

checkCIF (full publication check) running

checkCIF/PLATON (full publication check)

Structure factors have been supplied for datablock(s) L26-S-amine.HCl, L28-S-amine.HCl

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.

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

Structure factor report

Datablock: L26-S-amine.HCl

Bond precision: C-C = 0.0021 Å Wavelength=1.54184
Cell: a=8.3320(1) b=11.3877(2) c=22.1875(4)
alpha=90 beta=90 gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	2105.20(6)	2105.20(6)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C24 H30 N, Cl	C24 H30 Cl1 N1
Sum formula	C24 H30 Cl1 N	C24 H30 Cl1 N1
Mr	367.94	367.96
Dx, g cm ⁻³	1.161	1.161
Z	4	4
Mu (mm ⁻¹)	1.632	1.632
F000	792.0	792.0
F000'	795.22	
h, k, lmax	10, 14, 27	10, 14, 27
Nref	4416[2527]	4373
Tmin, Tmax	0.806, 0.937	0.840, 0.940
Tmin'	0.710	

Correction method= # Reported T Limits: Tmin=0.840 Tmax=0.940 AbsCorr = MULTI-SCAN

Data completeness= 1.73/0.99

Theta(max)= 76.114

R(reflections)= 0.0317(4106)

wR2(reflections)= 0.0852(4368)

S = 1.009

Npar= 309

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

[PLAT220_ALERT_2_C](#) Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.6 Ratio

[PLAT222_ALERT_3_C](#) Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range 5.0 Ratio

[PLAT410_ALERT_2_C](#) Short Intra H...H Contact H211 ..H22 . 1.98 Ang.

[PLAT922_ALERT_1_C](#) wR2 in the CIF and FCF Differ by 0.0023 Check

● Alert level G

[PLAT002_ALERT_2_G](#) Number of Distance or Angle Restraints on AtSite 20 Note

[PLAT007_ALERT_5_G](#) Number of Unrefined Donor-H Atoms 2 Report

[PLAT042_ALERT_1_G](#) Calc. and Reported MoietyFormula Strings Differ Please Check

[PLAT175_ALERT_4_G](#) The CIF-Embedded .res File Contains SAME Records 2 Report

[PLAT177_ALERT_4_G](#) The CIF-Embedded .res File Contains DELU Records 2 Report

[PLAT178_ALERT_4_G](#) The CIF-Embedded .res File Contains SIMU Records 2 Report

[PLAT301_ALERT_3_G](#) Main Residue Disorder(Resd 1) 32% Note

[PLAT720_ALERT_4_G](#) Number of Unusual/Non-Standard Labels 8 Note

[PLAT791_ALERT_4_G](#) Model has Chirality at C2 (Chiral SPGR) R Verify

[PLAT811_ALERT_5_G](#) No ADDSYM Analysis: Too Many Excluded Atoms ! Info

PLAT860_ALERT_3_G Number of Least-Squares Restraints 452 Note
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 10 Note
 PLAT960_ALERT_3_G Number of Intensities with I < - 2*sig(I) ... 1 Check

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

2 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
 6 ALERT type 4 Improvement, methodology, query or suggestion
 2 ALERT type 5 Informative message, check

Datablock: L28-S-amine.HCl

Bond precision: C-C = 0.0039 A Wavelength=1.54184
 Cell: a=11.4023(2) b=8.4460(1) c=12.1680(2)
 alpha=90 beta=117.387(2) gamma=90
 Temperature: 150 K

	Calculated	Reported
Volume	1040.49(3)	1040.49(3)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	C22 H20 F6 N, Cl	C22 H20 Cl1 F6 N1
Sum formula	C22 H20 Cl1 F6 N	C22 H20 Cl1 F6 N1
Mr	447.84	447.85
Dx, g cm-3	1.429	1.429
Z	2	2
Mu (mm-1)	2.190	2.190
F000	460.0	460.0
F000'	462.41	
h,k,lmax	14,10,15	14,10,15
Nref	4373[2342]	4288
Tmin,Tmax	0.749,0.858	0.710,0.860
Tmin'	0.660	

Correction method= # Reported T Limits: Tmin=0.710 Tmax=0.860 AbsCorr =
 MULTI-SCAN
 Data completeness= 1.83/0.98 Theta(max)= 76.206
 R(reflections)= 0.0357(4200) wR2(reflections)= 0.0950(4285)
 S = 1.003 Npar= 345

