
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**

PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on Cs1 1.52 eA-3

 **Alert level C**

PLAT245_ALERT_2_C U(iso) H2B Smaller than U(eq) C2 by 0.012 Ang**2
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.01025 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.16Ang From Cs1 1.63 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.98Ang From O1 . 0.62 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 1.09Ang From O1 . -0.65 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 1.09Ang From O1 . -0.65 eA-3

 **Alert level G**

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 2 Note
PLAT303_ALERT_2_G Full Occupancy Atom H2A with # Connections 2.00 Check
PLAT303_ALERT_2_G Full Occupancy Atom H8 with # Connections 2.00 Check
PLAT343_ALERT_2_G Unusual Angle Range in Main Residue for C1 Check
PLAT343_ALERT_2_G Unusual Angle Range in Main Residue for C2 Check
PLAT367_ALERT_2_G Long? C(sp?)-C(sp?) Bond C1 - C3 . 1.50 Ang.
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 2.07 Ratio
PLAT774_ALERT_1_G Check X-Y Bond in CIF: Cs1 --Cs1 .. 4.21 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 38.70 Deg.
O1 -C1 -CS1 1_555 1_555 5_666 # 80 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 35.50 Deg.
O1 -C1 -CS1 1_555 1_555 1_555 # 81 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). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 8 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.9 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
12 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
5 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Datablock: jrl3099

Bond precision: C-C = 0.0112 A

Wavelength=1.54184

Cell: a=13.3301(2) b=16.6470(2) c=28.3794(2)
alpha=73.521(1) beta=83.579(1) gamma=80.046(1)
Temperature: 160 K

	Calculated	Reported
Volume	5934.82(13)	5934.82(13)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C120.04 H126.08 Cs6 O12, 2(C0.50 H 00.13)	?
Sum formula	C124.54 H135.08 Cs6 O13.13	C20.76 H22.51 Cs O2.19
Mr	2639.36	439.89
Dx, g cm ⁻³	1.477	1.477
Z	2	12
Mu (mm ⁻¹)	14.669	14.669
F000	2634.6	2635.0
F000'	2632.94	
h, k, lmax	16, 20, 35	16, 20, 35
Nref	24054	23704
Tmin, Tmax	0.219, 0.532	0.083, 0.428
Tmin'	0.126	

Correction method= # Reported T Limits: Tmin=0.083 Tmax=0.428
AbsCorr = GAUSSIAN

Data completeness= 0.985 Theta(max)= 73.918

R(reflections)= 0.0507(19131)

wR2(reflections)=
0.1511(23704)

S = 1.082 Npar= 1394

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test-name_ALERT_alert-type_alert-level.
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 **Alert level A**

PLAT201_ALERT_2_A Isotropic non-H Atoms in Main Residue(s) 13 Report
O12A C77 C78 C79 C80 etc.

 **Alert level C**

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.9 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.9 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 07 Check

PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	011	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C27	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C29	Check
PLAT245_ALERT_2_C	U(iso)	H4B	Smaller than U(eq) C4	by 0.015	Ang**2
PLAT245_ALERT_2_C	U(iso)	H60A	Smaller than U(eq) C60	by 0.013	Ang**2
PLAT260_ALERT_2_C	Large Average	Ueq of Residue Including		O8 0.116	Check
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds	0.01116	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		2.382	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta (Min).			8	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600		5	Report
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.73Ang	From Cs1	-1.52	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H11F	.		-0.31	eA-3

● Alert level G

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
 CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
 From the CIF: _cell_formula_units_Z 12
 From the CIF: _chemical_formula_sum C20.76 H22.51 Cs O2.19
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	249.12	249.08	0.04
H	270.12	270.16	-0.04
Cs	12.00	12.00	0.00
O	26.28	26.25	0.03

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		25	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		35	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		1	Info
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...		0.167	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please	Check
PLAT153_ALERT_1_G	The s.u.'s on the Cell Axes are Equal ..(Note)		0.0002	Ang.
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)		0.001	Degree
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.		9	Note
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		14	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		8	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records		6	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records		6	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records		2	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used		0.0200	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used		0.0200	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used		0.0200	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used		0.0200	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used		0.0200	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of C77	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C78	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C79	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C80	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C77A	Constrained at	0.46	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C78A	Constrained at	0.46	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C79A	Constrained at	0.46	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C80A	Constrained at	0.46	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H77A	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H77B	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H78A	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H78B	Constrained at	0.55	Check

