checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait **..**

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) HN2980

> 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
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: HN2980

```
Bond precision:        C-C = 0.0049 A              Wavelength=1.54184
Cell:       a=6.49997(14)    b=11.1943(3)    c=14.0113(3)
            alpha=90         beta=95.358(2)  gamma=90
Temperature:100 K
```

	Calculated	Reported
Volume	1015.04(4)	1015.05(4)
Space group	P n	P 1 n 1
Hall group	P -2yac	P -2yac
Moiety formula	C20 H23 Cl N2 O2, 2(H2 O)	C20 H23 Cl N2 O2, 2(H2 O)
Sum formula	C20 H27 Cl N2 O4	C20 H27 Cl N2 O4
Mr	394.89	394.88
Dx,g cm-3	1.292	1.292
Z	2	2
Mu (mm-1)	1.895	1.895
F000	420.0	420.0
F000'	421.91	
h,k,lmax	8,13,17	7,13,17
Nref	4029[2021]	2216
Tmin,Tmax	0.651,0.876	0.399,1.000
Tmin'	0.201	

```
Correction method= # Reported T Limits: Tmin=0.399 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.10/0.55      Theta(max)= 72.781

R(reflections)= 0.0468( 2135)           wR2(reflections)= 0.1220(
                                        2216)

S = 1.024            Npar= 259
```

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

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.00489 Ang.
PLAT417_ALERT_2_C Short Inter D-H..H-D   H26B   ..H27A   .   2.14 Ang.
                            x,y,z =   1_555 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   27 Report
        6 0 0, 0 12 0, -5 0 1, 5 0 1, 6 0 2, 5 0 3,

```
      0 13  3,   4  0  4,   6  0  4,   4  5  4,   0 13  4,  -5  0  5,
      5  0  5,   7  0  5,  -2 12  5,   6  0  6,   5  0  7,  -4  0  8,
      4  0  8,   5  7  8,  -3  0  9,  -6  5  9,   3  9 10,   4  3 13,
     -1  6 15,   0  0 16,  -1  4 16,
```
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.83Ang From O19   .   0.40 eA-3

⬤ Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   6 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   1 Report
       H19
PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size ..   0.82 mm
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large   0.10 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records   2 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records   2 Report
PLAT650_ALERT_4_G SWAT Instruction Used to Model Solvent Disorder   ! Report
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   8 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600   61 Note
PLAT915_ALERT_3_G No Flack x Check Done: Low Friedel Pair Coverage   14 %
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ....   2.5 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ....   2.670 Note
      Predicted wR2: Based on SigI**2 4.57 or SHELX Weight 11.92
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.   4 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
 13 ALERT level G = General information/check it is not something unexpected


  0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  5 ALERT type 2 Indicator that the structure model may be wrong or deficient
  5 ALERT type 3 Indicator that the structure quality may be low
  5 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.
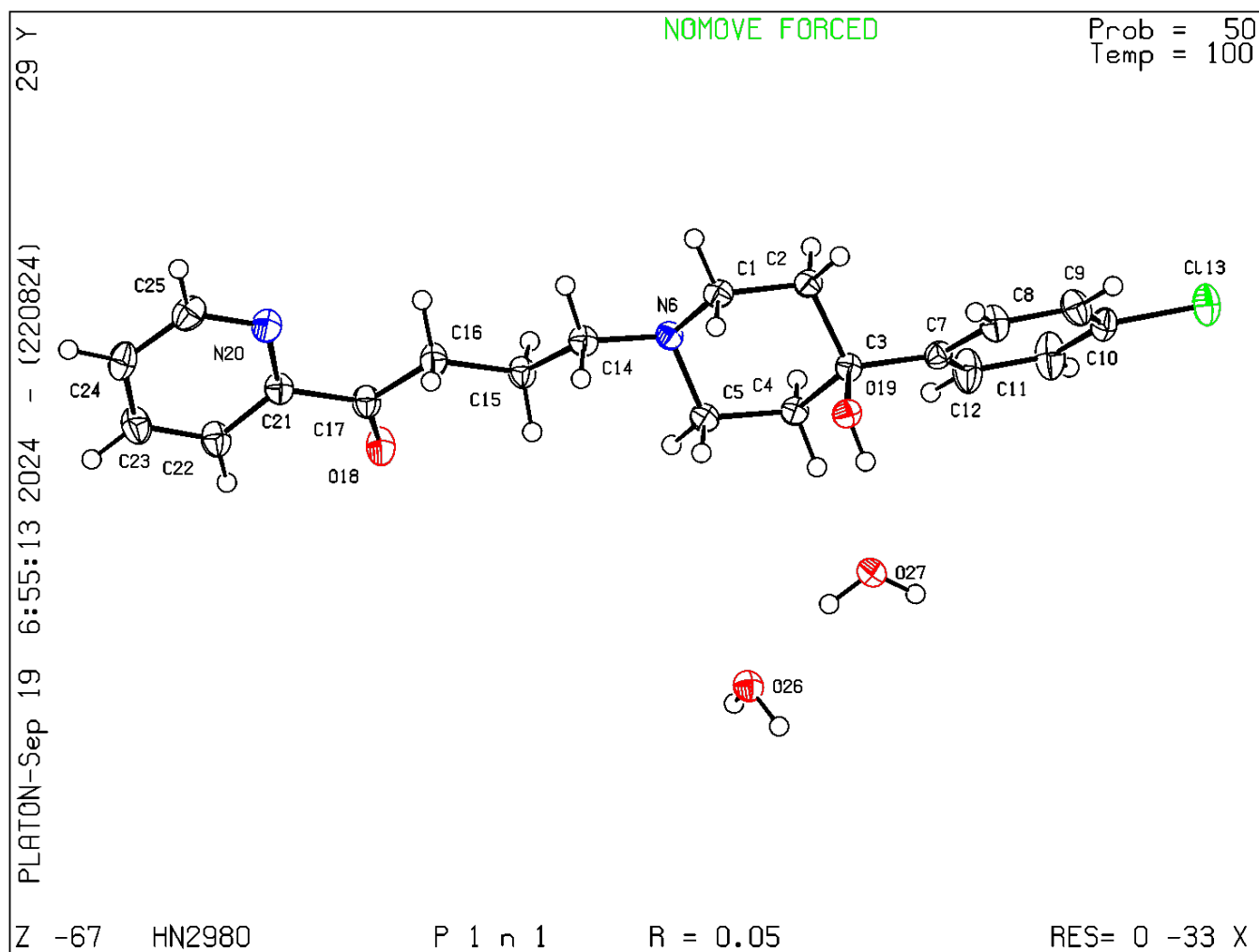
Publication of your CIF in IUCr journals

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 submission.

PLATON version of 22/08/2024; check.def file version of 21/08/2024

Datablock HN2980 - ellipsoid plot