



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.

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**Alert level C**

PLAT220_ALERT_2_C	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min) Range	3.5	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C25	--C26	.	0.16	Ang.
PLAT341_ALERT_3_C	Low Bond Precision on	C-C Bonds	.....		0.00991	Ang.

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**Alert level G**

PLAT012_ALERT_1_G	N.O.K.	_shelx_res_checksum	Found in CIF	.....		Please Check
PLAT013_ALERT_1_G	N.O.K.	_shelx_hkl_checksum	Found in CIF	.....		Please Check
PLAT014_ALERT_1_G	N.O.K.	_shelx_fab_checksum	Found in CIF	.....		Please Check
PLAT042_ALERT_1_G	Calc. and Reported	MoietyFormula	Strings	Differ		Please Check
PLAT045_ALERT_1_G	Calculated and Reported	Z	Differ by a Factor	...	2.00	Check
PLAT154_ALERT_1_G	The s.u.'s on the Cell	Angles are Equal	..(Note)		0.002	Degree
PLAT606_ALERT_4_G	Solvent Accessible	VOID(S) in Structure	.....		!	Info
PLAT791_ALERT_4_G	Model has Chirality at	C20	(Sohnke SpGr)		S	Verify
PLAT791_ALERT_4_G	Model has Chirality at	C59	(Sohnke SpGr)		R	Verify
PLAT794_ALERT_5_G	Tentative Bond Valency for	Co1	(II)	.	2.00	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for	Co2	(II)	.	2.04	Info
PLAT850_ALERT_4_G	Check Flack Parameter	Exact Value	0.00 with s.u.		0.00	Check
PLAT869_ALERT_4_G	ALERTS Related to the Use of	SQUEEZE	Suppressed		!	Info
PLAT933_ALERT_2_G	Number of OMIT Records in	Embedded .res File	...		3	Note
PLAT941_ALERT_3_G	Average HKL Measurement	Multiplicity	.....		3.1	Low

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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  
15 **ALERT level G** = General information/check it is not something unexpected

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
2 ALERT type 2 Indicator that the structure model may be wrong or deficient  
2 ALERT type 3 Indicator that the structure quality may be low  
6 ALERT type 4 Improvement, methodology, query or suggestion  
2 ALERT type 5 Informative message, check

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## Datablock: Co5

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Bond precision: C-C = 0.0088 A

Wavelength=0.71073

Cell: a=13.0704(7) b=19.0887(9) c=16.5809(7)  
alpha=90 beta=98.492(4) gamma=90

Temperature: 170 K

	Calculated	Reported
Volume	4091.5(3)	4091.5(3)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C45 H39 Cl2 Co N3 [+ solvent]	C45 H39 Cl2 Co N3
Sum formula	C45 H39 Cl2 Co N3 [+ solvent]	C45 H39 Cl2 Co N3
Mr	751.62	751.62
Dx,g cm-3	1.220	1.220
Z	4	4
Mu (mm-1)	0.583	0.583
F000	1564.0	1564.0
F000'	1567.01	
h,k,lmax	17,25,22	16,25,22
Nref	10623	9259
Tmin,Tmax	0.840,0.895	0.495,1.000
Tmin'	0.840	

Correction method= # Reported T Limits: Tmin=0.495 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.872                      Theta(max)= 28.745

R(reflections)= 0.0852( 5832)              wR2(reflections)= 0.2606( 9259)

S = 1.031                                      Npar= 464

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#### ● Alert level C

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) .....	0.26 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....	2.02 Report
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of	C24 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds .....	0.00881 Ang.

#### ● Alert level G

PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF .....	Please Check
PLAT013_ALERT_1_G N.O.K. _shelx_hkl_checksum Found in CIF .....	Please Check
PLAT014_ALERT_1_G N.O.K. _shelx_fab_checksum Found in CIF .....	Please Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large	0.13 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large	6.64 Why ?
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure	113 A**3
PLAT793_ALERT_4_G Model has Chirality at C20 (Centro SPGR)	R Verify
PLAT793_ALERT_4_G Model has Chirality at C38 (Centro SPGR)	R Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Co1 (II) .	2.05 Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed	! Info
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....	3.7 Low

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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.

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**PLATON version of 10/08/2020; check.def file version of 06/08/2020**



