checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3F-decomposition

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: 3F-decomposition

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Bond precision:  C-C = 0.0044 A          Wavelength=1.54178

Cell:            a=37.4781(16)     b=37.4781(16)     c=6.4871(3)
                 alpha=90          beta=90           gamma=120
Temperature:     180 K
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	Calculated	Reported
Volume	7891.1(9)	7891.1(8)
Space group	R -3	R -3
Hall group	-R 3	-R 3
Moiety formula	C42 H41.48 F0.52 N2 O6	C42 H41.48 F0.52 N2 O6
Sum formula	C42 H41.48 F0.52 N2 O6	C42 H41.48 F0.52 N2 O6
Mr	680.06	680.07
Dx,g cm-3	1.288	1.288
Z	9	9
Mu (mm-1)	0.711	0.711
F000	3241.2	3241.0
F000’	3251.10	
h,k,lmax	46,46,8	46,45,8
Nref	3562	3478
Tmin,Tmax	0.918,0.931	0.836,1.000
Tmin’	0.899	

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Correction method= # Reported T Limits: Tmin=0.836 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.976          Theta(max)= 74.018

R(reflections)= 0.0819( 2442)     wR2(reflections)= 0.2761( 3478)

S = 1.032                 Npar= 255
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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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PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..     Please Check
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..................       0.28 Report
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        4.7 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range        5.5 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C15      --C18             0.18 Ang.
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0044 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      5.057 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         5 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .         1 Check
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Alert level G

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CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
          From the CIF: _cell_formula_units_Z    9
          From the CIF: _chemical_formula_sum  C42 H41.48 F0.52 N2 O6
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        378.00    378.00    0.00
          H        373.32    373.36   -0.04
          F          4.68      4.64    0.04
          N         18.00     18.00    0.00
          O         54.00     54.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        16 Note
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.17 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       8.42 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records        10 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         3 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )       44% Note
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O1            107.9 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact  F3       ..C6             2.82 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  F3       ..C5             2.96 Ang.
PLAT793_ALERT_4_G Model has Chirality at C15         (Centro SPGR)        S Verify
PLAT793_ALERT_4_G Model has Chirality at C15'        (Centro SPGR)        R Verify
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....        ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       14 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).        1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        77 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        2 Info
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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
   9 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  19 ALERT level G = General information/check it is not something unexpected

   3 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
   9 ALERT type 3 Indicator that the structure quality may be low
   7 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 3F-decomposition - ellipsoid plot