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

PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) 6.70 Note
 PLAT911_ALERT_3_C Missing FCF Refl Between Tmin & STh/L= 0.600 6 Report

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 20 Note
 PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report
 PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
 PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 1 Report
 PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 2 Report
 PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 2 Report
 PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 28% Note
 PLAT432_ALERT_2_G Short Inter X...Y Contact F114 ..C26 2.97 Ang.
 PLAT791_ALERT_4_G Model has Chirality at C2 (Chiral SPGR) R Verify
 PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ! Info
 PLAT860_ALERT_3_G Number of Least-Squares Restraints 565 Note
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 26 Note

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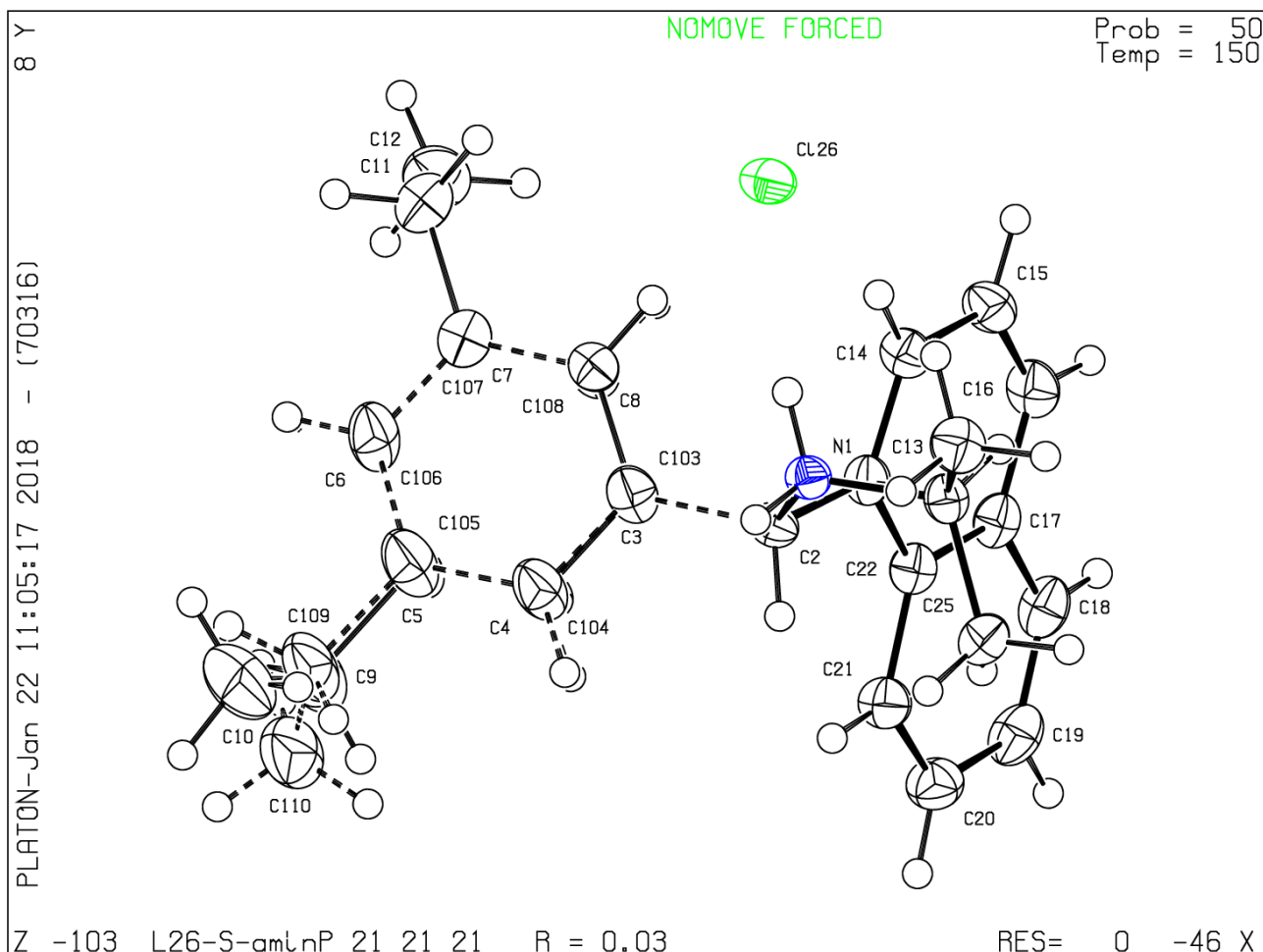
Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

