

No syntax errors found.
Please wait while processing

[CIF dictionary](#)
[Interpreting this report](#)

Datablock: oc1h-dlr-cat-012-c

Bond precision:	C-C = 0.0054 Å	Wavelength=1.54184
Cell:	a=5.4707(1) b=10.9139(1) c=24.3668(3)	
	alpha=90 beta=95.601(1) gamma=90	
Temperature: 170 K		

	Calculated	Reported
Volume	1447.92(3)	1447.91(3)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C32 H22 Br2 I2 N2 O2	?
Sum formula	C32 H22 Br2 I2 N2 O2	C16 H11 Br I N O
Mr	880.12	440.07
Dx, g cm ⁻³	2.019	2.019
Z	2	4
Mu (mm ⁻¹)	20.560	20.560
F000	840.0	840.0
F000'	838.03	
h,k,lmax	6,12,28	6,12,28
Nref	2560	2560
Tmin,Tmax	0.095,0.274	0.186,0.589
Tmin'	0.015	

Correction method= # Reported T Limits: Tmin=0.186 Tmax=0.589
AbsCorr = GAUSSIAN
Data completeness= 1.000 Theta(max)= 66.482
R(reflections)= 0.0267(2434) wR2(reflections)= 0.0738(2560)
S = 1.048 Npar= 181

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

PLAT230_ALERT_2_B	Hirshfeld Test Diff for I1	--Br1	.	12.3 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for I1	--Br1_a	.	15.0 s.u.

Alert level C

PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..	1 Check
	-3 0 17,	

Alert level G

PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500 Check
PLAT142_ALERT_4_G	s.u. on b - Axis Small or Missing	0.00010 Ang.
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O1	107.9 Degree
PLAT899_ALERT_4_G	SHELXL2018 is Deprecated and Succeeded by SHELXL	2019/3 Note
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	94% Note
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	133.0 Degree
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	1.967 Note
	Predicted wR2: Based on SigI**2 3.75 or SHELX Weight	7.04
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2 Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 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
2 ALERT type 4 Improvement, methodology, query or suggestion
2 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

PLATON version of 13/05/2024; check.def file version of 04/05/2024

Datablock oc1h-dlr-cat-012-c - ellipsoid plot

