checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 06F

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: 06F

Bond precision: C-C = 0.0088 A Wavelength=0.68882

Cell: a=7.44200 b=14.63500 c=19.31200
alpha=108.2700 beta=98.4900 gamma=93.6900
Temperature: 293 K

	Calculated	Reported
Volume	1961.668	1962
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C42 H34.46 F3.54 N2 O6, C42 H41.54 N2 O6, 3.246(F), 6(H)	C21 H20.23 F1.77 N O3, C21 H20.77 F1.62 N O3
Sum formula	C84 H82 F6.79 N4 O12	C42 H41 F3.37 N2 O6
Mr	1468.47	733.70
Dx,g cm-3	1.243	1.242
Z	1	2
Mu (mm-1)	0.086	0.088
F000	771.1	771.0
F000’	771.46	
h,k,lmax	8,16,22	7,16,22
Nref	6248	5738
Tmin,Tmax		
Tmin’		

Correction method= Not given

Data completeness= 0.918 Theta(max)= 23.320

R(reflections)= 0.1133(3582) wR2(reflections)= 0.3671(5738)

S = 1.367 Npar= 509

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 B

THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575
Calculated sin(theta_max)/wavelength = 0.5747
PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ..... 0.37 Report
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C35 Check
PLAT330_ALERT_2_B Large Average Phenyl C-C Dist C2AA -C21A 1.42 Ang.
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.575 378 Report

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Alert level C

PLAT018_ALERT_1_C _diffrn_measured_fraction_theta_max .NE. *_full ! Check
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT082_ALERT_2_C High R1 Value ..... 0.11 Report
PLAT141_ALERT_4_C s.u. on a - Axis Small or Missing ..... 0.00000 Ang.
PLAT142_ALERT_4_C s.u. on b - Axis Small or Missing ..... 0.00000 Ang.
PLAT143_ALERT_4_C s.u. on c - Axis Small or Missing ..... 0.00000 Ang.
PLAT144_ALERT_4_C s.u. on alpha Small or Missing ..... 0.0000 Degree
PLAT145_ALERT_4_C s.u. on beta Small or Missing ..... 0.0000 Degree
PLAT146_ALERT_4_C s.u. on gamma Small or Missing ..... 0.0000 Degree
PLAT151_ALERT_1_C No s.u. (esd) Given on Volume ..... Please Do !
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio
PLAT221_ALERT_2_C Solv./Anion Resd 2 C Ueq(max)/Ueq(min) Range 5.1 Ratio
PLAT223_ALERT_4_C Solv./Anion Resd 2 H Ueq(max)/Ueq(min) Range 6.1 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C34 --C37 . 5.4 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C13 --C32 . 5.1 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C14 --C20 . 7.0 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference C37 --C39A 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C32 --C36 0.19 Ang.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C13 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C36 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C38 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00883 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C4 - C26 . 1.54 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C1BA - C29 . 1.55 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C7 - C10 . 1.56 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C0BA - C27 . 1.54 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C10 - C20 . 1.54 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 10.792 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.260 Check
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 12 Note
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 2 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 1 Check

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Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: C42 H41 F3.37 N2 O6
Atom count from _chemical_formula_moiety:C42 H41 F3.39 N2 O6
FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C42 H41 F3.37 N2 O6
Atom count from the _atom_site data: C42 H41 F3.393 N2 O6
ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu

not performed for this radiation type.

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	12	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	7	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50	Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.20	Report
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.	Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	12	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	10	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	2	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	2	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1)	27%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	10%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
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
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 2	91.54	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 3	0.52	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 4	0.57	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 5	0.54	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 6	0.76	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 7	0.76	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 8	0.76	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 9	0.24	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 10	0.24	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 11	0.24	Check
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist. C1AA -C3AA_a	1.42	Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist. C2AA -C21	1.42	Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist. C9AA -C11_b	1.43	Ang.
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O0AA	107.9	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O3	107.6	Degree
PLAT432_ALERT_2_G	Short Inter X...Y Contact F24 ..C7AA	2.46	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact F25 ..C14	2.43	Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	15	Note
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C35 --C31A	1.73	Ang.
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # H	6	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # H	7	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # H	8	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # H	9	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # H	10	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # H	11	Note
PLAT793_ALERT_4_G	Model has Chirality at C32 (Centro SPGR)	R	Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	49	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	26	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	4	Info

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
5 **ALERT level B** = A potentially serious problem, consider carefully
33 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
50 **ALERT level G** = General information/check it is not something unexpected

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

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 30 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
 36 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 23/04/2018; check.def file version of 23/04/2018

Datablock 06F - ellipsoid plot