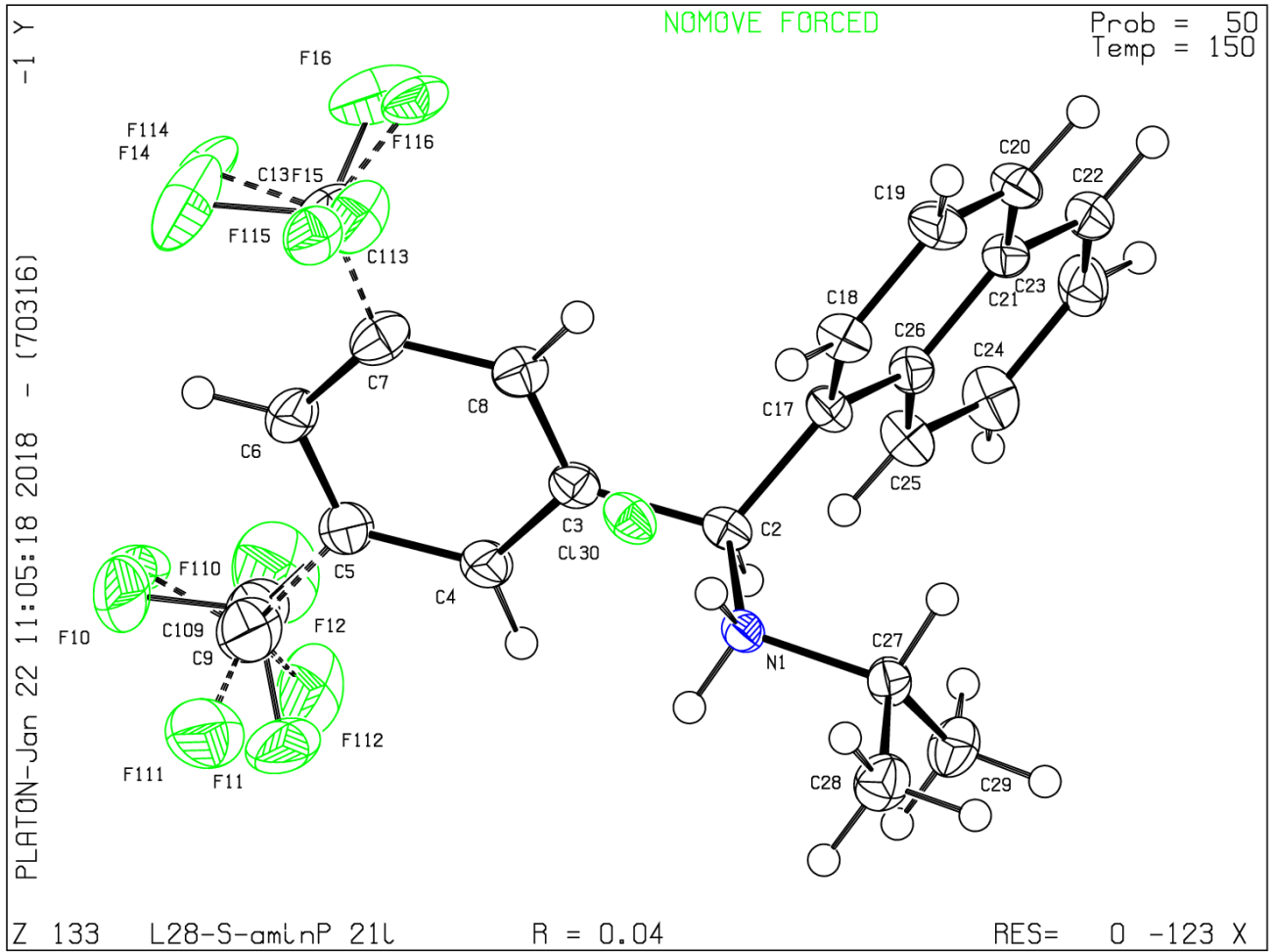
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PLATON version of 13/12/2017; check.def file version of 12/12/2017

Datablock L26-S-amine.HCl - ellipsoid plot



Datablock L28-S-amine.HCl - ellipsoid plot



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