CIF VALIDATION WITH THE PROGRAM PLATON (VERSION 01-10-2010)

See also:A.L.Spek, J.Appl.Cryst. 2003, 36, 7-13; A.L.Spek, Acta Cryst. 2009, D65, 148-155.

The structure validation report as generated with the program PLATON/CHECK depends on the external file *check.def*. That file contains the tests, error thresholds and short warning messages along with some text offering explanation and advise on the issues raised. This document collects and often expands on the text associated with each ALERT item in the file *check.def*.

Most but not all PLATON/CHECK ALERTS have been implemented in the Web-based IUCr CheckCIF/PLATON facility. Some duplicate named (i.e. not indicated as PLATxxx) Alerts or are warnings for issues taken care of by the software used for Acta Cryst. publications.

In this document, ALERTS are identified as ALERT_*n*_*mxx*, where *n* indicates the alert type, *m* the alert category number and xx a two digit serial number.

ALERT TYPES

ALERT_1_ = CIF Construction/Syntax Error, Inconsistent or Missing Data.
ALERT_2_ = Indicator that the Structure Model may be Wrong or Deficient.
ALERT_3_ = Indicator that the Structure Quality may be Low.
ALERT_4_ = Cosmetic improvement, Methodology, Query or Suggestion.
ALERT_5_ = Informative Message, Check.

ALERT CATEGORIES

n_0xx - general
n_1xx - cell/symmetry
n_2xx - adp-related
n_3xx - intra geometry
n_4xx - inter geometry
n_5xx - coordination geometry
n_6xx - void tests
n_7xx - varia
n_8xx - (Fatal) Software Errors/Problems
n_9xx - Reflection data issues

Notes:

- The terminology used is generally based on SHELXL practice. However, no other refinement packages are excluded. Where relevant, certain ALERTS are suppressed is such a case.
- FCF indicates an F(obs), F(calc) type of file (type 4 in case of SHELXL)
- Weight indicates the SHELXL weight expression.

EXAMPLE OUTPUT OF A NATIVE PLATON/CHECK VALIDATION RUN

```
#===============================================================================

# PLATON/CHECK-(190210) versus check.def version of 180210  for entry: ambi
# Data From: ambi.acc - Data Type: CIF          Bond Precision   C-C = 0.0016 A
# Refl Data: ambi.fcf - Data Type: SHELXL                          Temp = 293 K
#
# UCL  7.6421(10)   7.8306(8)   11.049(3)           90           90          90
# WaveLength 0.71073    Volume Reported      661.2(2)  Calculated      661.2(2)
# SpaceGroup from Symmetry P 21 21 21    Hall: P 2ac 2ab
#                 Reported P 21 21 21          P 2ac 2ab
# MoietyFormula C4 H5 O6, H4 N
#      Reported C4 H5 O6, H4 N
#    SumFormula C4 H9 N O6
#      Reported C16 H36 N4 O24
# Mr        =    167.12[Calc],    167.12[Rep]
# Dx,gcm-3  =     1.679[Calc],     1.679[Rep]
# Z         =         4[Calc],         4[Rep]
# Mu (mm-1) =     0.161[Calc],     0.161[Rep]
# F000      =     352.0[Calc],     352.0[Rep]  or F000' =    352.28[Calc]
# Reported   Hmax=  9, Kmax= 10, Lmax= 14, Nref=  1521        , Th(max)= 27.500
# Obs in FCF Hmax=  9, Kmax= 10, Lmax= 14, Nref=  1521        , Th(max)= 27.496
# Calculated Hmax=  9, Kmax= 10, Lmax= 14, Nref=   909[  1528], Ratio=1.67/1.00
# Reported   Rho(min) = -0.17, Rho(max) =  0.23 e/Ang**3 (From CIF)
# Calculated Rho(min) = -0.17, Rho(max) =  0.23 e/Ang**3 (From CIF+FCF data)
# w=1/[sigma**2(Fo**2)+(0.0350P)**2+  0.1164P], P=(Fo**2+2*Fc**2)/3
# R= 0.0239(  1501), wR2= 0.0636(  1521), S = 1.101      (From CIF+FCF data)
# R= 0.0239(  1501), wR2= 0.0636(  1521), S = 1.101      (From FCF data only)
# R= 0.0239(  1501), wR2= 0.0636(  1521), S = 1.101, Npar= 136, Flack   -0.1(8)
#                          Friedel Pair Coverage (Perc.) = 100, Hooft -0.05(16)
#===============================================================================
================================================================================
>>> The Following Improvement and Query ALERTS were generated - (Acta-Mode) <<<
================================================================================
035_ALERT_1_A No _chemical_absolute_configuration info given .          ?
052_ALERT_1_A (Proper) Absorption Correction Method Missing ..          ?
053_ALERT_1_A Minimum Crystal Dimension Missing (or Error) ...          ?
054_ALERT_1_A Medium  Crystal Dimension Missing (or Error) ...          ?
055_ALERT_1_A Maximum Crystal Dimension Missing (or Error) ...          ?
#===============================================================================
024_ALERT_4_C Merging of Friedel Pairs is Indicated ..........          !
032_ALERT_4_C Std. Uncertainty in Flack Parameter too High ...       0.80
041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
194_ALERT_1_C Missing _cell_measurement_reflns_used datum ....          ?
195_ALERT_1_C Missing _cell_measurement_theta_max   datum ....          ?
196_ALERT_1_C Missing _cell_measurement_theta_min   datum ....          ?
#===============================================================================
199_ALERT_1_G Check the Reported _cell_measurement_temperature        293 K
200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature        293 K
791_ALERT_4_G Note: The Model has Chirality at C2     (Verify)          R
791_ALERT_4_G Note: The Model has Chirality at C3     (Verify)          R
#===============================================================================


               ALERT_Level and ALERT_Type Summary
               ==================================
```

```
  5 ALERT_Level_A = In General: Serious Problem.
  8 ALERT_Level_C = Check & Explain.
  4 ALERT_Level_G = General Issues to Check, Not Necessarily Errors.

 11 ALERT_Type_1 CIF Construction/Syntax Error, Inconsistent or Missing Data.
  2 ALERT_Type_3 Indicator that the Structure Quality may be Low.
  4 ALERT_Type_4 Improvement, Methodology, Query or Suggestion.
#===============================================================================
===============================================================================
For Documentation See: http://www.cryst.chem.uu.nl/platon/CIF-VALIDATION.pdf
===============================================================================
>>> The Following Model and Quality ALERTS were generated     - (Acta-Mode) <<<
===============================================================================
     Format: alert-number_ALERT_alert-type_alert-level text
911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600          6
913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          5
#===============================================================================
```

