       2 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
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1        Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1'       Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O5         Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O5'        Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O6         Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O6'        Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N3         Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N3'        Constrained at     0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )     11% Note
PLAT343_ALERT_2_G Unusual sp?       Angle Range in Main Residue for      C3 Check
PLAT343_ALERT_2_G Unusual sp?       Angle Range in Main Residue for     C11 Check
PLAT343_ALERT_2_G Unusual sp?       Angle Range in Main Residue for     C13 Check
PLAT343_ALERT_2_G Unusual sp?       Angle Range in Main Residue for     C15 Check
PLAT343_ALERT_2_G Unusual sp?       Angle Range in Main Residue for     C16 Check
PLAT395_ALERT_2_G Deviating  X-O-Y    Angle From 120 for O2           114.0 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y    Angle From 120 for O3           110.5 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact  O5'      ..C15            2.85 Ang.
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure     209 A**3
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      42 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed         ! Info
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...       13 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  27 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  13 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
  14 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
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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 09/11/2017; check.def file version of 08/11/2017