checkCIF/PLATON (full publication check)

You have not supplied any structure factors. As a result the full set of tests cannot be run.

Sample Pz21, Bonazzi cell

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

CIF dictionary
Interpreting this report

Datablock: I

Bond precision: Sb- O = 0.0027 A Wavelength=0.71070

Cell: a=8.1416(3) b=10.6968(3) c=5.7835(2)
alpha=102.758(3) beta=110.657(3) gamma=101.020(3)

Temperature: 293 K

	Calculated	Reported
Volume	439.23(3)	439.23(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	O2 S4 Sb4	O1 S2 Sb2
Sum formula	O2 S4 Sb4	O1 S2 Sb2
Mr	647.32	323.60
Dx,g cm-3	4.894	4.892
Z	2	4
Mu (mm-1)	13.056	13.056
F000	568.0	568.0
F000'	564.49	
h,k,lmax	12,16,8	12,16,8
Nref	3231	4465
Tmin,Tmax	0.440,0.650	0.109,0.667
Tmin'	0.000	

Correction method= GAUSSIAN

Data completeness= 1.382 Theta(max)= 32.680

R(reflections)= 0.0244(2604) wR2(reflections)= wR= 0.0270(4465)

S = 1.120 Npar= 92

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

PLAT021_ALERT_4_B Ratio Unique / Expected Reflections too High ... 1.382

Comment: The structure is twinned. CheckCIF probably does not consider reflections belonging to the second twin individual.

Alert level C

PLAT155_ALERT_4_C The Triclinic Unitcell is NOT Reduced ..... ?
PLAT156_ALERT_4_C Axial System Input Cell not Standard ..... ?
Comment: We use the same unit cell as authors of the previous publication.

Alert level G

PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension . 2
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF ?
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ ?
PLAT045_ALERT_1_G Calculated and Reported Z Differ by ..... 0.50 Ratio
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size .... 0.65 mm
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal ..... 0.00300 Deg.
PLAT158_ALERT_4_G The Input Unitcell is NOT Standard/Reduced ..... ?
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature 293 K
PLAT200_ALERT_1_G Check the Reported _diffrn_ambient_temperature 293 K
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb3 -- S1_a .. 5.0 su
And 2 other PLAT232 Alerts
More ...
PLAT794_ALERT_5_G Note: Tentative Bond Valency for Sb3 (III) 3.25
PLAT794_ALERT_5_G Note: Tentative Bond Valency for Sb4 (III) 3.00
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found !

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
2 **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

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

checkCIF/PLATON (full publication check)

Sample Pz21, Kupcik cell

You have not supplied any structure factors. As a result the full set of tests cannot be run.
No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Datablock: I

Bond precision: Sb- O = 0.0020 A Wavelength=0.71070
Cell: a=21.6466(9) b=8.1416(3) c=20.3824(9)
alpha=90.079(4) beta=101.985(5) gamma=89.948(4)
Temperature: 293 K

	Calculated	Reported
Volume	3513.9(3)	3513.8(3)
Space group	F -1	X-1
Hall group	-F 1	-X
Moiety formula	O S2 Sb2	O1 S2 Sb2
Sum formula	O S2 Sb2	O1 S2 Sb2
Mr	323.66	323.60
Dx,g cm-3	3.671	4.892
Z	24	32
Mu (mm-1)	9.792	13.056
F000	3408.0	568.0
F000'	3386.91	
h,k,lmax	32,12,30	31,12,30
Nref	6455	4465
Tmin,Tmax	0.440,0.650	0.109,0.667
Tmin'	0.000	

Correction method= GAUSSIAN
Data completeness= 0.692 Theta(max)= 32.680
R(reflections)= 0.0243(2604) wR2(reflections)= wR= 0.0270(4465)
S = 1.110 Npar= 92