Comments

- The analysis was run as: **platon -U ambi.acc** from the command line. The result will be in files named **ambi.chk** and **ambi.ckf**.
- The Validation can be executed in several modes: (-U and -G switches)
    a) Acta mode, CIF + FCF data: This is the most extensive version
    b) Acta mode, CIF data: CIF's may also be those generated with the CSD software
    c) Non-Acta mode: CIF (+FCF) data: Acta specific ALERTS are left out
- G-Level ALERTS are generally no errors but issues to check
- Three R factor lines are shown. The reported values should be identical within rounding errors. Bottom up they show:

1a) The R, wR2 and S values reported in the CIF
2b) R, wR2 & S values as calculated with the SHELXL weight parameter values reported in the CIF and Fobs and Fcalc data from the FCF.
3c) R, wR2 & S values as calculated with the SHELXL weight parameter values reported in the CIF, Fobs data from the FCF and Fcalc data calculated from the model parameter values in the CIF.

Documentation of the ALERTS

Note: The material below will be updated and extended later-on

==========

ALERT_3_020 A High Rint Value is Reported

==========

Rint (i.e. the value associated with *_diffrn_reflns_av_R_equivalents*) is expected to have a value that is considerably less than 0.12 and in the order of magnitude of the reported wR2-value. Higher than expected Rint values should be accompanied by a suitable explanation in the *_publ_section_exptl_refinement* section of an Acta Crystallographica paper. However, authors should first ensure that there are no overlooked problems. Elevated values of Rint may also be indicative of a need to recollect the data from a higher quality crystal, at low temperature and/or with Copper radiation.

Reasons for high Rint values include:

- Wrong crystal system, Laue group or space-group assignment
- Rint value is based on a very limited reflection data redundancy.
- The correction for absorption is inadequate or inappropriate.
- The overall quality of the data is poor due to the crystal quality.
- The crystal is very weakly diffracting as indicated by high values of *_diffrn_reflns_av_sigmaI/netI*. Large proportion of essentially "unobserved" reflections with high s.u.'s are being used in the refinement.

==========

ALERT_1_021 A too High Actual/Expected number of Reflections Ratio is Reported

==========

Test for redundant reflection data. The actual number of reflections is the number specified with *_reflns_number_total* in the CIF. The expected number of reflections corresponds to the number of reflections in the asymmetric unit of the Laue group. This number is calculated by PLATON on the basis of the supplied values of the cell dimensions, space group and Θ(max). Expected ratios are : less-or-equal 1 for centro-symmetric structures and less than 2 for non-centro-symmetric structures.

Reasons to exceed those numbers can be:

- Systematic extinctions were not omitted from the reported *_reflns_number_total* data count
- The refinement is deliberately done with a redundant/not merged data set. This might be the case with HKLF 5 data.
-

==========

ALERT_3_022 A too Low Actual/Expected number of Reflections Ratio is Reported

==========

Test for data completeness. The ratio of the reported number of unique reflections *_reflns_number_total* and the expected number of reflections for the resolution given in the CIF is reported. This ratio can be low due to a missing cusp of data when collected with a 2D-detector. Alternatively, the wrong asymmetric part of reciprocal space was collected on a serial

detector system.

==========

ALERT_3_023 Low Resolution Data Set

==========

This Alert is issued when sin(theta)/lambda < 0.6. This corresponds to a theta(max) of about 25 degrees for MoKa radiation and is sometimes called 'the Acta Crystallographica or IUCr limit'.

==========

ALERT_4_024 Merging of the Friedel pairs is Indicated

==========

Averaging of Friedel pairs is advised when indicated by a large s.u. on the Flack parameter. Large s.u. values indicate that the anomalous scattering power is too small in combination with the data quality at hand to merit refinement with a non-averaged data set. This will generally be the case with MoKa data sets for structures containing atoms not heavier than Si. The value of the Flack parameter will be largely meaningless anyway for large s.u. values. Use MERG 3 or MERG 4 in case of refinement with the SHELXL97 program. Non-compliance with the above for valid scientific reasons should be discussed in detail in the experimental section of the paper.

==========

ALERT_1_025 The Reported and Calculated Hmin..Lmax Values Differ

==========

Check the reported h,k,l - range with the range calculated by PLATON based on reported theta-max.

==========

ALERT_3_026 Check for low Ratio of Observed/Unique Reflection Data

==========

This is a check whether a sufficient fraction of the unique data is above the 2 * sigma(I) level.

==========

ALERT_3_027 - *_diffrn_reflns_theta_full* (too) Low

==========

Ideally (and a requirement for publication in Acta Crystallographica), the dataset should be essentially complete, as defined by *-diffrn-measured-fraction-theta-full* (close to 1.0), up to sin(theta)/lambda = 0.6 (i.e. 25.24 degrees MoKa).

The major causes of incomplete data sets are:

- A missing cusp of data due to data collection by rotation around the spindle axis only (standard on some image-plate systems).
  Cure: collect an additional data set after remounting the crystal.
- The DENZO image processing package has problems with certain strong reflections. They are often excluded from the data set.
  Cure: Add an additional scan at lower power setting in order to include strong low order reflections.
- Incomplete scans.

==========

ALERT_3_028 Low value of _*diffrn_measured_fraction_theta_max*

==========

Ideally, the reported '*_diffrn_measured_fraction_theta_max*' value, corresponding to theta-max, should be close to 1.0.

