

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rl2102

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: rl2102

Bond precision:	C-C = 0.0149 Å	Wavelength=0.71073	
Cell:	a=17.6552(3)	b=17.0120(2)	c=17.4808(3)
	alpha=90	beta=90	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	5250.36(14)	5250.36(14)	
Space group	P n a 21	P n a 21	
Hall group	P 2c -2n	P 2c -2n	
Moiety formula	C24 B F20, C32 H55 Dy P	C32 H55 Dy P, B C24 F20	
Sum formula	C56 H55 B Dy F20 P	C56 H55 B Dy F20 P	
Mr	1312.28	1312.28	
Dx,g cm-3	1.660	1.660	
Z	4	4	
Mu (mm-1)	1.564	1.564	
F000	2628.0	2628.0	
F000'	2629.45		
h,k,lmax	23,22,23	23,21,22	
Nref	13553[6990]	13221	
Tmin,Tmax	0.829,0.925	0.633,0.725	
Tmin'	0.457		

Correction method= # Reported T Limits: Tmin=0.633 Tmax=0.725
AbsCorr = MULTI-SCAN

Data completeness= 1.89/0.98 Theta(max)= 28.697

R(reflections)= 0.0584(9603) wR2(reflections)= 0.1380(13221)

S = 1.026 Npar= 769

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

PLAT213_ALERT_2_C	Atom C47	has ADP max/min Ratio	3.2	oblate
PLAT214_ALERT_2_C	Atom DylA	(Anion/Solvent) ADP max/min Ratio	4.4	prolat
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds		0.0149	Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	8	Report



Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		85	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ			Please Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		33.82	Why ?
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records		1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records		2	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records		1	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Dyl --P1	.	6.1	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) DylA --P1	.	5.1	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) DylA --C4	.	6.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) DylA --C13	.	5.2	s.u.
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		18%	Note
PLAT328_ALERT_4_G	Possible Missing H on sp3? Phosphorus			P1 Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C1 - C5	.	1.51	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C2 - C7	.	1.50	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C3 - C9	.	1.52	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C4 - C11	.	1.50	Ang.
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F3 ..F17		2.74	Ang.
	3/2-x,1/2+y,-1/2+z =		4_654	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F7 ..F12		2.68	Ang.
	1-x,1-y,1/2+z =		2_665	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		900	Note
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..		!	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .			Please Do !
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	68	Note

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

2 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
4 ALERT type 3 Indicator that the structure quality may be low
7 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.

