

No syntax errors found.
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[CIF dictionary](#)
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Datablock: moc93sol2

Bond precision:	C-C = 0.0083 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, C F3 O3	C27 H24 Cu F3 N6 O12 S, C F3 O3
	S, 2(H2 O)	S, 2(H2 O)
Sum formula	C28 H28 Cu F6 N6 O17 S2	C28 H28 Cu F6 N6 O17 S2
Mr	962.23	962.22
Dx, g cm-3	1.715	1.715
Z	2	2
Mu (mm-1)	0.812	0.812
F000	978.0	978.0
F000'	979.80	
h, k, lmax	11, 16, 26	11, 15, 26
Nref	10357	8653
Tmin, Tmax	0.864, 0.922	0.951, 1.000
Tmin'	0.850	
Correction method=	# Reported T Limits: Tmin=0.951	
Tmax=1.000 AbsCorr =	MULTI-SCAN	
Data completeness=	0.835 Theta(max)= 29.459	
R(reflections)=	0.1091(7132)	wR2(reflections)=
		0.3109(8653)
S = 1.026	Npar= 534	

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 A

PLAT097_ALERT_2_A	Large Reported Max. (Positive) Residual Density	9.72 eA-3
PLAT417_ALERT_2_A	Short Inter D-H..H-D H2WB ..H1WA .	1.72 Ang.
	x, y, z =	1_555 Check
PLAT971_ALERT_2_A	Check Calcd Resid. Dens. 0.06Ang From C5T	9.63 eA-3
PLAT975_ALERT_2_A	Check Calcd Resid. Dens. 1.04Ang From O1T .	3.16 eA-3



Alert level B

PLAT094_ALERT_2_B	Ratio of Maximum / Minimum Residual Density ...	4.08 Report
PLAT417_ALERT_2_B	Short Inter D-H..H-D H1CA ..H1WA .	2.04 Ang.
	x, y, z =	1_555 Check
PLAT417_ALERT_2_B	Short Inter D-H..H-D H2WA ..H1WA .	1.89 Ang.
	x, y, z =	1_555 Check
PLAT971_ALERT_2_B	Check Calcd Resid. Dens. 1.04Ang From O1T	3.16 eA-3
PLAT971_ALERT_2_B	Check Calcd Resid. Dens. 0.91Ang From O4T	2.59 eA-3



Alert level C

CRYSC01_ALERT_1_C	The word below has not been recognised as a standard identifier. dull	
DIFMN02_ALERT_2_C	The minimum difference density is < -0.1*ZMAX*0.75 _refine_diff_density_min given = -2.382 Test value = -2.175	
DIFMN03_ALERT_1_C	The minimum difference density is < -0.1*ZMAX*0.75 The relevant atom site should be identified.	

DIFMX02_ALERT_1_C The maximum difference density is $> 0.1 \times Z_{MAX} \times 0.75$

The relevant atom site should be identified.

PLAT082_ALERT_2_C	High R1 Value	0.11	Report
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.31	Report
PLAT098_ALERT_2_C	Large Reported Min. (Negative) Residual Density	-2.38	eA-3
PLAT213_ALERT_2_C	Atom C16B has ADP max/min Ratio	3.1	prolat
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.6	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	4.3	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference F6T --C5T .	0.20	Ang.
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including O2W	0.150	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00828	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.774	Check
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
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	1	Check
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.30Ang From S2T	-2.32	eA-3

And 3 other PLAT972 Alerts

PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.50Ang From S2T	-2.04	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.19Ang From O1T	-1.82	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.24Ang From O4T	-1.56	eA-3

PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on Cu01	1.22	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.70Ang From O2W .	-1.11	eA-3

And 2 other PLAT976 Alerts

PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.80Ang From O2W .	-1.03	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.64Ang From O2W .	-0.73	eA-3

PLAT977_ALERT_2_C	Check Negative Difference Density on H2WA .	-0.53	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H2WB .	-0.55	eA-3



Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	6	Report
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.17	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	19.48	Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.003	Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	2	Report
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) S2T --O3T .	8.0	s.u.
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C5D	Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	C5T	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	7	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # C F3 O3 S	2	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu01 (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.	1	Info

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

- 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
29 ALERT type 2 Indicator that the structure model may be wrong or deficient
8 ALERT type 3 Indicator that the structure quality may be low
7 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

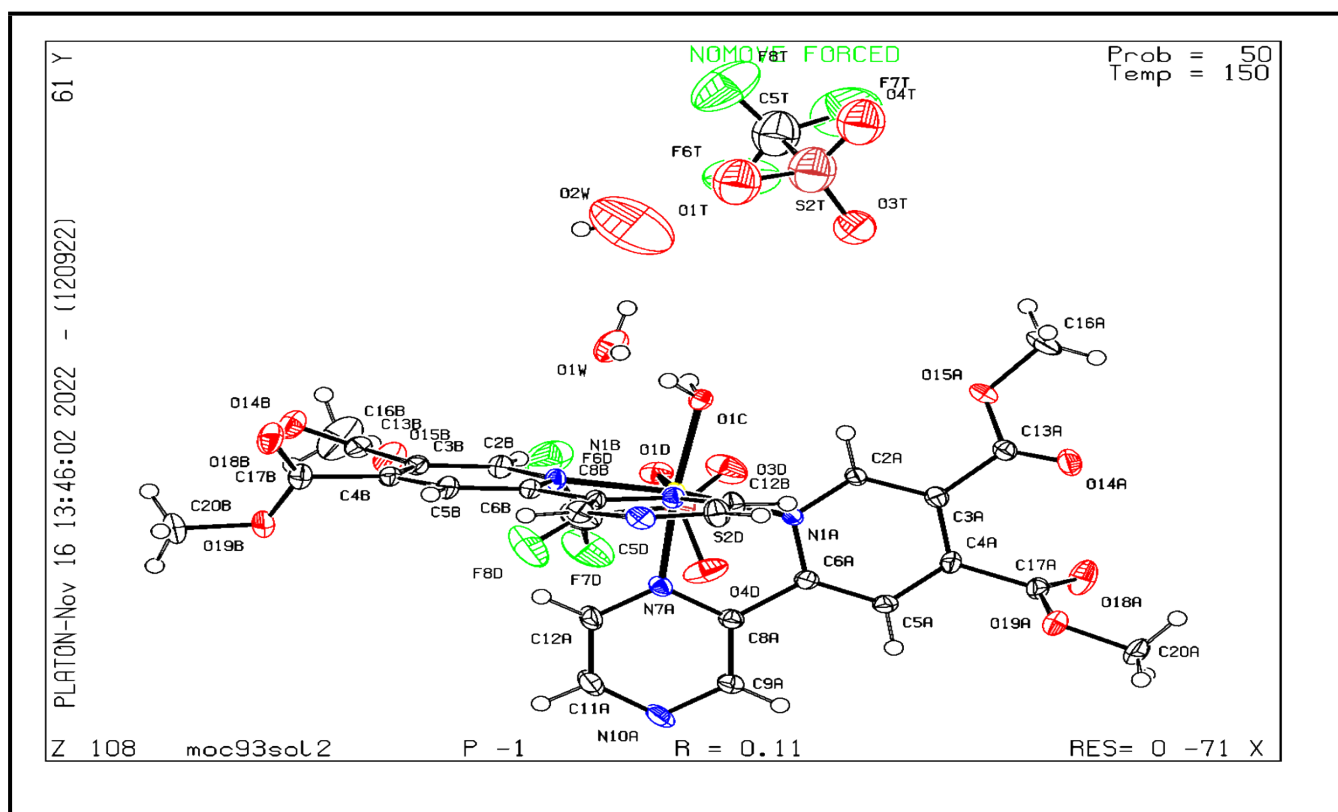
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

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Datablock moc93sol2 - ellipsoid plot



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