==========

ALERT_3_029 Low Value of _*diffrn_measured_fraction_theta_full*

==========

Ideally (and a requirement for publication in Acta Crystallographica), this fraction should be close to 1.0 for theta-full greater or equal to sin(theta/lambda) = 0.6 (i.e. 25.24 degrees for MoKa and 67.7 degrees for CuKa radiation).

Causes of incomplete data sets are:

- A missing cusp of data due to data collection by rotation around the spindle axis only (standard on some image-plate systems).
  Cure: collect an additional data set after remounting the crystal.
- Some image processing packages have problems with certain strong reflections. Those reflections are often excluded from the data set.
  Cure: Add an additional scan at lower power setting in order to include strong low order reflections.
- Incomplete scans, possibly based on erroneously assumed higher than actual symmetry.

Note: The default value of *_diffrn_measured_fraction_theta_full* that is automatically calculated and inserted in the CIF by SHELXL-97 might generate A-level ALERTS when significant numbers of reflections are missing at higher theta values. In order to avoid such an ALERT, substitute the values calculated with the SHELXL instruction 'ACTA 50' for *_diffrn_reflns_theta_full* and *_diffrn_measured_fraction_theta_full* respectively. For Mo-radiation, corresponding values of 25 degees (or higher) and 0.99 (or higher) are expected. PLATON may be used to analyse the case at hand (by invoking either the 'FCF-VALIDATION' mode or the 'ASYM-VIEW' mode).

==========

ALERT_1_030 - _*diffrn_reflns_number* Value less than _*reflns_number_total Value*

==========

The number of measured reflections should be equal or greater than the number of unique reflections.

==========

ALERT_4_031 - Refined Extinction Parameter within Range

==========

This test checks whether a refined extinction parameter is meaningful i.e. whether its value is significantly larger than its corresponding s.u. If not, this parameter should be removed from the model and the structure refined without this meaningless additional parameter.
The current default gives a warning when its value is within 3.33 s.u. SHELXL97-2 will not

allow negative values leading to ill-convergence and non-zero maximum shift/error values: remove extinction parameter from the refinement.

==========

ALERT_4_032 - Standard Uncertainty in Flack Parameter too High

==========

Check the validity of the absolute structure determination A high s.u. indicates that the experimental data do not support the determination of the absolute structure. This will generally be the case with light atom MoKa data where f'' is nearly zero.

Note: Use the TWIN & BASF 0.0 instructions in SHELXL97. The default FLACK parameter is not always reliable, in particular when strongly correlated with the position of the origin (e.g. along y in space-group P21).

Please refer to Flack,H.D. & Bernardinelli, G. (1999) Acta Cryst. A55, 908-915 and (2000) J. Appl. Cryst., 33, 1143-1148.

==========

ALERT_4_033 The Flack x Parameter Value Deviates from Zero

==========

Check the relevance/validity of the absolute structure determination. Please refer to Flack, H.D. & Bernardinelli, G. (1999) Acta Cryst. A55, 908-915 and (2000) J. Appl. Cryst., 33, 1143-1148.

A value of the Flack parameter that deviates significantly from zero (taking into account the associated s.u.) might indicate that the absolute structure should be inverted in case of a value closer to 1.0 than to zero. A value close to 0.5 may be indicative of an inversion twin or a missed centre of inversion.

For valid absolute structure assignments, abs(x) should be less thans 2 * s.u., with s.u. < 0.04. For enantiopure compounds, s.u. should be less than 0.1.

==========

ALERT_1_034 - No Flack Parameter Given. Z .GT. Si, NonCentro

==========

No Flack parameter value given for non-centrosymmetric structure with heaviest atom Z > Si. This might be intentional.

==========

ALERT_1_035 - No _chemical_absolute_configuration info given

==========

Options are 'rm', 'ad', 'rmad', 'syn', 'unk' or '.'

rm : absolute configuration established by the structure determination of a compound containing a chiral reference molecule of known absolute configuration.
ad : absolute configuration established by anomalous dispersion effects in diffraction measurements on the crystal.
rmad : absolute configuration established by the structure determination of a compound

containing a chiral reference molecule of known absolute configuration and confirmed by anomalous dispersion effects in diffraction measurements on the crystal.
syn : absolute configuration has not been established by anomalous dispersion effects in diffraction measurements on the crystal. The enantiomer has been assigned by reference to an unchanging chiral centre in the synthetic procedure.
unk : absolute configuration is unknown, there being no firm chemical evidence for its assignment to hand and it having not been established by anomalous dispersion effects in diffraction measurements on the crystal. An arbitrary choice of enantiomer has been made. . : inapplicable.

==========

ALERT_1_036 - No s.u. Given for Flack Parameter

==========

No standard uncertainty found for the Flack parameter. When the structure refinement was done with SHELXL97-2, the likely reason for this is a missing BASF instruction. This applies in particular when the associated Flack parameter has the value 0.000. No valid conclusions on the absolute structure can be drawn.

==========

ALERT_1_037 The Value of *_diffrn_reflns_theta_full* is not Given

==========

No information is given about the theta value for which the dataset is complete, subject to the percentage given with the dataname *_diffrn_measured_fraction_theta_full*.

==========

ALERT_1_038 The Value of *_diffrn_measured_fraction_theta_max* is Not Given

==========

The fraction *_diffrn_measured_fraction_theta_max* should be specified in combination with the theta value given with the data name *_diffrn_reflns_theta_full*.

==========

ALERT_1_039 The Value of *_diffrn_measured_fraction_theta_full* is Not Given

==========

This fraction should be specified in combination with the value for theta-max.

==========

ALERT_1_040 No H-Atoms found in CIF for Carbon Atom Containing Compound

==========

This is unusual for a carbon atom containing compound, but may be correct in special cases.

==========

ALERT_1_041 The Calculated and Reported *_chemical_formula_sum* Strings Differ

==========

In the ideal case, both strings (reported and calculated from the data in the CIF) should be identical. If not, the reason for the difference should be clear. Examples are cases where populations do not add up to integer numbers, or when solvent molecules have been SQUEEZED.