PLAT300_ALERT_4_G	Atom Site Occupancy of H79A	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H79B	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H80A	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H80B	Constrained at	0.55	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H77C	Constrained at	0.46	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H77D	Constrained at	0.46	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H78C	Constrained at	0.46	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H78D	Constrained at	0.46	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H79C	Constrained at	0.46	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H79D	Constrained at	0.46	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H80C	Constrained at	0.46	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H80D	Constrained at	0.46	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O14	Constrained at	0.125	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C120	Constrained at	0.125	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C121	Constrained at	0.125	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C122	Constrained at	0.125	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C123	Constrained at	0.125	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12A	Constrained at	0.125	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12B	Constrained at	0.125	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12C	Constrained at	0.125	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12D	Constrained at	0.125	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12E	Constrained at	0.125	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12F	Constrained at	0.125	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12G	Constrained at	0.125	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12H	Constrained at	0.125	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)		19%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)		100%	Note
PLAT303_ALERT_2_G	Full Occupancy Atom H24B with # Connections		2.00	Check
PLAT303_ALERT_2_G	Full Occupancy Atom H86 with # Connections		2.00	Check
PLAT303_ALERT_2_G	Full Occupancy Atom H94B with # Connections		2.00	Check
PLAT343_ALERT_2_G	Unusual Angle Range in Main Residue for		C81	Check
PLAT343_ALERT_2_G	Unusual Angle Range in Main Residue for		C82	Check
PLAT343_ALERT_2_G	Unusual Angle Range in Main Residue for		C91	Check
PLAT343_ALERT_2_G	Unusual Angle Range in Main Residue for		C94	Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C91 - C101		1.50	Ang.
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O8		109.7	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O14		109.8	Degree
PLAT410_ALERT_2_G	Short Intra H...H Contact H49 ..H56B		2.06	Ang.
		x,y,z =	1_555	Check
PLAT410_ALERT_2_G	Short Intra H...H Contact H54A ..H53D		1.70	Ang.
		x,y,z =	1_555	Check
PLAT410_ALERT_2_G	Short Intra H...H Contact H82 ..H85A		2.04	Ang.
		x,y,z =	1_555	Check
PLAT410_ALERT_2_G	Short Intra H...H Contact H84B ..H89B		2.08	Ang.
		x,y,z =	1_555	Check
PLAT411_ALERT_2_G	Short Inter H...H Contact H84B ..H12D		2.10	Ang.
		2-x,2-y,-z =	2_775	Check
PLAT722_ALERT_1_G	Angle Calc 112.00, Rep 110.90 Dev...		1.10	Degree
	H78A -C78 -H78B 1_555 1_555 1_555	#	943	Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)		1.14	Ratio
PLAT780_ALERT_1_G	Coordinates do not Form a Properly Connected Set			Please Do !
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group	#	13	Check
PLAT822_ALERT_4_G	CIF-embedded .res Contains Negative PART Numbers		1	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		334	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary			Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Deprecated and Succeeded by SHELXL		2019/3	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		337	Note

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 4.7 Low
 PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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

Datablock: wit_exp_820_auto

Bond precision: C-C = 0.0088 A Wavelength=1.54184

Cell: a=25.4358(3) b=15.8158(2) c=26.6220(3)
 alpha=90 beta=92.424(1) gamma=90

Temperature: 200 K

	Calculated	Reported
Volume	10700.1(2)	10700.1(2)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C228 H228 O21 Rb12	C57 H57 O5.25 Rb3
Sum formula	C228 H228 O21 Rb12	C57 H57 O5.25 Rb3
Mr	4329.75	1082.43
Dx, g cm ⁻³	1.344	1.344
Z	2	8
Mu (mm ⁻¹)	3.825	3.825
F000	4416.0	4416.0
F000'	4414.36	
h, k, lmax	31, 19, 33	31, 19, 33
Nref	10755	10480
Tmin, Tmax	0.751, 0.789	0.757, 0.900
Tmin'	0.595	

Correction method= # Reported T Limits: Tmin=0.757 Tmax=0.900
 AbsCorr = GAUSSIAN

Data completeness= 0.974 Theta(max)= 73.205

R(reflections)= 0.0482(6670)

wR2(reflections)=
0.1802(10480)

S = 1.076

Npar= 653

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test-name_ALERT_alert-type_alert-level.

