
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

PLAT307_ALERT_2_A Isolated Metal Atom found in Structure (Unusual) Co2A Check

Author Response: A 4% occupancy disorder for the three heavy Co atoms was applied based on residual peaks in the final difference map. No attached atoms could be located for this minor disorder component.

PLAT307_ALERT_2_A Isolated Metal Atom found in Structure (Unusual) Co3A Check

Author Response: A 4% occupancy disorder for the three heavy Co atoms was applied based on residual peaks in the final difference map. No attached atoms could be located for this minor disorder component.

PLAT307_ALERT_2_A Isolated Metal Atom found in Structure (Unusual) Co4A Check

Author Response: A 4% occupancy disorder for the three heavy Co atoms was applied based on residual peaks in the final difference map. No attached atoms could be located for this minor disorder component.

Alert level C

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT230_ALERT_2_C	Hirshfeld Test Diff for O10 --C25 .	7.0 s.u.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	6 Report

Alert level G

PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co1	--C19	.	7.4 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co1	--C20	.	11.8 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co1	--C21	.	9.8 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co2	--C21	.	6.4 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co2	--C22	.	18.2 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co2	--C24	.	9.0 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co2	--C25	.	17.2 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co3	--C19	.	8.0 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co3	--C23	.	17.6 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co3	--C24	.	9.4 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co3	--C29	.	14.2 s.u.
PLAT233_ALERT_4_G	Hirshfeld (M-X Solvent) Co4	--C26	.	17.4 s.u.
PLAT233_ALERT_4_G	Hirshfeld (M-X Solvent) Co4	--C27	.	15.2 s.u.
PLAT233_ALERT_4_G	Hirshfeld (M-X Solvent) Co4	--C28	.	16.8 s.u.
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)		5% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 2)		14% Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd 1)		56.04 Check

PLAT304_ALERT_4_G Non-Integer Number of Atoms in	(Resd 2)	6.96	Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C20	..C28 .	3.12	Ang.
	x,y,z =	1_555	Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd)	.	1.24	Ratio
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).		4	Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=	0.600	6	Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF		1	Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File		4	Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.		13	Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 18 ALERT type 2 Indicator that the structure model may be wrong or deficient
 4 ALERT type 3 Indicator that the structure quality may be low
 8 ALERT type 4 Improvement, methodology, query or suggestion
 0 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.

PLATON version of 18/05/2022; check.def file version of 17/05/2022

Datablock mo_b1959_0m - ellipsoid plot