Note: SHELXL97 reports population parameters in the CIF with two decimals only. This may lead to non-integer atom counts in cases of disorder due to rounding.

Note: Alerts _041, _042, _043, _044 & _045 can probably be ignored when the relevant values differ by the same factor. A valid reason can be a description of the composition with a different Z value.

==========

ALERT_1_042 The Calculated and Reported *_chemical_formula_moiety* Strings Differ

==========

In the ideal case, the *_chemical_formula_moiety* string as reported should be identical to the *_chemical_formula_moiety* string calculated from the data in the CIF. If not, the reason should be clear. Examples are cases where there is no separating space between two element names or cases where populations do not add up to integer numbers or when moieties are separated by '.' instead of ','.

Example: NO3 should be given as N O3

Note: Alerts _041, _042, _043, _044 & _045 can probably be ignored when the relevant values differ by the same factor.

==========

ALERT_1_043 - Reported and Calculated Molecular Weight Values Differ

==========

Note: atomic weights used in the calculation of the molecular weight are taken from Inorg. Chim. Acta. 217 (1994) 217-218 which deviate in a few cases slightly from the older values used in SHELXL97-2.

==========

ALERT_1_044 The Calculated and Reported Dx Values Differ

==========

In the ideal case, both data items should be the same within a small tolerance. If not, the reason should be clear.

==========

ALERT_1_045 The Calculated and Reported Z Values Differ

==========

In the ideal case, both data items (Z(calc) & Z(reported)) should be the same. If not, the reason for the difference should be clear. An example is the situation where PLATON gives Z = 1 when the program cannot work out a proper Z.

Note: Alerts _041, _042, _043, _044 & _045 can probably be ignored when the relevant values differ by the same factor.

==========

ALERT_1_046 The Reported Z, MW and D(calc) Values are Inconsistent

==========

D(calc) as calculated from the reported Z and MW is compared for consistency with the reported d(calc).

==========

ALERT_1_047 - The *_chemical_formula_sum* string is Not Given

==========

The *_chemical_formula_sum* string, corresponding with the *_chemical_formula_moiety* string, should be given.

==========

ALERT_1_048 - The *_chemical_formula_moiety* string is Not Given

==========

The *_chemical_formula_moiety* string (i.e. the specification of the various species in the structure) should be given in the CIF.

Example: '(Cd 2+)3, (C6 N6Cr 3-)2, 2(H2 O)'

==========

ALERT_1_049 The Calculated Density has a Value less than 1.0 g/cm3

==========

The calculated density will, with a few exceptions, be larger than 1.0. A smaller value may indicate either an incomplete model or incorrect symmetry. (e.g. a missing 'bar' for P-1 etc.) Large voids in a structure for which the enclosed disordered solvent was modeled with the SQUEEZE technique may be another cause for this ALERT.

==========

ALERT_1_050 - Absorption Coefficient mu Missing

==========

The linear absorption coefficient corresponding to the *_chemical_formula_sum* string should be given.

==========

ALERT_1_051 The Mu(calc) and Mu(CIF) Ratio Differs from 1.0

==========

In the ideal case, both data items should be the same within a small tolerance. If not, the reason should be clear.

==========

ALERT_1_052 - (Proper) Absorption Correction Method Missing

==========

The treatment/method of absorption(correction) should be given explicitly Set *_exptl_absorpt_correction_type* to 'none when no correction is done. Other recognized values are '*psi-scan*', '*empirical*', '*multi-scan*', '*refdelf*', '*analytical*', '*numerical*', '*gaussian*'.

==========

ALERT_1_053 - Minimum Crystal Dimension Missing (or Error)

==========

The smallest crystal dimension should be supplied in the CIF. The expected value should be a real number (i.e. not 0.35mm)

==========

ALERT_1_054 - Medium Crystal Dimension Missing (or Error)

==========

The medium crystal dimension should be supplied in the CIF. The expected value should be a real number (i.e. not 0.35mm)

==========

ALERT_1_055 - Maximum Crystal Dimension Missing (or Error)

==========

The largest crystal dimension should be supplied in the CIF. The expected value should be a real number (i.e. not 0.35mm)

ALERT_1_056 Crystal Radius Missing

==========

Either three linear crystal dimensions or a crystal radius should be given.

==========

ALERT_3_057 - Correction for Absorption Required

==========

You have indicated that an absorption correction has not been applied. (*_exptl_absorpt_correction_type* '*none*'). However, the predicted values of Tmin & Tmax, based on the crystal dimensions given in the CIF, are sufficiently unequal that absorption effects appear to be significant. Therefore, the application of a suitable absorption correction would appear to be required. Also check that the crystal dimensions given in the CIF do represent the actual crystal dimensions as closely as possible. Inaccuracies here can lead to a poor prediction of Tmin & Tmax and give rise to these alerts. It should normally be possible to estimate the crystal dimensions to 2 decimal places. Rough estimates to only 1 decimal place may be too inaccurate to provide reliable estimates of Tmin & Tmax.

==========

ALERT_1_058 - Maximum Transmission Factor Missing

==========

The Maximum transmission factor should be specified in the case a correction for absorption was done. This is NOT the value that is calculated automatically with SHELXL when a SIZE instruction is given in the SHELXL instruction file. The values reported by SHELXL represent the EXPECTED correction range. Some correction packages (e.g. SADABS) will provide only one 'relative- correction-factor'. In such cases, Tmax should be given as Tmax-expected and Tmin = relative-correction-factor * Tmax.

==========

ALERT_1_059 Minimum Transmission Factor Missing

==========

The Minimum transmission factor should be specified in case a correction for absorption was

done. This is NOT the value that is calculated automatically with SHELXL when a SIZE instruction is given in the SHELXL instruction file. The values reported by SHELXL represent the EXPECTED correction range. Some correction packages (e.g. SADABS) will provide only one 'relative-correction-factor'. In such cases, Tmax should be given as Tmax-expected and Tmin = relative-correction-factor * Tmax.

