checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 0800

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: 0800

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Bond precision:  C-C = 0.0035 A          Wavelength=0.71073

Cell:            a=9.5760(14)     b=9.7100(17)     c=41.176(4)
                 alpha=90         beta=90          gamma=90
Temperature:     173 K
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	Calculated	Reported
Volume	3828.7(9)	3828.7(9)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C17 H22 N Si, C2 F3 O2	C17 H22 N Si, C2 F3 O2
Sum formula	C19 H22 F3 N O2 Si	C19 H22 F3 N O2 Si
Mr	381.47	381.47
Dx,g cm-3	1.324	1.324
Z	8	8
Mu (mm-1)	0.163	0.163
F000	1600.0	1600.0
F000’	1601.57	
h,k,lmax	11,11,48	11,11,48
Nref	6752[3851]	6661
Tmin,Tmax	0.962,0.968	0.938,0.968
Tmin’	0.937	

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Correction method= # Reported T Limits: Tmin=0.938 Tmax=0.968
AbsCorr = MULTI-SCAN

Data completeness= 1.73/0.99      Theta(max)= 25.000

R(reflections)= 0.0340( 4893)     wR2(reflections)= 0.0592( 6661)

S = 1.000                 Npar= 566
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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 A

PLAT214_ALERT_2_A Atom F2B (Anion/Solvent) ADP max/min Ratio 7.5 prolat
PLAT214_ALERT_2_A Atom F3B (Anion/Solvent) ADP max/min Ratio 7.8 prolat

Alert level B

PLAT230_ALERT_2_B Hirshfeld Test Diff for C15 -- C16 .. 9.5 s.u.
PLAT353_ALERT_3_B Long N-H (N0.87,N1.01A) N2 - H3N .. 1.08 Ang.
PLAT412_ALERT_2_B Short Intra XH3 .. XHn H35C .. H36A .. 1.77 Ang.

Alert level C

PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) ..... 6.76 Note
PLAT214_ALERT_2_C Atom F5B (Anion/Solvent) ADP max/min Ratio 4.2 prolat
PLAT221_ALERT_2_C Solv./Anion Resd 3 F Ueq(max)/Ueq(min) Range 5.6 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 8.3 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for Si2 -- C20 .. 5.1 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for Si2 -- C33 .. 5.8 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C29 -- C30 .. 6.5 s.u.
PLAT231_ALERT_4_C Hirshfeld Test (Solvent) O4 -- C37 .. 6.5 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference F4B -- C38 .. 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F5B -- C38 .. 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F6B -- C38 .. 0.16 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C16 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C18 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C37 Check
PLAT245_ALERT_2_C U(iso) H4N Smaller than U(eq) N2 by ... 0.018 AngSq
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 3.0 Note
PLAT353_ALERT_3_C Long N-H (N0.87,N1.01A) N1 - H1N .. 1.05 Ang.
PLAT353_ALERT_3_C Long N-H (N0.87,N1.01A) N1 - H2N .. 1.01 Ang.
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.595 24 Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C19 Check
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C38 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C35A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C35B is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H35A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H35B is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H35C is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H35D is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F1A is Constrained at 0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F2A is Constrained at 0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F3A is Constrained at 0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F1B is Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F2B is Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F3B is Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4A is Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F5A is Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F6A is Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4B is Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F5B is Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F6B is Constrained at 0.35 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1).. 5% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3).. 43% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4).. 43% Note
PLAT367_ALERT_2_G Long? C(sp?)-C(sp?) Bond C33 - C34 .. 1.54 Ang.

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PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.16 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        30 Check
              F2B  -C19  -F2A     1.555   1.555   1.555             35.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        36 Check
              F3B  -C19  -F3A     1.555   1.555   1.555             40.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        66 Check
              C35B -C34  -C35A    1.555   1.555   1.555             31.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        72 Check
              C35B -C36  -C35A    1.555   1.555   1.555             30.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        81 Check
              F4B  -C38  -F4A     1.555   1.555   1.555             22.90 Deg.
PLAT791_ALERT_4_G The Model has Chirality at C14     (Chiral SPGR)         S Verify
PLAT791_ALERT_4_G The Model has Chirality at C33     (Chiral SPGR)         S Verify
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        31% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         3 Note
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  2 ALERT level A = Most likely a serious problem - resolve or explain
  3 ALERT level B = A potentially serious problem, consider carefully
 20 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 36 ALERT level G = General information/check it is not something unexpected

  1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 14 ALERT type 2 Indicator that the structure model may be wrong or deficient
  9 ALERT type 3 Indicator that the structure quality may be low
 36 ALERT type 4 Improvement, methodology, query or suggestion
  1 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 13/08/2017; check.def file version of 27/07/2017

Datablock 0800 - ellipsoid plot