checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Bi8TlAlCl43_170K

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: Bi8TlAlCl43_170K

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Bond precision:  Cl-Al = 0.0367 A        Wavelength=0.71073

Cell:           a=26.1108(11)    b=26.1108(11)    c=31.2199(13)
                alpha=90         beta=90          gamma=120
Temperature:    170 K

                Calculated                Reported
Volume          18433(2)                  18433.3(17)
Space group     P 65                      P 65
Hall group      P 65                      P 65
                Al3 Bi0.74 Cl12, Al3
Moiety formula  Bi0.80 Cl12, 3(Bi2.51     ?
                Tl4), 3(Al Bi0.46 Cl
Sum formula     Al36 Bi96 Cl144 Tl12      Al3 Bi8 Cl12 Tl
Mr              28590.71                  2382.55
Dx,g cm-3       5.151                     5.151
Z               2                         24
Mu (mm-1)       51.992                    51.992
F000            23712.0                   23712.0
F000'           23002.68
h,k,lmax        31,31,37                  31,31,37
Nref            21992[ 11217]             21762
Tmin,Tmax       0.011,0.049               0.097,0.250
Tmin'           0.004

Correction method= # Reported T Limits: Tmin=0.097 Tmax=0.250
AbsCorr = NUMERICAL

Data completeness= 1.94/0.99      Theta(max)= 25.141

R(reflections)= 0.0488( 6278)     wR2(reflections)= 0.0583( 21762)

S = 0.932                 Npar= 637
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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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RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
          Rint given   0.169
STRVA01_ALERT_4_C          Flack test results are ambiguous.
          From the CIF: _refine_ls_abs_structure_Flack    0.466
          From the CIF: _refine_ls_abs_structure_Flack_su    0.019
PLAT018_ALERT_1_C _diffrn_measured_fraction_theta_max .NE. *_full          ! Check
PLAT214_ALERT_2_C Atom B303      (Anion/Solvent) ADP max/min Ratio       4.4 prolat
PLAT214_ALERT_2_C Atom B203      (Anion/Solvent) ADP max/min Ratio       4.4 prolat
PLAT214_ALERT_2_C Atom Bi03      (Anion/Solvent) ADP max/min Ratio       4.4 prolat
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of      Cl21 Check
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        64 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         1 Info
PLAT017_ALERT_1_G Check Scattering Type Consistency of B117     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B118     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B119     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B120     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B121     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B122     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B123     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B124     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B201     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B202     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B203     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B204     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B205     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B206     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B207     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B208     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B217     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B218     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B219     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B220     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B221     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B222     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B223     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B224     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B301     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B302     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B303     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B304     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B305     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B306     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B307     as        BI
PLAT017_ALERT_1_G Check Scattering Type Consistency of B308     as        BI
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 .....      0.169 Report
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .   0.466 Note
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...    0.08 Check
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...       3 Units
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records       21 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records       32 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )       5% Note
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  2  )       5% Note
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PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )        39% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )         8% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 14  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 15  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 16  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 17  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 18  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 19  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 20  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 21  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 22  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 23  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 24  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 25  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 26  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 27  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 28  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 29  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 30  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 31  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 32  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 33  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 34  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 35  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 36  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 37  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 46  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 47  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 48  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 49  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 50  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 51  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 52  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 53  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 54  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 55  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 56  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 57  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 58  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 59  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 60  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 61  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 62  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 63  )       100% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........         59 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Tl1       (I)       .      0.80 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Tl2       (I)       .      0.68 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Tl3       (I)       .      0.76 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Tl4       (I)       .      0.80 Info
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....         ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       450 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...        20 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
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
94 **ALERT level G** = General information/check it is not something unexpected

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

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  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
 50 ALERT type 4 Improvement, methodology, query or suggestion
  6 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 18/02/2019; check.def file version of 18/02/2019

Datablock Bi8TlAlCl43_170K - ellipsoid plot