

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 14be55-p-1_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: 14be55-p-1_a

Bond precision: C-C = 0.0022 Å Wavelength=0.79990

Cell: a=7.9750 (16) b=11.781 (2) c=17.767 (4)
 alpha=75.65 (3) beta=82.14 (3) gamma=87.48 (3)
Temperature: 100 K

	Calculated	Reported
Volume	1601.9 (6)	1601.9 (6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C28 H22 F9 N9 O12	C28 H22 F9 N9 O12
Sum formula	C28 H22 F9 N9 O12	C28 H22 F9 N9 O12
Mr	847.55	847.54
Dx, g cm ⁻³	1.757	1.757
Z	2	2
Mu (mm ⁻¹)	0.227	0.232
F000	860.0	860.0
F000'	860.97	
h, k, lmax	9, 14, 22	9, 14, 22
Nref	6540	5885
Tmin, Tmax	0.986, 0.993	0.962, 0.993
Tmin'	0.961	

Correction method= # Reported T Limits: Tmin=0.962 Tmax=0.993
AbsCorr = MULTI-SCAN

Data completeness= 0.900 Theta(max)= 29.995

R(reflections)= 0.0426 (5436)	wR2(reflections)=
S = 1.063	0.1192 (5885)
Npar= 550	

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

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.919 Why?

Author Response: The data were collected on MX14-2 beamline (Bessy II, Berlin) and spindle axis rotation was the only available strategy resulting in slightly lowered completeness for triclinic and sometimes also monoclinic crystals.

Alert level B

PLAT430_ALERT_2_B Short Inter D...A Contact O18 ..O18 . 2.78 Ang.
1-x,-y,-z = 2_655 Check
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 473 Report

Alert level C

PLAT213_ALERT_2_C Atom F10 has ADP max/min Ratio 3.4 prolat
PLAT213_ALERT_2_C Atom F11 has ADP max/min Ratio 3.2 prolat
PLAT213_ALERT_2_C Atom F12 has ADP max/min Ratio 3.2 prolat

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 2 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.79990 Ang.
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.03 Degree
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 2 Report
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C3A Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C20A Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C34A Check
PLAT300_ALERT_4_G Atom Site Occupancy of F7 Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F8 Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F9 Constrained at 0.7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F10 Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F11 Constrained at 0.3 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F12 Constrained at 0.3 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 5% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact O22 ..C18 . 2.97 Ang.
-x,-y,-z = 2_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O22 ..C19 . 2.98 Ang.
-x,-y,-z = 2_555 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F1 ..F7 . 2.76 Ang.
1-x,1-y,1-z = 2_666 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F1 ..F12 . 2.80 Ang.

	1+x,1+y,z =	1_665	Check
PLAT767_ALERT_4_G	INS Embedded LIST 6 Instruction Should be LIST 4		Please Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	12	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT898_ALERT_4_G	Second Reported H-M Symbol in CIF Ignored		! Check
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	183	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.4	Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	7	Info
PLAT984_ALERT_1_G	The C-f' = 0.0033 Deviates from the B&C-Value	0.0043	Check
PLAT984_ALERT_1_G	The F-f' = 0.0186 Deviates from the B&C-Value	0.0225	Check
PLAT984_ALERT_1_G	The N-f' = 0.0063 Deviates from the B&C-Value	0.0082	Check
PLAT984_ALERT_1_G	The O-f' = 0.0113 Deviates from the B&C-Value	0.0142	Check

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

8 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
 5 ALERT type 3 Indicator that the structure quality may be low
 11 ALERT type 4 Improvement, methodology, query or suggestion
 1 ALERT type 5 Informative message, check

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.