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

CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as calculated from the _atom_site* data lies outside the range 0.90 <> 1.10
From the CIF: _cell_formula_units_Z 32

```
          From the CIF: _chemical_formula_weight          323.60
          TEST: Calculate formula weight from _atom_site_*
          atom     mass    num     sum
          O        16.00    0.50    8.00
          S        32.07    1.00   32.07
          Sb      121.75    1.00  121.75
          Calculated formula weight             161.82
SYMMG01_ALERT_1_A          Unrecognised _symmetry_space_group_name_H-M
           International Tables space group number is not in the CIF
          From the CIF: _symmetry_space_group_name_H-M      X-1
          Int. Tables space group number for X-1 is   0
SYMMG02_ALERT_1_A        Supplied _symmetry_space_group_name_H-M not recognised
          From the CIF: _symmetry_equiv_pos_as_xyz
                                       x,y,z
                                       -x+1/2,-y+1/2,-z
                                       x+3/4,y+1/4,z+1/2
                                       -x+1/4,-y+3/4,-z+1/2
                                       x+1/2,y+1/2,z
                                       -x,-y,-z
                                       x+1/4,y+3/4,z+1/2
                                       -x+3/4,-y+1/4,-z+1/2
                                       x+1/4,y+1/4,z
                                       -x+3/4,-y+3/4,-z
                                       x,y+1/2,z+1/2
                                       -x+1/2,-y,-z+1/2
                                       x+3/4,y+3/4,z
                                       -x+1/4,-y+1/4,-z
                                       x+1/2,y,z+1/2
                                       -x,-y+1/2,-z+1/2
          These symops generate the Hall space group symbol   -f
           which is equivalent to the H-M space group symbol
PLAT043_ALERT_1_A Check Reported Molecular Weight ...............     323.60
PLAT044_ALERT_1_A Calculated and Reported Dx Differ .............          ?
PLAT051_ALERT_1_A Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .      25.00 %
PLAT129_ALERT_4_A Unusual Space-group Specified .................        X-1
```

Comment: All these differences are due to the non-standard axial setting of Kupcík. Platon does not consider the extra centering points (in addition to the F-centering), so some values are calculated incorrectly. Reason why the non-standard cell is used is justified in the text.

Alert level C

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT120_ALERT_1_C Reported SPGR X-1     Inconsistent with Explicit      F-1
PLAT126_ALERT_1_C Error in or Uninterpretable Hall Symbol  .......         -X
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .         71 Ang3
```

Comment: Also these alerts are due to the non-standard axial setting.

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:O1 S2 Sb2
           Atom count from the _atom_site data:  O0.5 S1 Sb1
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   32
From the CIF: _chemical_formula_sum  O1 S2 Sb2
TEST: Compare cell contents of formula and atom_site data

atom    Z*formula  cif sites diff
O         32.00     16.00   16.00
S         64.00     32.00   32.00
Sb        64.00     32.00   32.00
```

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF ?
PLAT045_ALERT_1_G Calculated and Reported Z Differ by ..... 0.75 Ratio
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size .... 0.65 mm
PLAT104_ALERT_1_G The Reported Crystal System is Inconsistent with F-1
PLAT110_ALERT_2_G ADDSYM Detects Potential Lattice Centering or Halving . ?
PLAT112_ALERT_2_G ADDSYM Detects Additional (Pseudo) Symm. Elem... m
And 3 other PLAT112 Alerts
More ...
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space-group. P-1
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature 293 K
PLAT200_ALERT_1_G Check the Reported _diffrn_ambient_temperature 293 K
PLAT794_ALERT_5_G Note: Tentative Bond Valency for Sb1 (III) 2.20
And 3 other PLAT794 Alerts
More ...
PLAT804_ALERT_5_G ARU-Pack Problem in PLATON Analysis ..... 1021 Times
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found !

