

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) JW1132_01, JW1132_02, JW1132_03, JW1144a_01_sq_sq, JW1144b_01, as-hiwi-007a_03, jw1110_01, jw1110_02, pd_si01_01, pd_si03_01, pd_si03l_01, sb-si01_01a

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 Interpreting this report

Datablock: pd_si01_01

Bond precision: C-C = 0.0028 A Wavelength=0.71073

Cell: a=10.6121 (6) b=17.1874 (9) c=11.2970 (6)
 alpha=90 beta=92.385 (4) gamma=90

Temperature: 180 K

	Calculated	Reported
Volume	2058.73 (19)	2058.72 (19)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C22 H19 N3 O3 Si	C22 H19 N3 O3 Si
Sum formula	C22 H19 N3 O3 Si	C22 H19 N3 O3 Si
Mr	401.49	401.49
Dx, g cm ⁻³	1.295	1.295
Z	4	4
Mu (mm ⁻¹)	0.142	0.142
F000	840.0	840.0
F000'	840.66	
h, k, lmax	14, 22, 14	14, 22, 14
Nref	4965	4961
Tmin, Tmax	0.958, 0.979	0.958, 0.987
Tmin'	0.952	

Correction method= # Reported T Limits: Tmin=0.958 Tmax=0.987
AbsCorr = INTEGRATION

Data completeness= 0.999 Theta(max)= 27.999

R(reflections)= 0.0423(3853)

wR2(reflections)=
0.1176(4961)

S = 1.118

Npar= 263

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

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	Si1	--C16	.	5.1 s.u.
PLAT601_ALERT_2_C	Unit Cell Contains Solvent Accessible VOIDS of	.			50 Ang**3



Alert level G

PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	? Check
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary	Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	4 Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities	Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	56.0 Degree
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	5 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
6 **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
1 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

Datablock: sb-si01_01a

Bond precision: C-C = 0.0039 A

Wavelength=0.71073

Cell:	a=9.7675(8)	b=10.6315(8)	c=17.7868(16)
	alpha=78.951(6)	beta=88.972(7)	gamma=77.779(6)
Temperature:	180 K		

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	12	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	3	Report
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records	2	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	4	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	5	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	12%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	12%	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	20	Note

PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	45%	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.7	Low
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities		Please Check
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	50.0	Degree
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info

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

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 4 ALERT type 2 Indicator that the structure model may be wrong or deficient
 7 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: jw1110_01

Bond precision:	C-C = 0.0034 A	Wavelength=0.71073
Cell:	a=9.1764(4)	b=18.4453(10)
	alpha=90	beta=91.991(3)
Temperature:	200 K	c=13.3241(5)
		gamma=90
	Calculated	Reported
Volume	2253.90(18)	2253.89(18)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	2(C21 H17 Cl Cu N3 O3 Si),	2(C21 H17 Cl Cu N3 O3 Si),
	C4 H8 O	C4 H8 O
Sum formula	C46 H42 Cl2 Cu2 N6 O7 Si2	C46 H42 Cl2 Cu2 N6 O7 Si2
Mr	1045.04	1045.04
Dx, g cm ⁻³	1.540	1.540
Z	2	2
Mu (mm ⁻¹)	1.175	1.175
F000	1072.0	1072.0
F000'	1074.53	
h,k,lmax	12,24,17	12,24,17
Nref	5440	5437
Tmin,Tmax	0.809,0.868	0.754,0.898
Tmin'	0.703	

Correction method= # Reported T Limits: Tmin=0.754 Tmax=0.898
 AbsCorr = INTEGRATION

Data completeness= 0.999

Theta(max)= 28.000

R(reflections)= 0.0341(4343)

wR2(reflections)=
0.0848(5437)

S = 1.068

Npar= 316

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

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.682 Check



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 5 Note
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 2 Report
PLAT300_ALERT_4_G Atom Site Occupancy of O4 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C22 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C23 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C24 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C25 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H23A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H23B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H24A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H24B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H25A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H25B Constrained at 0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 2) 6.50 Check
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O1 . 139.9 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O2 . 141.7 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O3 . 134.2 Degree
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O4 . 104.4 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact Si1 ..04 . 3.39 Ang.
x,y,l+z = 1_556 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group # 13 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints 4 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 3 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 4.3 Low
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 56.0 Degree
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
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1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
31 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 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
17 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

