

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ot086_263_e

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: ot086_263_e

Bond precision: C-C = 0.0143 Å Wavelength=0.71073

Cell: a=21.474(4) b=26.428(5) c=14.176(3)
 alpha=90 beta=90 gamma=90
Temperature: 263 K

	Calculated	Reported
Volume	8045(3)	8045(3)
Space group	F d d 2	F d d 2
Hall group	F 2 -2d	F 2 -2d
Moiety formula	C34 H34 Cr N10, 2(B F4), 2(C2 H3 N)	?
Sum formula	C38 H40 B2 Cr F8 N12	C38 H40 B2 Cr F8 N12
Mr	890.44	890.44
Dx,g cm-3	1.470	1.470
Z	8	8
Mu (mm-1)	0.368	0.368
F000	3664.0	3664.0
F000'	3668.38	
h,k,lmax	28,35,18	28,35,18
Nref	4961[2579]	4596
Tmin,Tmax	0.846,0.895	0.893,1.172
Tmin'	0.838	

Correction method= # Reported T Limits: Tmin=0.893 Tmax=1.172
AbsCorr = MULTI-SCAN

Data completeness= 1.78/0.93 Theta(max)= 28.236

R(reflections)= 0.0455(3489) wR2(reflections)= 0.1394(4596)

S = 1.032 Npar= 357

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

PLAT111_ALERT_2_B	ADDSYM Detects New (Pseudo) Centre of Symmetry .	100	%Fit
PLAT112_ALERT_2_B	ADDSYM Detects New (Pseudo) Symm. Elem d	100	%Fit
PLAT113_ALERT_2_B	ADDSYM Suggests Possible Pseudo/New Space Group	Fddd	Check

Alert level C

STRVA01_ALERT_4_C	Flack test results are ambiguous.		
	From the CIF: <code>_refine_ls_abs_structure_Flack</code>	0.390	
	From the CIF: <code>_refine_ls_abs_structure_Flack_su</code>	0.070	
PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18)	7.18	Note
PLAT234_ALERT_4_C	Large Hirshfeld Difference C2 --C3	0.16	Ang.
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01433	Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	2	Report
PLAT915_ALERT_3_C	No Flack x Check Done: Low Friedel Pair Coverage	85	%

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	16	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	11	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	15.60	Why ?
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	2	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	2	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	2	Report
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	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	2.91	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 3	2.09	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 4	3.44	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 5	2.56	Check
PLAT721_ALERT_1_G	Bond Calc 0.97000, Rep 0.96000 Dev...	0.01	Ang.
	C12A -H12B 1.555 1.555 #	69	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Cr1 (III) .	2.82	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	122	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	14	Note
PLAT916_ALERT_2_G	Hooft y and Flack x Parameter Values Differ by .	0.10	Check
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	11	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	4	Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 9 ALERT type 2 Indicator that the structure model may be wrong or deficient
 6 ALERT type 3 Indicator that the structure quality may be low
 14 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.