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

15 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 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
2 ALERT type 4 Improvement, methodology, query or suggestion
7 ALERT type 5 Informative message, check

checkCIF/PLATON (full publication check)

Sample Pz24, Bonazzi cell

You have not supplied any structure factors. As a result the full set of tests cannot be run.
No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Datablock: I

Bond precision: Sb- O = 0.0053 A Wavelength=0.71070
Cell: a=8.1372(2) b=10.6969(3) c=5.7840(1)
alpha=102.787(2) beta=110.6063(19) gamma=100.9833(19)
Temperature: 293 K

	Calculated	Reported
Volume	439.24(2)	439.24(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	O2 S4 Sb4	O1 S2 Sb2
Sum formula	O2 S4 Sb4	O1 S2 Sb2
Mr	647.32	323.60
Dx,g cm-3	4.894	4.892
Z	2	4
Mu (mm-1)	13.056	13.056
F000	568.0	568.0
F000'	564.49	
h,k,lmax	12,16,8	12,16,8
Nref	3244	4591
Tmin,Tmax	0.347,0.878	0.048,0.779
Tmin'	0.000	

Correction method= GAUSSIAN
Data completeness= 1.415 Theta(max)= 32.710
R(reflections)= 0.0321(3769) wR2(reflections)= wR= 0.0382(4591)
S = 2.190 Npar= 92

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

PLAT021_ALERT_4_B Ratio Unique / Expected Reflections too High ... 1.415

Comment: The structure is twinned. CheckCIF probably does not consider reflections belonging to the second twin individual.

Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00
Goodness of fit given = 2.190

PLAT155_ALERT_4_C	The Triclinic Unitcell is NOT Reduced	?
PLAT156_ALERT_4_C	Axial System Input Cell not Standard	?

Comment: The sample studied is not of good quality (mineral), thus the thus the goodness of fit parameter is somewhat above the allowed range.
We use the same unit cell as authors of the previous publication.

Alert level G

PLAT004_ALERT_5_G	Info: Polymeric Structure Found with Dimension .	2
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	?
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	?
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by	0.50 Ratio
PLAT063_ALERT_4_G	Crystal Size Likely too Large for Beam Size	0.95 mm
PLAT158_ALERT_4_G	The Input Unitcell is NOT Standard/Reduced	?
PLAT199_ALERT_1_G	Check the Reported _cell_measurement_temperature	293 K
PLAT200_ALERT_1_G	Check the Reported _diffrn_ambient_temperature	293 K
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Sb4 -- S3_d ..	6.4 su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Sb4 -- S4_d ..	6.7 su
PLAT794_ALERT_5_G	Note: Tentative Bond Valency for Sb3 (III)	3.24
PLAT794_ALERT_5_G	Note: Tentative Bond Valency for Sb4 (III)	3.01
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found	!

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

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checkCIF/PLATON (full publication check)

Sample Pz24, Kupcik cell

You have not supplied any structure factors. As a result the full set of tests cannot be run.
No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Datablock: I

Bond precision: Sb- O = 0.0060 A Wavelength=0.71070
Cell: a=21.6558(5) b=8.1372(2) c=20.3859(8)
alpha=90.028(3) beta=101.994(3) gamma=89.986(2)
Temperature: 293 K

	Calculated	Reported
Volume	3513.93(19)	3513.92(19)
Space group	F -1	X-1
Hall group	-F 1	-X
Moiety formula	O S2 Sb2	O1 S2 Sb2
Sum formula	O S2 Sb2	O1 S2 Sb2
Mr	323.66	323.60
Dx,g cm-3	3.671	4.892
Z	24	32
Mu (mm-1)	9.792	13.056
F000	3408.0	4544.0
F000'	3386.91	
h,k,lmax	32,12,30	32,12,30
Nref	6476	4591
Tmin,Tmax	0.347,0.878	0.048,0.779
Tmin'	0.000	

Correction method= GAUSSIAN
Data completeness= 0.709 Theta(max)= 32.710
R(reflections)= 0.0321(3769) wR2(reflections)= wR= 0.0381(4591)
S = 2.190 Npar= 93