Datablock: pd_si03_01

Bond precision: C-C = 0.0046 A Wavelength=0.71073

Cell: a=15.3617(7) b=8.6072(5) c=16.3936(7)
alpha=90 beta=90 gamma=90

Temperature: 200 K

	Calculated	Reported
Volume	2167.58(19)	2167.58(18)
Space group	P c a 21	P c a 21
Hall group	P 2c -2ac	P 2c -2ac
Moiety formula	C22 H19 Cl Cu N3 O3 Si	C22 H19 Cl Cu N3 O3 Si
Sum formula	C22 H19 Cl Cu N3 O3 Si	C22 H19 Cl Cu N3 O3 Si
Mr	500.49	500.48
Dx, g cm ⁻³	1.534	1.534
Z	4	4
Mu (mm ⁻¹)	1.216	1.216
F000	1024.0	1024.0
F000'	1026.50	
h, k, lmax	20, 11, 21	20, 11, 21
Nref	5247[2717]	5100
Tmin, Tmax	0.747, 0.833	0.765, 0.841
Tmin'	0.694	

Correction method= # Reported T Limits: Tmin=0.765 Tmax=0.841
AbsCorr = INTEGRATION

Data completeness= 1.88/0.97 Theta(max)= 27.998

R(reflections)= 0.0235(4772) wR2(reflections)=
0.0583(5100)

S = 1.087 Npar= 280

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

PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cu1	--Cl1	.	5.2 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cu1	--N3	.	5.7 s.u.
PLAT395_ALERT_2_G	Deviating X-O-Y	Angle From 120 for O1	.	135.2 Degree	
PLAT395_ALERT_2_G	Deviating X-O-Y	Angle From 120 for O2	.	135.0 Degree	
PLAT395_ALERT_2_G	Deviating X-O-Y	Angle From 120 for O3	.	132.8 Degree	
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary	.		Please Do !	
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).			3 Note	
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF			1 Note	
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities			Please Check	
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..			56.0 Degree	
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.			7 Info	

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 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
0 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

Datablock: JW1132_01

Bond precision:	Cu-Cl = 0.0006 A	Wavelength=0.71073	
Cell:	a=9.0369(2)	b=23.5711(6)	c=9.6583(2)
	alpha=90	beta=108.839(2)	gamma=90
Temperature:	200 K		

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	27	Note
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	25	Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	3	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	13	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cul --Cll .	5.7	s.u.
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	93%	Note
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O1 .	137.2	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O2 .	144.9	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O3 .	138.8	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O2A .	149.5	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O3A .	148.1	Degree
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	27	Note

PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 56.0 Degree

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1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
15 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

Datablock: JW1132_03

Bond precision: C-C = 0.0031 A Wavelength=0.71073

Cell: a=8.7413(3) b=10.4028(3) c=10.7168(3)
alpha=80.052(3) beta=80.903(2) gamma=89.273(3)
Temperature: 180 K

	Calculated	Reported
Volume	947.69(5)	947.69(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C18 H17 Cl Cu N3 O3 Si	C18 H17 Cl Cu N3 O3 Si
Sum formula	C18 H17 Cl Cu N3 O3 Si	C18 H17 Cl Cu N3 O3 Si
Mr	450.44	450.42
Dx, g cm-3	1.579	1.578
Z	2	2
Mu (mm-1)	1.381	1.381
F000	460.0	460.0
F000'	461.23	
h, k, lmax	11, 13, 14	11, 13, 14
Nref	4570	4570
Tmin, Tmax	0.725, 0.871	0.747, 0.876
Tmin'	0.654	

Correction method= # Reported T Limits: Tmin=0.747 Tmax=0.876
AbsCorr = INTEGRATION

Data completeness= 1.000 Theta(max)= 27.993

R(reflections)= 0.0303(4149)

wR2(reflections)=
0.0753(4570)

S = 1.101

Npar= 244

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

PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cu1 --N2	.	11.3 s.u.
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O1	.	135.5 Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O2	.	131.0 Degree
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1 (I)	.	1.03 Info
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF		1 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		4.2 Low
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities		Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..		56.0 Degree
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
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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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 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
0 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

