checkCIF/PLATON report

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

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: I

```
Bond precision:   Mo- O = 0.0225 A         Wavelength=0.71073

Cell:          a=6.09721(10)       b=7.50731(16)     c=7.6779(2)
               alpha=110.4285(13)  beta=93.1670(13)  gamma=113.5086(14)
Temperature:   0 K
```

	Calculated	Reported
Volume	294.172(12)	294.171(12)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	Ag2 Mo2 O7	?
Sum formula	Ag2 Mo2 O7	Ag2 Mo2 O7
Mr	519.62	519.62
Dx,g cm-3	5.866	0.000
Z	2	2
Mu (mm-1)	10.706	0.000
F000	468.0	0.0
F000'	457.70	
h,k,lmax		
Nref		
Tmin,Tmax		
Tmin'		

```
Correction method= Not given

Data completeness=                  Theta(max)=

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

EXPT001_ALERT_1_A _exptl_crystal_density_diffrn is missing
Density calculated from unit cell and contents (Mg m-3).
The following tests will not be performed.
DENSD_01,DENSX_01
DIFF001_ALERT_1_A _diffrn_radiation_type is missing
The radiation type should contain one of the following
* 'Cu K\a'
* 'Mo K\a'
* 'Ag K\a'
* neutron
* synchrotron
The following tests will not be performed.
ABSMU_01,ABSTM_02,CRYSS_01,RADNW_01
DIFF002_ALERT_1_A _diffrn_radiation_wavelength is missing
Radiation wavelength (A).
The following tests will not be performed.
RADNW_01,REFLT_03,REFNR_01,THETM_01
CELL003_ALERT_1_A _cell_measurement_reflns_used is missing
Number of reflections used to measure unit cell.
CELL004_ALERT_1_A _cell_measurement_theta_min is missing
Minimum theta of reflections used to measure unit cell.
The following tests will not be performed.
CELLT_01
CELL005_ALERT_1_A _cell_measurement_theta_max is missing
Maximum theta of reflections used to measure unit cell.
The following tests will not be performed.
CELLT_01
CELL006_ALERT_1_A _cell_measurement_temperature is missing
Measurement temperature (K).
The following tests will not be performed.
CELLK_01
EXPT004_ALERT_1_A _exptl_absorpt_coefficient_mu is missing
Linear absorption coefficient (mm-1).
The following tests will not be performed.
ABSMU_01,ABSTM_02
EXPT005_ALERT_1_A _exptl_crystal_description is missing
Crystal habit description.
The following tests will not be performed.
CRYSR_01
EXPT009_ALERT_1_A No crystal dimensions have been given.
The following tests will not be performed.
CRYSS_01,CRYSS_02
EXPT010_ALERT_1_A _exptl_crystal_colour (_pd_char_colour for powder) is missing
Crystal colour.
The following tests will not be performed.
CRYSC_01
DIFF003_ALERT_1_A _diffrn_measurement_device_type is missing
Diffractometer make and type. Replaces _diffrn_measurement_type.
DIFF005_ALERT_1_A _diffrn_measurement_method is missing
Mode of intensity measurement and scan.
DIFF007_ALERT_1_A _diffrn_reflns_number is missing

```
            Total number of reflections measured.
            The following tests will not be performed.
            REFLG_01,REFLT_01
REFL001_ALERT_1_A  _reflns_number_total is missing
            Number of symmetry-independent reflections.
            The following tests will not be performed.
            REFLT_01,REFLT_02,REFLT_03,REFNR_01
REFL002_ALERT_1_A  _reflns_number_gt is missing
            Number of reflections > sigma threshold.
            The following tests will not be performed.
            REFLG_01,REFLT_02
REFL004_ALERT_1_A  _reflns_threshold_expression is missing
            Sigma expression for F, F2 or I threshold.
            The following tests will not be performed.
            REFLE_01
DIFF008_ALERT_1_A  _diffrn_reflns_theta_max is missing
            Maximum theta of measured reflections.
            The following tests will not be performed
            REFLT_03,REFNR_01,THETM_01
DIFF013_ALERT_1_A  _diffrn_reflns_limit_h_min is missing
            Minimum h index of measured data.
            The following tests will not be performed
            REFLL_01
DIFF014_ALERT_1_A  _diffrn_reflns_limit_h_max is missing
            Maximum h index of measured data.
            The following tests will not be performed
            REFLL_01
DIFF015_ALERT_1_A  _diffrn_reflns_limit_k_min is missing
            Minimum k index of measured data.
            The following tests will not be performed
            REFLL_01
DIFF016_ALERT_1_A  _diffrn_reflns_limit_k_max is missing
            Maximum k index of measured data.
            The following tests will not be performed
            REFLL_01
DIFF017_ALERT_1_A  _diffrn_reflns_limit_l_min is missing
            Minimum l index of measured data.
            The following tests will not be performed
            REFLL_01
DIFF018_ALERT_1_A  _diffrn_reflns_limit_l_max is missing
            Maximum l index of measured data.
            The following tests will not be performed
            REFLL_01
DIFF019_ALERT_1_A  _diffrn_standards_number is missing
            Number of standards used in measurement.
DIFF020_ALERT_1_A  _diffrn_standards_interval_count and
            _diffrn_standards_interval_time are missing. Number of measurements
            between standards or time (min) between standards.
DIFF022_ALERT_1_A  _diffrn_standards_decay_% is missing
            Percentage decrease in standards intensity.
REFI001_ALERT_1_A  _refine_ls_structure_factor_coef is missing
            The structure factor coefficient should be one of the following
            *  Inet
            *  Fsqd
            *  F
            The following tests will not be performed
            FCOEF_01
```