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● Alert level C

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT213_ALERT_2_C	Atom C58 has ADP max/min Ratio	3.5 prolat
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.2 Ratio
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0088 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.190 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	90 Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	2 Check
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..	1 Check

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	23 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	10 Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	4 Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250 Check
PLAT073_ALERT_1_G	H-atoms ref, but _hydrogen_treatment Reported as	constr Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	11.18 Why ?
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	6 Note
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	6 Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	9 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
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0200 Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0200 Report
PLAT300_ALERT_4_G	Atom Site Occupancy of O6 Constrained at	0.125 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O7 Constrained at	0.125 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C57 Constrained at	0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C58 Constrained at	0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C59 Constrained at	0.125 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C60 Constrained at	0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C61 Constrained at	0.125 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6A Constrained at	0.125 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6B Constrained at	0.125 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H7A Constrained at	0.125 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H7B Constrained at	0.125 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H57A Constrained at	0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H57B Constrained at	0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H58A Constrained at	0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H58B Constrained at	0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H60A Constrained at	0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H60B Constrained at	0.25 Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	8% Note
PLAT343_ALERT_2_G	Unusual Angle Range in Main Residue for	C17 Check

PLAT343_ALERT_2_G Unusual	Angle Range in Main Residue for	C33	Check
PLAT367_ALERT_2_G Long?	C(sp?)-C(sp?) Bond C17 - C21	1.51	Ang.
PLAT764_ALERT_4_G Overcomplete	CIF Bond List Detected (Rep/Expd)	1.26	Ratio
PLAT789_ALERT_4_G Atoms with Negative	_atom_site_disorder_group #	17	Check
PLAT822_ALERT_4_G CIF-embedded	.res Contains Negative PART Numbers	1	Check
PLAT860_ALERT_3_G Number of Least-Squares	Restraints	112	Note
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	185	Note
PLAT933_ALERT_2_G Number of HKL-OMIT	Records in Embedded .res File	4	Note
PLAT941_ALERT_3_G Average HKL	Measurement Multiplicity	3.3	Low
PLAT978_ALERT_2_G Number C-C	Bonds with Positive Residual Density.	3	Info

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10 ALERT type 3 Indicator that the structure quality may be low
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Datablock: jw-78_1_auto

Bond precision:	C-C = 0.0204 A	Wavelength=1.54184
Cell:	a=18.6607(4)	b=6.0929(2) c=22.6838(7)
	alpha=90	beta=90 gamma=90
Temperature:	220 K	

	Calculated	Reported
Volume	2579.10(13)	2579.10(13)
Space group	P c a 21	P c a 21
Hall group	P 2c -2ac	P 2c -2ac
Moiety formula	C28 H24 Cs2 N2 O2	0.25(C56 H48 Cs4 N4 O4)
Sum formula	C28 H24 Cs2 N2 O2	C14 H12 Cs N O
Mr	686.31	343.16
Dx, g cm-3	1.768	1.768
Z	4	8
Mu (mm-1)	22.254	22.254
F000	1328.0	1328.0
F000'	1326.04	
h, k, lmax	23, 7, 28	23, 7, 28
Nref	5295[2719]	5087
Tmin, Tmax	0.162, 0.211	0.216, 0.474
Tmin'	0.072	

Correction method= # Reported T Limits: Tmin=0.216 Tmax=0.474
AbsCorr = GAUSSIAN

Data completeness= 1.87/0.96 Theta(max)= 74.464

R(reflections)= 0.0389(4496)

wR2(reflections)=
0.1147(5087)

S = 1.194 Npar= 308

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**

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds 0.02043 Ang.
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 7 Check

 **Alert level C**

STRVA01_ALERT_4_C Flack test results are ambiguous.
 From the CIF: _refine_ls_abs_structure_Flack 0.478
 From the CIF: _refine_ls_abs_structure_Flack_su 0.015
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Cs1 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 3 Report

 **Alert level G**

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.500 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 7.69 Why ?
PLAT303_ALERT_2_G Full Occupancy Atom H26 with # Connections 2.00 Check
PLAT343_ALERT_2_G Unusual Angle Range in Main Residue for C5 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.75 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 40.50 Deg.
 O1 -C1 -CS1 1_555 1_555 1_555 # 152 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 36.60 Deg.
 O1 -C1 -CS2 1_555 1_555 3_565 # 153 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 41.10 Deg.
 CS2 -C9 -H9 3_575 1_555 1_555 # 200 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 24.60 Deg.
 CS2 -C26 -H26 1_555 1_555 1_555 # 293 Check
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 50 Note
PLAT953_ALERT_1_G Reported (CIF) and Actual (FCF) Hmax Differ by . 1 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

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

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 01 Check

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing 0.00010 Ang.
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 2 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 2.05 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 38.60 Deg.
RB1 -C10 -H10 3_666 1_555 1_555 # 120 Check
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
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 7 Info

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
5 ALERT type 4 Improvement, methodology, query or suggestion
1 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 06/07/2023; check.def file version of 30/06/2023