Datablock: jw1110_02

Bond precision: C-C = 0.0036 A

Wavelength=0.71073

Cell: a=15.7556(8) b=18.2565(7) c=17.2013(6)
alpha=90 beta=90 gamma=90

Temperature: 200 K

PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O1	.	130.5 Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O2	.	132.3 Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O4	.	130.4 Degree
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary	.	Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above Sth/L= 0.600		2 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF		1 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		4.4 Low
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities		Please Check
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..		56.0 Degree
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		9 Info

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

Datablock: pd_si03l_01

Bond precision: C-C = 0.0036 A Wavelength=0.71073
 Cell: a=15.8215(9) b=9.8221(4) c=17.4885(10)
 alpha=90 beta=109.961(4) gamma=90
 Temperature: 200 K

	Calculated	Reported
Volume	2554.5(2)	2554.5(2)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C27 H23 Cl Cu N4 O4 Si	C27 H23 Cl Cu N4 O4 Si
Sum formula	C27 H23 Cl Cu N4 O4 Si	C27 H23 Cl Cu N4 O4 Si
Mr	594.58	594.57
Dx, g cm ⁻³	1.546	1.546
Z	4	4
Mu (mm ⁻¹)	1.049	1.049
F000	1220.0	1220.0
F000'	1222.59	
h, k, lmax	19, 12, 21	19, 12, 21
Nref	5020	5012
Tmin, Tmax	0.828, 0.900	0.832, 0.929
Tmin'	0.730	

Correction method= # Reported T Limits: Tmin=0.832 Tmax=0.929
 AbsCorr = INTEGRATION

Data completeness= 0.998 Theta(max)= 26.000

R(reflections)= 0.0291(4064) wR2(reflections)=
 0.0747(5012)
 S = 1.081 Npar= 343

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

PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	7	Note
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..	1	Check



Alert level G

PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cu1 --Si1 .	8.3	s.u.
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O1 .	130.7	Degree
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	2	Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities		Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	52.0	Degree
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	5	Info

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3 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

Datablock: JW1132_02

Bond precision: C-C = 0.0042 A

Wavelength=0.71073

Cell: a=15.2140(3) b=9.6459(2) c=17.0865(3)

alpha=90 beta=108.677(1) gamma=90

Temperature: 200 K

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	6	Note
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records	1	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	2	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cul --Sil .	5.0	s.u.
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	9%	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	2	Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities		Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	52.0	Degree
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
 3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 10 **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
 3 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

Datablock: as-hiwi-007a_03

Bond precision: C-C = 0.0033 A

Wavelength=0.71073

Cell: a=9.6434(6) b=10.4351(6) c=12.0659(7)
 alpha=100.595(5) beta=110.075(5) gamma=106.546(5)
 Temperature: 180 K

	Calculated	Reported
Volume	1038.34(13)	1038.34(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C44 H36 Cl2 Cu2 N4 O4 Si2	C44 H36 Cl2 Cu2 N4 O4 Si2
Sum formula	C44 H36 Cl2 Cu2 N4 O4 Si2	C44 H36 Cl2 Cu2 N4 O4 Si2
Mr	938.95	938.93
Dx, g cm ⁻³	1.502	1.502
Z	1	1
Mu (mm ⁻¹)	1.259	1.259
F000	480.0	480.0
F000'	481.23	
h, k, lmax	12, 13, 15	12, 13, 15
Nref	5009	5010
Tmin, Tmax	0.710, 0.797	0.776, 0.909
Tmin'	0.696	

Correction method= # Reported T Limits: Tmin=0.776 Tmax=0.909
 AbsCorr = INTEGRATION

Data completeness= 1.000

Theta(max)= 27.996

R(reflections)= 0.0334(4492)

wR2(reflections)=
 0.0865(5010)

S = 1.072

Npar= 262

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

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.01 Report



Alert level G

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.005 Degree
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1 --Cl1 . 20.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1 --Cl1_a . 50.5 s.u.
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O1 . 131.9 Degree
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O2 . 131.4 Degree
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.3 Low
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 56.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 13 Info

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1 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

Datablock: JW1144a_01_sq_sq

Bond precision: C-C = 0.0033 A

Wavelength=0.71073

Cell: a=9.6236(3) b=12.6110(4) c=12.8592(4)
alpha=110.726(2) beta=107.692(2) gamma=98.836(2)
Temperature: 180 K

