No syntax errors found.
Please wait while processing ....

CIF dictionary
Interpreting this report

Datablock: Rh_curcumin

Bond precision: C-C = 0.0045 A Wavelength=1.54178
Cell: a=17.3703(3) b=23.7039(4) c=15.7300(3)
alpha=90 beta=90 gamma=90
Temperature: 103 K

	Calculated	Reported
Volume	6476.7(2)	6476.7(2)
Space group	P b c n	P b c n
Hall group	-P 2n 2ab	-P 2n 2ab
Moiety formula	C31 H34 Cl O6 Rh, 2(C H4 O)	C31 H34 Cl O6 Rh, 2(C H4 O)
Sum formula	C33 H42 Cl O8 Rh	C33 H42 Cl O8 Rh
Mr	705.03	705.02
Dx,g cm-3	1.446	1.446
Z	8	8
Mu (mm-1)	5.431	5.431
F000	2928.0	2928.0
F000'	2939.55	
h,k,lmax	20,28,18	20,28,18
Nref	5934	5928
Tmin,Tmax	0.177,0.337	0.893,0.931
Tmin'	0.053	

Correction method= # Reported T Limits: Tmin=0.893 Tmax=0.931
AbsCorr = NUMERICAL
Data completeness= 0.999 Theta(max)= 68.242
R(reflections)= 0.0426(5766) wR2(reflections)= 0.0930(5928)
S = 1.267 Npar= 397

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

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 4.873 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 4 Report

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 4 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 14.23 Why ?
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 2 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 5 Info

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

0 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
1 ALERT type 4 Improvement, methodology, query or suggestion
1 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

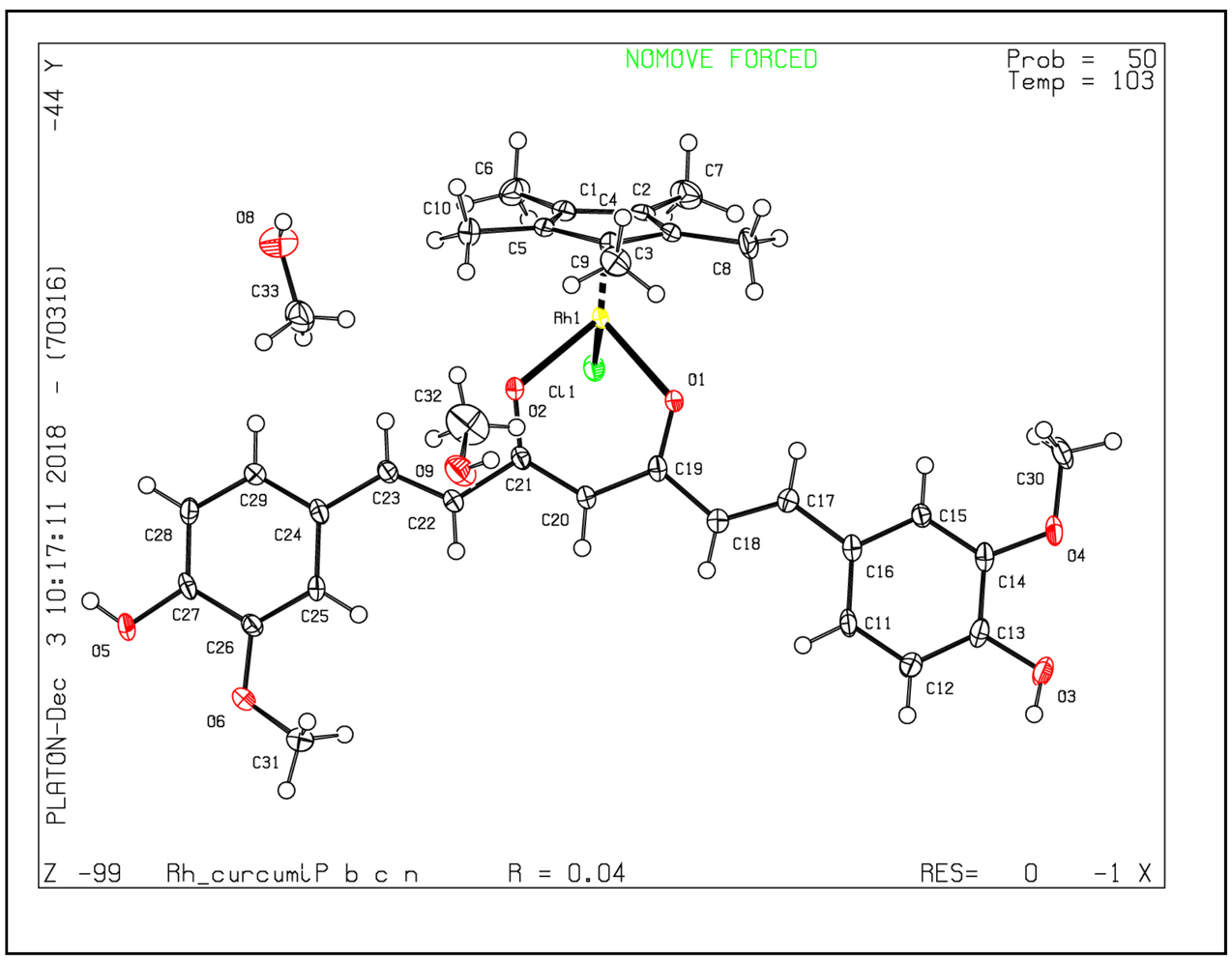
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 19/10/2018; check.def file version of 15/10/2018

Datablock Rh_curcumin - ellipsoid plot



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