```
REFI003_ALERT_1_A  _refine_ls_R_factor_gt is missing
            R factor of F for reflections > threshold.
            The following tests will not be performed
            RFACG_01
REFI005_ALERT_1_A  _refine_ls_wR_factor_ref is missing
            R factor of coefficient for refinement reflections.
            The following tests will not be performed
            RFACR_01
REFI007_ALERT_1_A  _refine_ls_goodness_of_fit_ref is missing
            Goodness of fit S for refinement reflections.
            The following tests will not be performed
            GOODF_01
REFI009_ALERT_1_A  _refine_ls_number_reflns is missing
            Number of reflections used in refinement.
            The following test will not be performed
            REFNR_01
REFI010_ALERT_1_A  _refine_ls_number_parameters is missing
            Number of parameters refined.
            The following tests will not be performed
            REFNR_01
REFI011_ALERT_1_A  _refine_ls_weighting_scheme is missing
            The weighting scheme should be one of the following
            *  sigma
            *  calc
            The following tests will not be performed
            WEIGH_01
REFI015_ALERT_1_A  _refine_ls_shift/su_max is missing
            Maximum shift/s.u. ratio after final refinement cycle.
            The following tests will not be performed
            SHFSU_01
REFI017_ALERT_1_A  _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
REFI018_ALERT_1_A  _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
ATOM007_ALERT_1_A  _atom_site_aniso_label is missing
            Unique label identifying the atom site.
GEOM001_ALERT_1_A  _geom_bond_atom_site_label_1 is missing
            Label identifying the atom site 1.
GEOM002_ALERT_1_A  _geom_bond_atom_site_label_2 is missing
            Label identifying the atom site 2.
GEOM003_ALERT_1_A  _geom_bond_distance is missing
            Distance between atom sites 1 and 2.
GEOM005_ALERT_1_A  _geom_angle_atom_site_label_1 is missing
            Label identifying the atom site 1.
GEOM006_ALERT_1_A  _geom_angle_atom_site_label_2 is missing
            Label identifying the atom site 2.
GEOM007_ALERT_1_A  _geom_angle_atom_site_label_3 is missing
            Label identifying the atom site 3.
ABSTY01_ALERT_1_A  The absorption correction should be one of the following
            *  none
            *  analytical
            *  integration
            *  numerical
```

```
            *  gaussian
            *  empirical
            *  psi-scan
            *  multi-scan
            *  refdelf
            *  sphere
            *  cylinder
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low .      0.000 Why?
PLAT044_ALERT_1_A Calculated and Reported Density Dx  Differ by ..     5.8663 Check
PLAT050_ALERT_1_A Absorption Coefficient mu Not Given .............    Please Do !
PLAT086_ALERT_2_A Unsatisfactory S Value (Too Low or Not Given) ..       0.00 Check
PLAT183_ALERT_1_A Missing _cell_measurement_reflns_used Value ....     Please Do !
PLAT184_ALERT_1_A Missing _cell_measurement_theta_min Value ......     Please Do !
PLAT185_ALERT_1_A Missing _cell_measurement_theta_max Value ......     Please Do !
PLAT197_ALERT_1_A Missing _cell_measurement_temperature Datum ....     Please Add
PLAT198_ALERT_1_A Missing _diffrn_ambient_temperature   Datum ....     Please Add
              Ag1       Ag2       Mo1       Mo2       O1                 etc.
PLAT699_ALERT_1_A Missing _exptl_crystal_description Value .......     Please Do !
PLAT880_ALERT_1_A No datum for _diffrn_reflns_number supplied ....     Please Do !
PLAT881_ALERT_1_A No Datum for _diffrn_reflns_av_R_equivalents ...     Please Do !
```

Alert level B