	Calculated	Reported
Volume	1329.53(8)	1329.53(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C44 H36 Cl4 Cu4 N4 O4 Si2 [+ solvent]	C44 H36 Cl4 Cu4 N4 O4 Si2, 2 (C4 H8 O)
Sum formula	C44 H36 Cl4 Cu4 N4 O4 Si2 [+ solvent]	C52 H52 Cl4 Cu4 N4 O6 Si2
Mr	1136.95	1281.11
Dx, g cm ⁻³	1.420	1.600
Z	1	1
Mu (mm ⁻¹)	1.864	1.877
F000	572.0	652.0
F000'	574.16	
h,k,lmax	12,16,16	12,16,16
Nref	6424	6424
Tmin,Tmax	0.668,0.713	0.717,0.758
Tmin'	0.655	

Correction method= # Reported T Limits: Tmin=0.717 Tmax=0.758

AbsCorr = INTEGRATION

Data completeness= 1.000

Theta(max)= 27.996

R(reflections)= 0.0346(5224)

wR2(reflections)=
0.0876(6424)

S = 1.038

Npar= 316

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

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance

2.554 Check



Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the

_chemical_formula_sum and the formula from the _atom_site* data.

Atom count from _chemical_formula_sum: C52 H52 Cl4 Cu4 N4 O6 Si2

Atom count from the _atom_site data: C44 H36 Cl4 Cu4 N4 O4 Si2

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G ALERT: Large difference may be due to a

symmetry error - see SYMMG tests

From the CIF: _cell_formula_units_Z 1

From the CIF: _chemical_formula_sum C52 H52 Cl4 Cu4 N4 O6 Si2

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	52.00	44.00	8.00
H	52.00	36.00	16.00
Cl	4.00	4.00	0.00
Cu	4.00	4.00	0.00
N	4.00	4.00	0.00
O	6.00	4.00	2.00
Si	2.00	2.00	0.00

PLAT041_ALERT_1_G	Calc. and Reported SumFormula	Strings Differ	Please Check
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)		0.002 Degree
PLAT300_ALERT_4_G	Atom Site Occupancy of Cu1	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cu2	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cu3	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cu4	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl1	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl2	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl3	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl4	Constrained at	0.5 Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)		13% Note
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure		271 A**3
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #		8 Check
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed		! Info
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		4.0 Low
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities	Please Check	
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..		56.0 Degree
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		7 Info

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 3 ALERT type 3 Indicator that the structure quality may be low
 11 ALERT type 4 Improvement, methodology, query or suggestion
 2 ALERT type 5 Informative message, check

Datablock: JW1144b_01

Bond precision: C-C = 0.0070 A Wavelength=0.71073

Cell: a=8.9766(2) b=19.8415(3) c=13.5256(3)
 alpha=90 beta=92.846(2) gamma=90

Temperature: 180 K

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite				8	Note
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records				2	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records				2	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cu1	--Cl1	.	6.9	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cu1	--Cl2	.	33.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cu2	--Cl2	.	67.7	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cu2	--Cl3	.	8.2	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cu3	--Cl2	.	18.2	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cu3	--Cl3	.	23.0	s.u.
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)				100%	Note

PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 2)	3.25	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 3)	1.75	Check
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O3 .	132.4	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O4 .	130.3	Degree
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	32	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	6	Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities		Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	56.0	Degree
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info

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checkCIF publication errors

Alert level A

PUBL004_ALERT_1_A The contact author's name and address are missing,
_publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A _publ_contact_author_email, _publ_contact_author_fax and
_publ_contact_author_phone are all missing.
At least one of these should be present.
PUBL006_ALERT_1_A _publ_requested_journal is missing
e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A _publ_section_abstract is missing.
Abstract of paper in English.

Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or
empty.

7 **ALERT level A** = Data missing that is essential or data in wrong format
1 **ALERT level G** = General alerts. Data that may be required is missing

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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
```


i

```
vrf PUBL012 GLOBAL
```

i

PROBLEM: `_publ_section_abstract` is missing.

RESPONSE: . . .

i

```
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 18/11/2022; check.def file version of 09/08/2022

Datablock pd si01 01 - ellipsoid plot























