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

CIF dictionary
Interpreting this report

Datablock: moc93sol1

Bond precision: C-C = 0.0031 A Wavelength=0.71073
Cell: a=8.2856(3) b=12.1191(5) c=19.2393(6)
alpha=82.105(3) beta=86.220(3) gamma=77.071(3)
Temperature: 150 K

	Calculated	Reported
Volume	1863.83(12)	1863.83(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C27 H24 Cu F3 N6 O12 S, H2 O [+ solvent]	C27 H24 Cu F3 N6 O12 S, H2 O
Sum formula	C27 H26 Cu F3 N6 O13 S [+ solvent]	C27 H26 Cu F3 N6 O13 S
Mr	795.15	795.14
Dx,g cm-3	1.417	1.417
Z	2	2
Mu (mm-1)	0.723	0.723
F000	812.0	812.0
F000'	813.37	
h,k,lmax	11,16,26	11,15,26
Nref	10357	8653
Tmin,Tmax	0.878,0.930	0.951,1.000
Tmin'	0.865	

Correction method= # Reported T Limits: Tmin=0.951
Tmax=1.000 AbsCorr = MULTI-SCAN
Data completeness= 0.835 Theta(max)= 29.459
R(reflections)= 0.0390(7132) wR2(reflections)= 0.0916(8653)
S = 1.026 Npar= 468

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 B

PLAT230_ALERT_2_B	Hirshfeld Test Diff for	S2D	--C5D	.	7.4 s.u.
PLAT417_ALERT_2_B	Short Inter D-H..H-D	H1CA	..H1WA	.	2.07 Ang.
			x,y,z =		1_555 Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O1W	--H1WA	.	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O1W	--H1WB	.	Please Check

Alert level C

CRYSC01_ALERT_1_C The word below has not been recognised as a standard identifier.
dull

PLAT220_ALERT_2_C	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min) Range	3.3 Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1	H	Uiso(max)/Uiso(min) Range	4.1 Ratio
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).				6 Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=			0.600	10 Report
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.97Ang	From	O1W .	0.43 eA-3

Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	4 Report
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.003 Degree
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C5D Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	314 A**3

```
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....          4 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)      .     2.32 Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600     1608 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....           1.7 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.     6 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   4 ALERT level B = A potentially serious problem, consider carefully
   6 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

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 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
   3 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

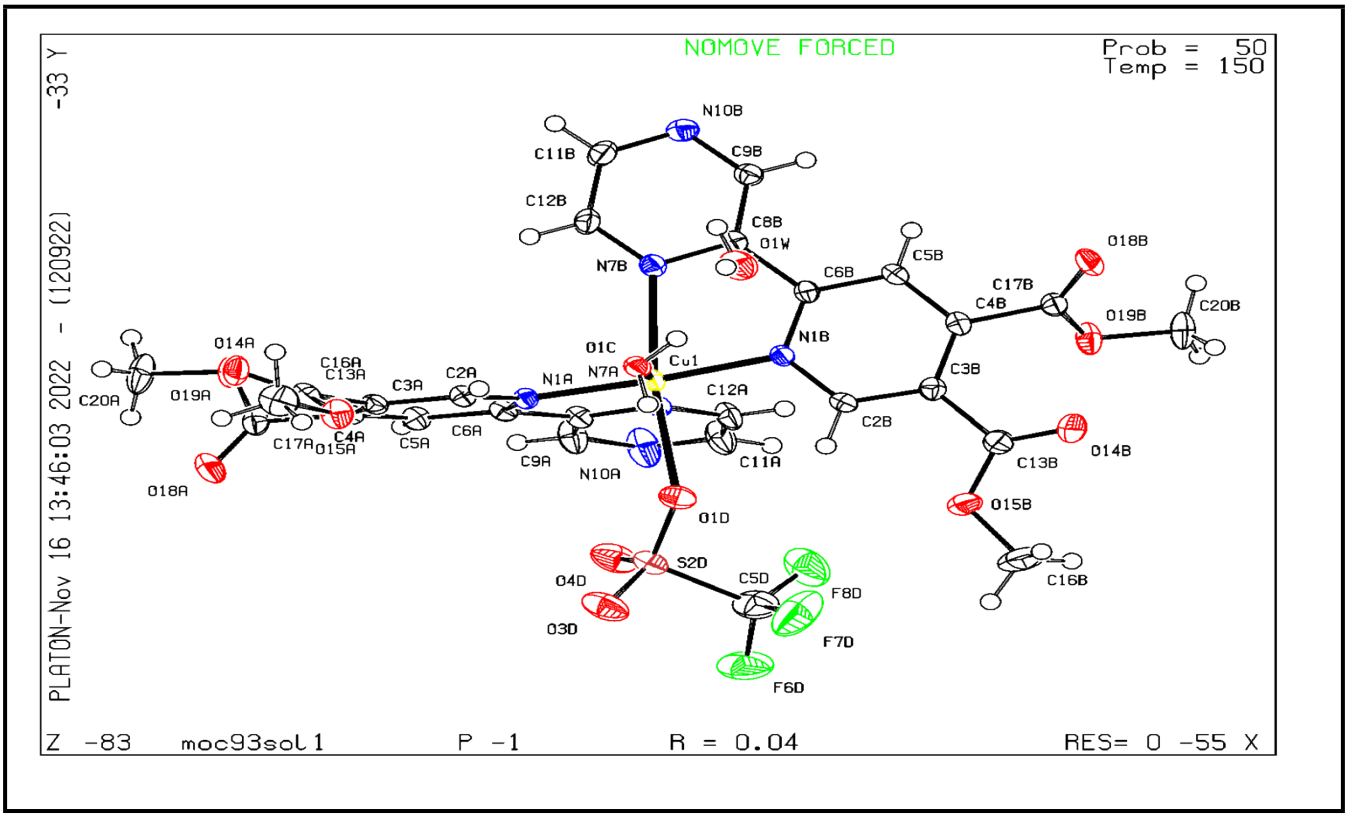
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 12/09/2022; check.def file version of 09/08/2022

Datablock moc93sol1 - ellipsoid plot



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