

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) quercetin_imidazole_ipa_1a1_secondocrystallo

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: quercetin_imidazole_ipa_1a1_secondocrystallo

Bond precision: C-C = 0.0034 Å

Wavelength=1.54184

Cell: a=10.9581(8) b=12.1229(10) c=13.0804(12)
 alpha=114.659(8) beta=93.308(7) gamma=113.045(7)
Temperature: 298 K

	Calculated	Reported
Volume	1401.5(3)	1401.5(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C15 H10 O7), C3 H4 N2	2(C15 H10 O7), C3 H4 N2
Sum formula	C33 H24 N2 O14	C33 H24 N2 O14
Mr	672.54	672.54
Dx, g cm ⁻³	1.594	1.594
Z	2	2
Mu (mm ⁻¹)	1.082	1.082
F000	696.0	696.0
F000'	698.60	
h,k,lmax	13,14,15	13,14,15
Nref	4990	4941
Tmin,Tmax	0.759,0.897	0.957,1.000
Tmin'	0.554	

Correction method= # Reported T Limits: Tmin=0.957 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.990

Theta(max)= 66.901

R(reflections)= 0.0503(3160)

wR2(reflections)=
0.1459(4941)

S = 1.011

Npar= 482

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

PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd	1)	2.6	Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd	2)	2.6	Note
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		6.521	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.597	49	Report
-12	1 0, -13 6 0, -13 7 0, -6 -8 1,	8 5 1,	6 7 1,	
5	8 1, 9-13 2, 11 0 2, -2 1 2,	3 9 2,	9-13 3,	
-12	0 3, 7 5 3, 6 6 3, 9-13 4,	7 4 4,	5 5 4,	
6	5 4, 5 6 4, 4 7 4, 6 4 5,	5 5 5,	4 6 5,	
3	7 5, 11-11 6, 4 5 6, -9 9 6,	-8 -7 7,	7 2 7,	
6	3 7, 5 4 7, 1 7 7, -5 9 7,	7 1 8,	6 2 8,	
5	3 8, 4 4 8, -11 2 9, 4 3 9,	0-13 10,	8 -5 11,	
-3	0 11, 3-13 12, -2-11 12, -3-10 13,	-4 2 13,	2 -9 15,	
2	-5 15,			



Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms		1	Report
H14A				
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		1	Note
H2IA				
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		2	Note
C15 H10 O7				
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still		42%	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		3.4	Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value		2.780	Note
Predicted wR2: Based on SigI**2	5.25 or SHELX Weight	14.43		
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		1	Info

- 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
7 **ALERT level G** = General information/check it is not something unexpected
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 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
2 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check
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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.