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

CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as calculated from the _atom_site* data lies outside the range 0.90 <> 1.10
From the CIF: _cell_formula_units_Z 32

```
          From the CIF: _chemical_formula_weight          323.60
          TEST: Calculate formula weight from _atom_site_*
          atom     mass    num     sum
          O        16.00    0.50    8.00
          S        32.07    1.00   32.07
          Sb      121.75    1.00  121.75
          Calculated formula weight             161.82
SYMMG01_ALERT_1_A          Unrecognised _symmetry_space_group_name_H-M
           International Tables space group number is not in the CIF
          From the CIF: _symmetry_space_group_name_H-M      X-1
          Int. Tables space group number for X-1 is   0
SYMMG02_ALERT_1_A        Supplied _symmetry_space_group_name_H-M not recognised
          From the CIF: _symmetry_equiv_pos_as_xyz
                                          x,y,z
                                          -x+1/2,-y+1/2,-z
                                          x+3/4,y+1/4,z+1/2
                                          -x+1/4,-y+3/4,-z+1/2
                                          x+1/2,y+1/2,z
                                          -x,-y,-z
                                          x+1/4,y+3/4,z+1/2
                                          -x+3/4,-y+1/4,-z+1/2
                                          x+1/4,y+1/4,z
                                          -x+3/4,-y+3/4,-z
                                          x,y+1/2,z+1/2
                                          -x+1/2,-y,-z+1/2
                                          x+3/4,y+3/4,z
                                          -x+1/4,-y+1/4,-z
                                          x+1/2,y,z+1/2
                                          -x,-y+1/2,-z+1/2
          These symops generate the Hall space group symbol   -f
           which is equivalent to the H-M space group symbol
PLAT043_ALERT_1_A Check Reported Molecular Weight ...............     323.60
PLAT044_ALERT_1_A Calculated and Reported Dx Differ .............          ?
PLAT051_ALERT_1_A Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .      25.00 %
PLAT129_ALERT_4_A Unusual Space-group Specified .................        X-1
```

Comment: All these differences are due to the non-standard axial setting of Kupcík. Platon does not consider the extra centering points (in addition to the F-centering), so some values are calculated incorrectly. Reason why the non-standard cell is used is justified in the text.

Alert level C

```
GOODF01_ALERT_2_C  The least squares goodness of fit parameter lies
           outside the range 0.80 <> 2.00
           Goodness of fit given =      2.190
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT120_ALERT_1_C Reported SPGR X-1     Inconsistent with Explicit      F-1
PLAT126_ALERT_1_C Error in or Uninterpretable Hall Symbol  .......         -X
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .         71 Ang3
```

Comment: The sample studied is not of ideal quality (mineral), thus the goodness of fit parameter is somewhat above the allowed range.
Other alerts are due to the non-standard axial setting.

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:O1 S2 Sb2
           Atom count from the _atom_site data: O0.5 S1 Sb1
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   32
           From the CIF: _chemical_formula_sum O1 S2 Sb2
           TEST: Compare cell contents of formula and atom_site data

           atom   Z*formula cif sites diff
           O   32.00   16.00   16.00
           S   64.00   32.00   32.00
           Sb   64.00   32.00   32.00
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF   ?
PLAT045_ALERT_1_G Calculated and Reported Z Differ by .....   0.75 Ratio
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size .... 0.95 mm
PLAT104_ALERT_1_G The Reported Crystal System is Inconsistent with   F-1
PLAT110_ALERT_2_G ADDSYM Detects Potential Lattice Centering or Halving .   ?
PLAT112_ALERT_2_G ADDSYM Detects Additional (Pseudo) Symm. Elem...   m
And 3 other PLAT112 Alerts
More ...
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space-group.   P-1
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature   293 K
PLAT200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature   293 K
PLAT794_ALERT_5_G Note: Tentative Bond Valency for Sb1   (III)   2.21
And 3 other PLAT794 Alerts
More ...
PLAT804_ALERT_5_G ARU-Pack Problem in PLATON Analysis .....   1021 Times
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found   !

---

   7 **ALERT level A** = Most likely a serious problem - resolve or explain
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  21 **ALERT level G** = General information/check it is not something unexpected

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  10 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
   2 ALERT type 4 Improvement, methodology, query or suggestion
   7 ALERT type 5 Informative message, check