==========

ALERT_4_063 - Crystal Size may be too Large for the Beam Size

==========

Alert for crystals with at least one dimension probably too large for the homogeneous part of the X-ray beam when used for data collection using monochromated radiation. An exception might be data collected using a beta-filter in combination with a sufficiently large collimator. The diffracting volume varies during the rotation of the crystal when the crystal is too large for the primary beam. An inhomogeneous beam may complicate the issue even further for highly absorbing crystals. The scaling function in programs like SADABS may successfully minimize the problem given sufficiently redundant data for a not to high mu structure. Eventually, inspection of the difference density map may validate the analysis.

See also: C.H. Gorbitz (1999), Acta Cryst. B55, 1090-1098.

==========

ALERT_1_064 The Reported T(min) is Greater than Reported T(max)

==========

Check that the values entered under *_exptl_correction_T_min* and *_exptl_correction_T_max* have not been reversed or if there is a typographical error for one of these two items.

==========

ALERT_3_065 - Crystal Requires Numerical Correction

==========

For high mu * r values, numerical absorption correction procedures are recommended.

==========

ALERT_1_066 - Predicted and Reported Transmissions Identical

==========

The predicted and reported transmission ranges are found to be identical which is not to be expected. CIF's generated with SHELXL97 report transmission ranges based on the crystal dimensions supplied on the SIZE card. Those values have nothing to do with the actual corrections for absorption as applied to the data: they just report the EXPECTED range. Some correction packages (e.g. SADABS) will provide only one 'relative-correction-factor'. In such cases, Tmax should be given as Tmax-expected and Tmin = relative-correction-factor * Tmax.

==========

ALERT_1_067 - Maximum Dimension Less Than Minimum Crystal Dimension

==========

Minimum an Maximum dimensions are likely exchanged in the CIF.

==========

ALERT_1_068 The Reported F000 Differs from the Calculated Value (or Missing)

==========

In the ideal case, both data items should have the same value. If not, the reason should be clear. A reason might be the output by SHELXL-97 of population parameters to the CIF with only two decimals.

Note: SHELXL counts the number of electrons in the unit cell. The result will in general be an integer. This is also the number checked for here. The official definition calls for 'The effective number of electrons in the crystal unit cell contributing to F(000)'. It may contain dispersion contributions and is calculated as:

$F(000) = [(\text{sum fr})^2 + (\text{sum fi})^2]^{1/2}$

fr = real part of the scattering factors at theta = 0
fi = imaginary part of the scattering factors at theta = 0

==========

ALERT_1_069 - Atom Label without Numerical Part

==========

The Acta Crystallographica *Notes for Authors* requires atom labels to contain a numerical part. E.g. A label of the type 'O' should be given as 'O1'. This is not necessarily a requirement for other journals.

==========

ALERT_1_070 - Duplicate Atomic Label on Input

==========

The CIF contains duplicate labels posing interpretation problems for PLATON/CHECK. Derived geometry ALERTS may have their origin in this problem.

==========

ALERT_1_071 - Uninterpretable Atom Label on Input

==========

The CIF contains labels posing problems for PLATON/CHECK. Example: label HN1 with no scattering type information supplied. Validation is aborted.

==========

ALERT_2_072 The SHELXL97 First Parameter in the WGHT Line is Unusually Large

==========

The first parameter on the SHELXL weighting line has an exceptionally large value. This may indicate either improper reflection s.u.'s or an unresolved problem such as missed twinning.

==========

ALERT_1_073 - H-atoms refined, but *_refine_ls_hydrogen_treatment* Reports Differently

==========

The structure contains refined hydrogen atoms. However the data item *_refine_ls_hydrogen_treatment* has the value '*constr*'. The value 'mixed' is more appropriate.

==========

ALERT_1_074 Atom with Reported Occupancy Parameter Value = 0.0

==========

The CIF contains an atom with occupancy less than 0.0001

==========

ALERT_1_075 Atom with an Occupancy greater than 1.0 Detected

==========

The reported atom has an occupancy greater than 1.0. This can be caused by an improper assignment of the population parameter to an atom in the least squares refinement model. Note: The definition of 'occupancy' is different for SHELXL and CIF. Populations in SHELXL include site symmetry numbers for atoms in special positions.

==========

ALERT_1_076 - Occupancy less than 1.0 Reported for an Atom on a Special Position

==========

The CIF contains an atom sitting on a special position with an occupancy specified as less than 1.0. This is often an error and the result of the confusion of the notions 'occupancy' and 'population parameter'. The first should be 1.0 for a fully occupied site. The latter multiplies the site-symmetry with the occupancy. Thus, for a fully occupied site on a mirror plane the site-symmetry will be 0.5 * 1.0 = 0.5.

Note: a wrong occupancy number will lead to an incorrect expected chemical formula.

==========

ALERT_4_077 The Unit-cell Contains a Non-integer Number of Atoms

==========

The unit cell contains a non-integer number of atoms of a given atom type. Valid reasons include partially occupied (solvent) sites and substitutional disorder.

==========

ALERT_1_078 - No H-atoms in CIF, but *_atom_sites_solution_hydrogens* Reported

==========

The structure contains no hydrogen atoms. However the data item *_atom_sites_solution_hydrogen* had the value 'geom'. This value is likely the SHELXL default and should be replaced by '.'.

==========

ALERT_1_079 - No H-atoms in CIF, but *_refine_ls_hydrogen_treatment* Reported

==========

The structure contains no hydrogen atoms. However the data item *_refine_ls_hydrogen_treatment* has the value 'mixed'. This value is likely the SHELXL default and should be replaced by '.'.

==========

ALERT_2_080 A Significant Maximum Shift/Error Value Reported

==========

Convergence of the refinement is proven with a close to zero shift/error value for all refined parameters. Such a convergence is easily achieved with a few additional refinement cycles at little cost. Note: Some SHELXL-97 versions do not allow for negative Flack parameter values.

Convergence in such a case may be never reached because the Flack parameter value is reset to zero.

==========

ALERT_1_081 - No Maximum Shift/Error Given

==========

A maximum shift/error should be specified in order to judge convergence.