```
PLAT025_ALERT_1_B Hmin..Lmax Data Incomplete or Missing ..........     Please Check
```

Alert level C

```
ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
            a literature citation. This should be contained in the
            _exptl_absorpt_process_details field.
            Absorption correction given as Not Given
PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given .....     Please Do !
```

Alert level G

```
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT794_ALERT_5_G Tentative Bond Valency for Ag1       (I)       .       1.08 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Ag2       (I)       .       1.10 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Mo1       (VI)      .       6.03 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Mo2       (VI)      .       5.95 Info
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found     Please Check
PLAT882_ALERT_1_G No Datum for _diffrn_reflns_av_unetI/netI ......     Please Do !
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT980_ALERT_1_G No Anomalous Scattering Factors Found in CIF ...     Please Check
```

```
  57 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
  10 ALERT level G = General information/check it is not something unexpected

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

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.
PUBL016_ALERT_1_A  Details of the refinement are missing.
           e.g. _publ_section_exptl_refinement
           _computing_data_collection
           _computing_cell_refinement , etc.
ATOM001_ALERT_1_A  _atom_type_scat_source is missing
           Reference to scattering factors applied.
```

Alert level G

```
PUBL017_ALERT_1_G The _publ_section_references section is missing or
           empty.
```

9 **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).
```

```
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
_vrf_PUBL016_GLOBAL
;
PROBLEM: Details of the refinement are missing.
RESPONSE: ...
;
_vrf_ATOM001_GLOBAL
;
PROBLEM: _atom_type_scat_source is missing
RESPONSE: ...
;
_vrf_EXPT001_I
;
PROBLEM: _exptl_crystal_density_diffrn is missing
RESPONSE: ...
;
_vrf_DIFF001_I
;
PROBLEM: _diffrn_radiation_type is missing
RESPONSE: ...
;
_vrf_DIFF002_I
;
PROBLEM: _diffrn_radiation_wavelength is missing
RESPONSE: ...
;
_vrf_CELL003_I
;
PROBLEM: _cell_measurement_reflns_used is missing
RESPONSE: ...
;
_vrf_CELL004_I
;
PROBLEM: _cell_measurement_theta_min is missing
RESPONSE: ...
;
_vrf_CELL005_I
;
PROBLEM: _cell_measurement_theta_max is missing
RESPONSE: ...
;
_vrf_CELL006_I
;
PROBLEM: _cell_measurement_temperature is missing
RESPONSE: ...
;
_vrf_EXPT004_I
;
PROBLEM: _exptl_absorpt_coefficient_mu is missing
RESPONSE: ...
;
```

```
_vrf_EXPT005_I
;
PROBLEM: _exptl_crystal_description is missing
RESPONSE: ...
;
_vrf_EXPT009_I
;
PROBLEM: No crystal dimensions have been given.
RESPONSE: ...
;
_vrf_EXPT010_I
;
PROBLEM: _exptl_crystal_colour (_pd_char_colour for powder) is missing
RESPONSE: ...
;
_vrf_DIFF003_I
;
PROBLEM: _diffrn_measurement_device_type is missing
RESPONSE: ...
;
_vrf_DIFF005_I
;
PROBLEM: _diffrn_measurement_method is missing
RESPONSE: ...
;
_vrf_DIFF007_I
;
PROBLEM: _diffrn_reflns_number is missing
RESPONSE: ...
;
_vrf_REFL001_I
;
PROBLEM: _reflns_number_total is missing
RESPONSE: ...
;
_vrf_REFL002_I
;
PROBLEM: _reflns_number_gt is missing
RESPONSE: ...
;
_vrf_REFL004_I
;
PROBLEM: _reflns_threshold_expression is missing
RESPONSE: ...
;
_vrf_DIFF008_I
;
PROBLEM: _diffrn_reflns_theta_max is missing
RESPONSE: ...
;
_vrf_DIFF013_I
;
PROBLEM: _diffrn_reflns_limit_h_min is missing
RESPONSE: ...
;
_vrf_DIFF014_I
;
```

```
PROBLEM: _diffrn_reflns_limit_h_max is missing
RESPONSE: ...
;
_vrf_DIFF015_I
;
PROBLEM: _diffrn_reflns_limit_k_min is missing
RESPONSE: ...
;
_vrf_DIFF016_I
;
PROBLEM: _diffrn_reflns_limit_k_max is missing
RESPONSE: ...
;
_vrf_DIFF017_I
;
PROBLEM: _diffrn_reflns_limit_l_min is missing
RESPONSE: ...
;
_vrf_DIFF018_I
;
PROBLEM: _diffrn_reflns_limit_l_max is missing
RESPONSE: ...
;
_vrf_DIFF019_I
;
PROBLEM: _diffrn_standards_number is missing
RESPONSE: ...
;
_vrf_DIFF020_I
;
PROBLEM: _diffrn_standards_interval_count and
RESPONSE: ...
;
_vrf_DIFF022_I
;
PROBLEM: _diffrn_standards_decay_% is missing
RESPONSE: ...
;
_vrf_REFI001_I
;
PROBLEM: _refine_ls_structure_factor_coef is missing
RESPONSE: ...
;
_vrf_REFI003_I
;
PROBLEM: _refine_ls_R_factor_gt is missing
RESPONSE: ...
;
_vrf_REFI005_I
;
PROBLEM: _refine_ls_wR_factor_ref is missing
RESPONSE: ...
;
_vrf_REFI007_I
;
PROBLEM: _refine_ls_goodness_of_fit_ref is missing
RESPONSE: ...
```

```
;
_vrf_REFI009_I
;
PROBLEM: _refine_ls_number_reflns is missing
RESPONSE: ...
;
_vrf_REFI010_I
;
PROBLEM: _refine_ls_number_parameters is missing
RESPONSE: ...
;
_vrf_REFI011_I
;
PROBLEM: _refine_ls_weighting_scheme is missing
RESPONSE: ...
;
_vrf_REFI015_I
;
PROBLEM: _refine_ls_shift/su_max is missing
RESPONSE: ...
;
_vrf_REFI017_I
;
PROBLEM: _refine_diff_density_max is missing
RESPONSE: ...
;
_vrf_REFI018_I
;
PROBLEM: _refine_diff_density_min is missing
RESPONSE: ...
;
_vrf_ATOM007_I
;
PROBLEM: _atom_site_aniso_label is missing
RESPONSE: ...
;
_vrf_GEOM001_I
;
PROBLEM: _geom_bond_atom_site_label_1 is missing
RESPONSE: ...
;
_vrf_GEOM002_I
;
PROBLEM: _geom_bond_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM003_I
;
PROBLEM: _geom_bond_distance is missing
RESPONSE: ...
;
_vrf_GEOM005_I
;
PROBLEM: _geom_angle_atom_site_label_1 is missing
RESPONSE: ...
;
_vrf_GEOM006_I
```

