

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: BrBPSSEt_4.91GPa

Bond precision: = 0.0000 A

Wavelength=0.61795

Cell: a=15.81103(17) b=15.81103(17) c=3.69185(6)
 alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	922.92(9)	922.92(2)
Space group	P -4 21 m	P -4 21 m
Hall group	P -4 2ab	P -4 2ab
Moiety formula	C7 H5 Br N3 Se4	C7 H5 Br N3 Se4
Sum formula	C7 H5 Br N3 Se4	C7 H5 Br N3 Se4
Mr	526.88	526.88
Dx, g cm-3	3.792	3.792
Z	4	4
Mu (mm-1)	13.902	0.000
F000	956.0	0.0
F000'	959.27	
h, k, lmax		0, 0, 0
Nref		81
Tmin, Tmax		1.000, 1.000
Tmin'		

Correction method= ?

Data completeness= Theta(max)= 0.000

R(reflections)= wR2(reflections)=

S = Npar=

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

PLAT431_ALERT_2_A Short Inter HL..A Contact Br1 .. Br1 .. 3.00 Ang.

Alert level C

REFI023_ALERT_1_C _refine_diff_density_max is missing
Maximum value of final difference map (e A-3).

The following tests will not be performed
DIFMN_01,DIFMX_01,DIFMX_02
REFI024_ALERT_1_C _refine_diff_density_min is missing
Minimum value of final difference map (e A-3).
The following tests will not be performed
DIFMN_01,DIFMN_02,DIFMN_03

PLAT413_ALERT_2_C	Short Inter XH3 .. XHn	H4A .. H5B	..	2.14 Ang.
PLAT152_ALERT_1_C	The Supplied and Calc. Volume s.u. Differ by ...			7 Units
PLAT161_ALERT_4_C	Missing or Zero su (esd)	on x-coordinate for ...		SE1
PLAT161_ALERT_4_C	Missing or Zero su (esd)	on x-coordinate for ...		SE2
PLAT161_ALERT_4_C	Missing or Zero su (esd)	on x-coordinate for ...		C2
PLAT161_ALERT_4_C	Missing or Zero su (esd)	on x-coordinate for ...		C1
PLAT161_ALERT_4_C	Missing or Zero su (esd)	on x-coordinate for ...		N1
PLAT162_ALERT_4_C	Missing or Zero su (esd)	on y-coordinate for ...		SE1
PLAT162_ALERT_4_C	Missing or Zero su (esd)	on y-coordinate for ...		SE2
PLAT162_ALERT_4_C	Missing or Zero su (esd)	on y-coordinate for ...		C2
PLAT162_ALERT_4_C	Missing or Zero su (esd)	on y-coordinate for ...		C1
PLAT162_ALERT_4_C	Missing or Zero su (esd)	on y-coordinate for ...		N1
PLAT163_ALERT_4_C	Missing or Zero su (esd)	on z-coordinate for ...		SE1
PLAT163_ALERT_4_C	Missing or Zero su (esd)	on z-coordinate for ...		SE2
PLAT163_ALERT_4_C	Missing or Zero su (esd)	on z-coordinate for ...		C2
PLAT163_ALERT_4_C	Missing or Zero su (esd)	on z-coordinate for ...		C1
PLAT163_ALERT_4_C	Missing or Zero su (esd)	on z-coordinate for ...		N1

● Alert level G

PLAT432_ALERT_2_G	Short Inter X...Y Contact	C4 .. C5	..	3.11 Ang.
PLAT981_ALERT_1_G	No non-zero f" Anomalous Scattering Values Found			?
PLAT982_ALERT_1_G	The reported f' Value Deviates from the IT-value			C
PLAT982_ALERT_1_G	The reported f' Value Deviates from the IT-value			Br
PLAT982_ALERT_1_G	The reported f' Value Deviates from the IT-value			N
PLAT982_ALERT_1_G	The reported f' Value Deviates from the IT-value			Se
PLAT983_ALERT_1_G	The Reported f" Value Deviates from the IT-value			C
PLAT983_ALERT_1_G	The Reported f" Value Deviates from the IT-value			Br
PLAT983_ALERT_1_G	The Reported f" Value Deviates from the IT-value			N
PLAT983_ALERT_1_G	The Reported f" Value Deviates from the IT-value			Se

1 **ALERT level A** = In general: serious problem

0 **ALERT level B** = Potentially serious problem

19 **ALERT level C** = Check and explain

10 **ALERT level G** = General alerts; check

12 **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

0 **ALERT type 3** Indicator that the structure quality may be low

15 **ALERT type 4** Improvement, methodology, query or suggestion

0 **ALERT type 5** Informative message, check

Datablock BrBPSSEt_4.91GPa - ellipsoid plot