==========

ALERT_2_082 A High R1 Value is Reported

==========

A higher than usual R1 indicates either an insufficient model or poor quality data.

==========

ALERT_2_083 - SHELXL 97 Second Parameter in the WGHT Line is Unusually Large

==========

The second parameter on the SHELXL weighting line has an exceptionally large value. This may indicate either improper reflection s.u.'s or an unresolved problem such as missed twinning.

==========

ALERT_2_084 High wR2 Value

==========

wR2 will in general have a value of in the order of twice that of R1 with refinement on F**2. Significantly larger values usually indicate a poor or incorrect refinement model. Also check for unaccounted for twinning.

==========

ALERT_2_085 The SHELXL Default Weighting Scheme is not Optimized

==========

The weighting scheme is found to be left at the SHELXL default.

==========

ALERT_2_086 - Unsatisfactory S Value (Too Low or Not Given)

==========

S should in general be close to 1.00 at the end of a refinement with a proper weighting scheme. If not, there might be significant unresolved problems with the model.

==========

ALERT_2_087 - Unsatisfactory S value (Too High)

==========

S should in general be close to 1 at the end of a refinement with a proper weighting scheme. If not, there might be significant unresolved problems with the model.

==========

ALERT_3_088 - Poor Data / Parameter Ratio

==========

The data/parameter ratio should in general be higher than 10 for a quality structure

determination. This ratio can be improved by not refining C-H parameters other than riding on their carrier atom.

==========

ALERT_3_089 - Poor Data / Parameter Ratio (Zmax .LT. 18)

==========

The data/parameter ratio should in general be higher than 8 for a quality determination of a structure containing atoms with Z less than 18. This ratio can be improved by not refining C-H parameters other than riding on their carrier atom.

Note that with light atom non-centro-symmetric structures where anomalous dispersion effects are insignificant, it is unwise to attempt to use unmerged Friedel-related reflections simply to boost the r/p ratio.

==========

ALERT_3_090 - Poor Data / Parameter Ratio (Zmax .GT. 18)

==========

The data/parameter ratio should in general be higher than 10 for a quality determination for a structure containing heavy atoms with ZMAX greater than 17. This ratio can be improved by not refining C-H parameters other than riding on their carrier atom.

==========

ALERT_1_091 - No Wavelength found in CIF - 0.71073 Ang Assumed

==========

No Wavelength specification found in the CIF.

==========

ALERT_4_092 - Check: Wavelength given is not Cu, Mo or Ag Ka

==========

Warning: specified wavelength is not Cu, Mo or Ag Ka radiation. Valid exceptions are Neutron and Synchrotron data.

==========

ALERT_1_093 - No s.u.'s on H-atoms, but their Refinement Reported

==========

The '*mixed*' type of Hydrogen atom refinement is reported (SHELXL-97 default). However, no Hydrogen atoms with freely refined positions are found in the CIF. Likely, the value '*constr*' for '*_refine_ls_hydrogen_treatment*' will be more appropriate (e.g. when all Hydrogen atoms have been refined in the riding mode on their carrier atom).

==========

ALERT_2_094 Unusual Ratio of Maximum / Minimum Residual Density

==========

The ratio of the maximum and minimum residual density excursions is unusual. This might indicate unaccounted for twinning or missing atoms (e.g. associated with disordered solvent).

==========

ALERT_1_095 No Maximum Residual Density Datum Found

==========

No residual electron density maximum given in the CIF.

==========

ALERT_1_096 No Minimum Residual Density Datum Found

==========

No residual electron density minimum given in the CIF.

==========

ALERT_2_097 - Large Reported Maximum (Positive) Residual Density

==========

Residual density maximum larger than expected. This might be caused by residual absorption artifacts, unaccounted for twinning, wrongly assigned atom types and other model errors.

==========

ALERT_2_098 - Large Reported Minimum (Negative) Residual Density

==========

Residual density minimum larger than expected. This might be caused by residual absorption artifacts, wrongly assigned atom types and other model errors.

==========

ALERT_1_099 Reported Minimum (Negative) Residual Density .GE. 0 !!

==========

Likely interchanged maximum and minimum values.Alternatively, the minimum residual density has the (unlikely) value zero.

==========

ALERT_2_101 Insufficient Number of Digits Given for Special Position x-Coordinate

==========

Fractions of the type 1/3 and 2/3 for the positional parameters of atoms in special positions should be provided with sufficient digits. (i.e. 0.66667 and 0.33333). Otherwise, they might be treated by the software as off the symmetry element.

==========

ALERT_2_102 Insufficient Number of Digits Given for Special Position y-Coordinate

==========

Fractions of the type 1/3 and 2/3 for the positional parameters of atoms in special positions should be provided with sufficient digits. (i.e. 0.66667 and 0.33333). Otherwise, they might be treated by the software as off the nearly symmetry element.

==========

ALERT_2_103 Insufficient Number of Digits Given for Special Position z-Coordinate

==========

Fractions of the type 1/3 and 2/3 for the positional parameters of atoms in special positions should be provided with sufficient digits. (i.e. 0.66667 and 0.33333). Otherwise, they might be treated by the software as off the nearby symmetry element.

==========

ALERT_2_110 - ADDSYM Detects Potential Lattice Centering or Halving

==========

Tests for missed symmetry are done with ADDSYM, an expanded MISSYM (C) clone. These tests warn for missed or possible higher (pseudo) symmetry in the structural model (i.e. based on the coordinate data). Close examination of the situation at hand is indicated in order to prove/disprove the issue (usually in combination with the reflection data). Report on potential (pseudo/real) lattice centering or cell halving. Note: H-atoms and disordered atoms are not taken into account in the tests.

==========

ALERT_2_111 - ADDSYM Detects a (Pseudo) Center of Symmetry

==========

Tests for missed symmetry are done with ADDSYM, an expanded MISSYM (C) clone. These tests warn for missed or possible higher (pseudo) symmetry in the structural model (i.e. based on the coordinate data). Close examination of the situation at hand is indicated in order to prove/disprove the issue (usually in combination with the reflection data). This ALERT reports on a potential additional (pseudo/real) inversion center. A pseudo-center may be incompatible with existing symmetry elements. Chiral molecules are incompatible with an inversion center. Note: H-atoms and disordered atoms are not taken into account in the test.

