

No syntax errors found.
Please wait while processing

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

Datablock: moca108_auto

Bond precision: C-C = 0.0020 Å Wavelength=0.71073
Cell: a=8.3598(5) b=8.8785(4) c=10.0104(5)
alpha=88.538(4) beta=82.936(4) gamma=83.704(4)

Temperature: 150 K

	Calculated	Reported
Volume	732.86(7)	732.86(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C15 H10 F6 N2 O2	C15 H10 F6 N2 O2
Sum formula	C15 H10 F6 N2 O2	C15 H10 F6 N2 O2
Mr	364.25	364.25
Dx, g cm ⁻³	1.651	1.651
Z	2	2
Mu (mm ⁻¹)	0.162	0.162
F000	368.0	368.0
F000'	368.31	
h, k, lmax	11, 12, 14	11, 12, 14
Nref	4477	3938
Tmin, Tmax	0.943, 0.968	0.820, 1.000
Tmin'	0.922	

Correction method= # Reported T Limits: Tmin=0.820
Tmax=1.000 AbsCorr = MULTI-SCAN

Data completeness= 0.880 Theta(max)= 30.505

R(reflections)= 0.0466(2957) wR2(reflections)=
0.1179(3938)

S = 1.031 Npar= 227

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 G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1 Report
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.004 Degree
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C00M Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C00M Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	35 Note
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	538 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.4 Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	11 Info

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

1 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
2 ALERT type 3 Indicator that the structure quality may be low
2 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

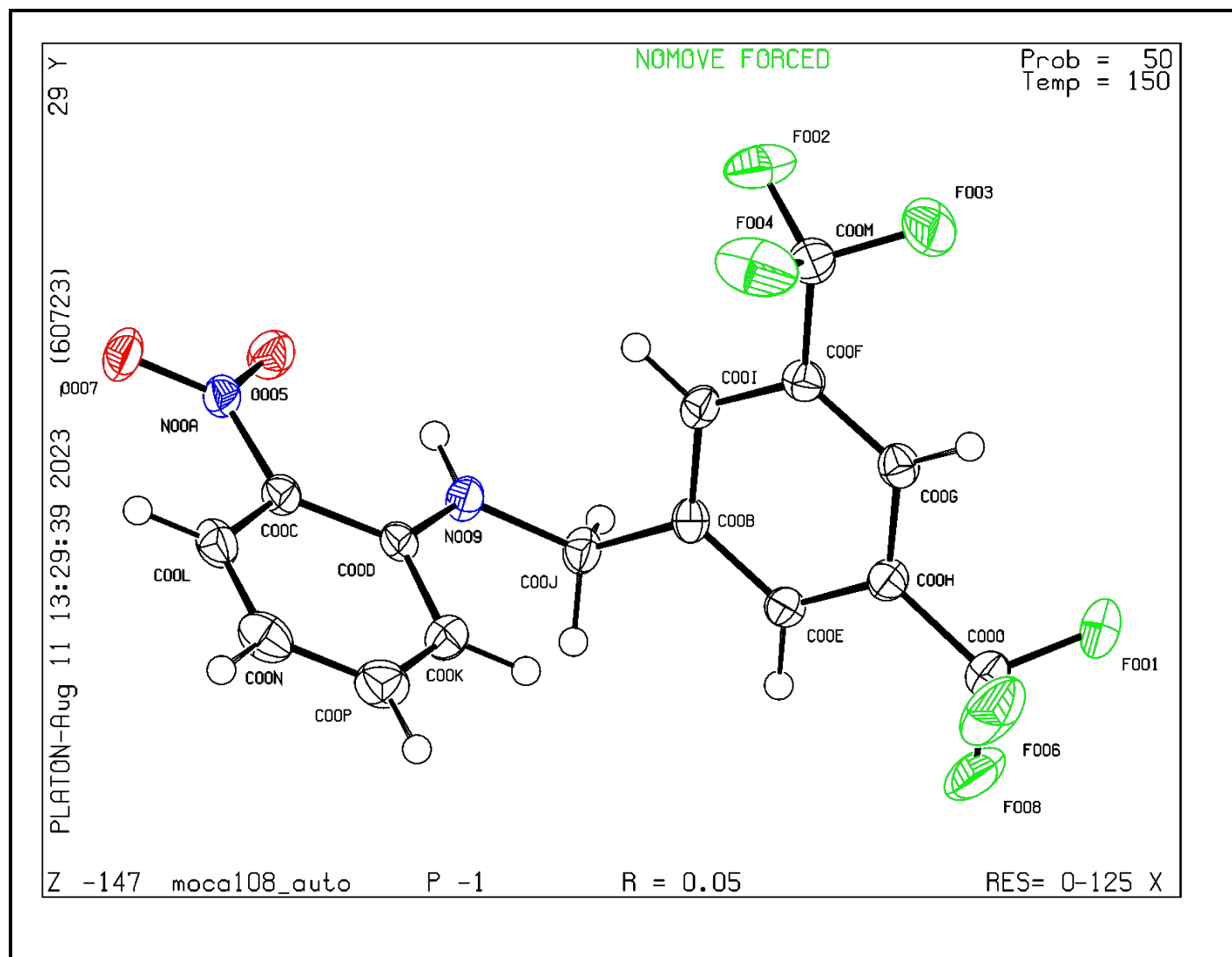
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 06/07/2023; check.def file version of 30/06/2023

Datablock moca108_auto - ellipsoid plot



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