checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mdx1_a

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: mdx1_a

Bond precision: C-C = 0.0182 A Wavelength=0.71073

Cell: a=22.513(5) b=12.233(3) c=37.764(16)
alpha=90 beta=102.01(3) gamma=90
Temperature: 120 K

	Calculated	Reported
Volume	10173(6)	10173(6)
Space group	I 2/c	I 2 / c
Hall group	-I 2yc	?
Moiety formula	C34 H34 N10 V, 3(F6 P), 3(C2 H3 N)	?
Sum formula	C40 H43 F18 N13 P3 V	C40 H43 F18 N13 P3 V
Mr	1191.72	1191.72
Dx,g cm-3	1.556	1.556
Z	8	8
Mu (mm-1)	0.401	0.401
F000	4832.0	4832.0
F000’	4840.03	
h,k,lmax	30,16,50	30,16,50
Nref	12883	12717
Tmin,Tmax	0.930,0.984	0.861,1.147
Tmin’	0.880	

Correction method= # Reported T Limits: Tmin=0.861 Tmax=1.147
AbsCorr = MULTI-SCAN

Data completeness= 0.987 Theta(max)= 28.483

R(reflections)= 0.1357(4529) wR2(reflections)= 0.3895(12717)

S = 1.039 Npar= 780

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

RINTA01_ALERT_3_A The value of Rint is greater than 0.25
Rint given 0.277
PLAT020_ALERT_3_A The Value of Rint is Greater Than 0.12 ..... 0.277 Report
PLAT214_ALERT_2_A Atom F13A (Anion/Solvent) ADP max/min Ratio 6.2 prolat

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Alert level B

PLAT026_ALERT_3_B Ratio Observed / Unique Reflections (too) Low .. 36% Check
PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ..... 0.39 Report
PLAT214_ALERT_2_B Atom F14A (Anion/Solvent) ADP max/min Ratio 5.7 prolat
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.01822 Ang.

Alert level C

PLAT082_ALERT_2_C High R1 Value ..... 0.14 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.13 Report
PLAT234_ALERT_4_C Large Hirshfeld Difference C32 --C33 0.16 Ang.
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C201 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C101 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C301 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 3.8 Note
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of . 58 Ang**3
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 23.281 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 3.759 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.116 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 37 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check
PLAT921_ALERT_1_C R1 in the CIF and FCF Differ by ..... 0.0012 Check
PLAT922_ALERT_1_C wR2 in the CIF and FCF Differ by ..... 0.0014 Check
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

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Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 23 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 14 Report
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.11 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 152.04 Why ?
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 3 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 3 Report
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of P1 Check
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of P2 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 5) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 6) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 7) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 4 3.57 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 5 3.66 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 6 3.43 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd 7 3.34 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact F5 ..C22 2.96 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact F7 ..C28 2.88 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact F18 ..C202 2.74 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact N100 ..C302 3.04 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact N200 ..C302 2.61 Ang.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 4 Note

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              F6 P
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          6 Note
              F6 P
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         10 Note
              C2 H3 N
PLAT794_ALERT_5_G Tentative Bond Valency for V1        (III)     .       2.86 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         84 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        126 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          4 Note
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   3 ALERT level A = Most likely a serious problem - resolve or explain
   4 ALERT level B = A potentially serious problem, consider carefully
  16 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  29 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  17 ALERT type 2 Indicator that the structure model may be wrong or deficient
  12 ALERT type 3 Indicator that the structure quality may be low
  20 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 23/04/2018; check.def file version of 23/04/2018

Datablock mdx1_a - ellipsoid plot