==========

ALERT_2_112 - ADDSYM Detects Additional (Pseudo) Symmetry Element

==========

Tests for missed symmetry are done with ADDSYM, an expanded MISSYM (C) clone. These tests warn for missed or possible higher (pseudo) symmetry in the structural model (i.e. based on the coordinate data). Close examination of the situation at hand is indicated in order to prove/disprove the issue (usually in combination with the reflection data). This ALERT reports on potential additional (pseudo/real) rotation axes and mirrors.

In addition, (pseudo/real) lattice centering/translations are reported as A, B, C, I, X, Y, Z, S. (Here S stands for special and not covered by the preceding types). Full details on the situation at hand should be gleaned from an actual PLATON/ADDSYM run.

Chiral molecules are incompatible with an inversion center or (glide)planes. Note: H-atoms and disordered atoms are not taken into account in the tests.

==========

ALERT_2_113 - ADDSYM Suggests Possible Pseudo/New Space-Group

==========

Tests for missed symmetry are done with ADDSYM, an extended clone of Yvon LePage's MISSYM (C) algorithm. These tests warn for missed or possibly higher (pseudo-) symmetry in the structural model (i.e. based on the coordinate data). A close examination of the situation at hand is indicated in order to prove/disprove the issue (preferably in combination with the reflection data). Chiral molecules are incompatible with an inversion center or (glide)planes. For an example of reported pseudo-symmetry see I.A.Guzei et al, (2002). Acta Cryst. C58, m141-m143.

Note: H-atoms and disordered atoms (i.e. atoms with population less than 1.0) are not taken into account in the tests. This may artificially lead to a symmetry higher than the actual one.

Note: Atoms are treated as having the same atom type in order to catch certain types of disorder or incorrect atom type assignment.
See also:
P1 or P-1? Or something else?, R.E. Marsh (1999). Acta Cryst. B55, 931-936.

More Space-Group Corrections: From Triclinic to Centered Monoclinic and to Rhombohedral; Also From P1 to P-1 and From Cc to C2/c. F.H. Herbstein & R.E. Marsh (1998). Acta Cryst. B54, 677-686.

Topical Review: Some Thoughts on Choosing the Correct Space-Group. R.E. Marsh (1995). B51, 897-907.

==========

ALERT_2_114 - ADDSYM Suggests Possible Pseudo/New Space-Group

==========

ADDSYM has problems to reconstruct a space-group from the symmetry operation found in the symmetry expanded coordinate set. The reason being either intricate additionally detected pseudo-symmetry or serious errors in the data set.

==========

ALERT_5_115 - ADDSYM Detects a Non-crystallographic Inversion Center

==========

Tests for missed symmetry are done with ADDSYM, an expanded MISSYM (C) clone. This ALERT reports on local inversion symmetry, not compatible with the reported space-group symmetry.

Note: H-atoms and disordered atoms are not taken into account in the test.

==========

ALERT_1_119 - Problem found with the Syntax of a Symmetry Operation

==========

A symmetry operation should be specified in the CIF either without spaces or between quotes.

==========

ALERT_1_120 Reported Space-Group is Inconsistent with the Explicit Space-Group

==========

Space-group symmetry should be provided in the CIF both explicitly with a *_symmetry_equiv_pos_as_xyz* loop and implicitly with *_symmetry_space_group_name-H-M*.

An unusual (non-standard) choice of origin may also raise this ALERT. Please check and Explain.

==========

ALERT_1_121 - Invalid *_symmetry_space_group_name_H-M*

==========

Symmetry in the CIF should be provided both explicitly with a *_symmetry_equiv_pos_as_xyz* loop and implicitly with *_symmetry_space_group_name_H-M*. Test for valid *_symmetry_space_group_name_H-M symbol*.

==========

ALERT_1_122 - No *_symmetry_space_group_name_H-M* Given

==========

Symmetry in the CIF should be provided both explicitly with a *_symmetry_equiv_pos_as_xyz* loop and implicitly with *_symmetry_space_group_name_H-M*. Test for missing (i.e. ?) *_symmetry_space_group_name_H-M symbol*.

==========

ALERT_1_123 - Uninterpretable or Inconsistent Space-Group Info

==========

The space-group symmetry should be provided in the CIF both explicitly with a *_symmetry_equiv_pos_as_xyz* loop and implicitly with _symmetry_space_group_name_H-M. This ALERT reports on uninterpretable or inconsistent Space-group information.

==========

ALERT_1_124 - Uninterpretable or Absent *_symmetry_equiv_pos_as_xyz*

==========

Symmetry in the CIF should be provided in the CIF both explicitly with a *_symmetry_equiv_pos_as_xyz* loop and implicitly with *_symmetry_space_group_name_H-M*. Test for uninterpretable or absent explicit symmetry records

==========

ALERT_1_125 - No *_symmetry_space_group_name_Hall* Given

==========

Optionally specify the Hall symbol. The Hall symbol provides an unambiguous definition of the space-group symmetry where the Hermann- Mauguin symbol leaves room for alternative choices of the origin. E.g. for space-group P21, the screw axis is in general taken to coincide with the b-axis. However, sometimes it is chosen to be shifted by 1/4 in the c-axis direction to bring out the relation with P21/c. The Hall symbols will be 'P 2yb' and 'P 2ybc' respectively.

Refer to: S.R.Hall, Space-Group Notation with an Explicit Origin; Acta Cryst. (1981), A37, 517-525.

or: http://www.kristall.ethz.ch/LFK/software/sginfo/hall_symbols.html

==========

ALERT_1_126 - Error in or Uninterpretable Hall Symbol

==========

The reported Hall-symbol is found to be in error or uninterpretable.