;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_I
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_ABSTY01_I
;
PROBLEM: The absorption correction should be one of the following
RESPONSE: ...
;
_vrf_PLAT029_I
;
PROBLEM: _diffrn_measured_fraction_theta_full value Low .   0.000 Why?
RESPONSE: ...
;
_vrf_PLAT044_I
;
PROBLEM: Calculated and Reported Density Dx Differ by ..   5.8663 Check
RESPONSE: ...
;
_vrf_PLAT050_I
;
PROBLEM: Absorption Coefficient mu Not Given .....   Please Do !
RESPONSE: ...
;
_vrf_PLAT086_I
;
PROBLEM: Unsatisfactory S Value (Too Low or Not Given) ..   0.00 Check
RESPONSE: ...
;
_vrf_PLAT183_I
;
PROBLEM: Missing _cell_measurement_reflns_used Value ....   Please Do !
RESPONSE: ...
;
_vrf_PLAT184_I
;
PROBLEM: Missing _cell_measurement_theta_min Value ......   Please Do !
RESPONSE: ...
;
_vrf_PLAT185_I
;
PROBLEM: Missing _cell_measurement_theta_max Value ......   Please Do !
RESPONSE: ...
;
_vrf_PLAT197_I
;
PROBLEM: Missing _cell_measurement_temperature Datum ....   Please Add
RESPONSE: ...
;
_vrf_PLAT198_I
;
PROBLEM: Missing _diffrn_ambient_temperature   Datum ....   Please Add

```
RESPONSE: ...
;
_vrf_PLAT699_I
;
PROBLEM: Missing _exptl_crystal_description Value .......     Please Do !
RESPONSE: ...
;
_vrf_PLAT880_I
;
PROBLEM: No datum for _diffrn_reflns_number supplied ....     Please Do !
RESPONSE: ...
;
_vrf_PLAT881_I
;
PROBLEM: No Datum for _diffrn_reflns_av_R_equivalents ...     Please Do !
RESPONSE: ...
;
# 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 13/07/2021; check.def file version of 13/07/2021

Datablock I - ellipsoid plot