Refer to: S.R.Hall, Space-Group Notation with an Explicit Origin; Acta Cryst. (1981), A37, 517-525.

or: http://www.kristall.ethz.ch/LFK/software/sginfo/hall_symbols.html

==========

ALERT_1_127 - Implicit Hall Symbol Inconsistent with Explicit

==========

The reported Hall-symbol is found to be inconsistent with the one derived from the explicit symmetry operations.

Alternatively, no Hall-symbol could be derived by PLATON for the explicit set of symmetry operations. This may be the case when an unusual origin is chosen.

Refer to: S.R.Hall, Space-Group Notation with an Explicit Origin; Acta Cryst. (1981), A37, 517-525.

or: http://www.kristall.ethz.ch/LFK/software/sginfo/hall_symbols.html

==========

ALERT_4_128 Alternate Monoclinic Space-group Setting

==========

The reported structure is described in a monoclinic space-group with a non-standard (alternate) setting. Transformation to the conventional setting is indicated unless there is a good (scientific) reason not to do so. Valid reasons can be a closer to 90 degrees monoclinic beta angle or a structural relationship with another temperature phase.

==========

ALERT_4_129 - Unusual Space-group Specified

==========

The reported space-group name is unusual.

==========

ALERT_1_130 Test for Cubic System Axial Constraints

==========

The cell dimensions do not conform with the symmetry constraints (a = b = c) for cubic cells.

==========

ALERT_1_131 Test for Cubic System Angle Constraints

==========

The cell angles do not conform with the symmetry constrainnts (alpha = beta = gamma = 90.0) for cubic cells.

==========

ALERT_1_132 The Trigonal/Hexagonal a and b axis lengths Differ

==========

Symmetry constraints on cell dimensions are checked.

==========

ALERT_1_133 - Trigonal/Hexagonal alpha and beta Angles should be 90 Degrees Exact

==========

Symmetry constraints on cell dimensions are checked.

==========

ALERT_1_134 - Trigonal/Hexagonal gamma Angle should be 120 Degree Exact

==========

Symmetry constraints on cell dimensions are checked.

==========

ALERT_1_135 - Tetragonal: a and b Axial Lengths should be Equal

==========

Symmetry constraints on cell dimensions are checked.

==========

ALERT_1_136 - Tetragonal: alpha, beta & gamma Angles should be 90 Degrees Exact

==========

Symmetry constraints on cell dimensions are checked.

==========

ALERT_1_137 - Orthorhombic: alpha, beta & gamma Angles should be 90 Degrees Exact

==========

Symmetry constraints on cell dimensions are checked.

==========

ALERT_1_138 - Monoclinic: More than one Angle Unequal 90.0 Degrees

==========

Symmetry constraints on cell dimensions are checked.

==========

ALERT_1_139 - Rhombohedral: a, b & c Axial Lengths are not all Exactly Equal

==========

Symmetry constraints on cell dimensions are checked.

==========

ALERT_1_140 - Rhombohedral: alpha, beta & gamma Angles are Not All Equal

==========

Symmetry constraints on cell dimensions are checked.

==========

ALERT_4_141 s.u. on a - Axis Small or Missing

==========

The s.u. on the a-axis is small or missing. The presence of s.u.'s (where required) and value are checked. S.u.'s as given by the diffractometer software are often much smaller then realistic.

See also:
*How precise are measurements of unit-cell dimensions from single crystal*s. F.H. Herbstein

(2000). Acta Cryst. B56, 547-557.

==========

ALERT_4_142 s.u. on b - Axis Small or Missing

==========

The s.u. on the b-axis is small or missing. The presence of s.u.'s (where required) and value are checked. S.u.'s as given by the diffractometer software are often much smaller then realistic.

==========

ALERT_4_143 s.u. on c - Axis Small or Missing

==========

The s.u. on the c-axis is small or missing. The presence of s.u.'s (where required) and value are checked. S.u.'s as given by the diffractometer software are often much smaller then realistic.

==========

ALERT_4_144 s.u. on alpha Angle Small or Missing

==========

The s.u. on alpha is small or missing. The presence of s.u.'s (where required) and value are checked. S.u.'s as given by the diffractometer software are often much smaller then realistic.

==========

ALERT_4_145 s.u. on beta Angle Small or Missing

==========

The s.u. on beta is small or missing. The presence of s.u.'s (where required) and value are checked. S.u.'s as given by the diffractometer software are often much smaller then realistic.

==========

ALERT_4_146 - su on gamma Angle Small or Missing

==========

The s.u. on gamma is small or missing. The presence of s.u.'s (where required) and value are checked. S.u.'s as given by the diffractometer software are often much smaller then realistic.

==========

ALERT_1_147 s.u. on Symmetry Constrained Cell Angle(s)

==========

There should be no s.u. on symmetry constrained cell angles. Example: No s.u. on alpha, beta and gamma for orthorhombic symmetry.

==========

ALERT_3_148 s.u. on Cell Axis too Large

==========

The s.u. on the reported -axis is unexpectedly large.

==========

ALERT_3_149 s.u. on Cell Angle too Large

==========

The s.u. on the reported angle is too large.

==========

ALERT_1_150 - Volume as Calculated Differs from that Given

==========

An ALERT is issued when the reported unit cell volume differs significantly from the volume calculated on the basis of the supplied unit-cell dimensions.

==========

ALERT_1_151 - No s.u. Given on Volume

==========

Missing s.u. on the unit-cell volume.

==========

ALERT_1_152 - The Supplied and Calculated Volume s.u.'s Differ

==========

Some software packages calculate Volume s.u.'s incorrectly. The correct formula (based on the propagation of error expression) may be found in:

M. Nardelli, Computer & Chemistry, (1983), 7, 95-98.C. Giacovazzo ed. in 'Fundamentals of Crystallography', Second Edition, Oxford University Press, 2003, p135.

==========

ALERT_1_153 - The su's on the Cell Axes are Equal

==========

The reported cell axes s.u.'s are reported equal. Please check whether this is correct or a software default value.

==========

ALERT_1_154 - The su's on the Cell Angles are Equal

==========

The reported cell angle s.u.'s are reported equal. Please check whether this is correct or a software default value.

==========

ALERT_4_155 - The Triclinic Unit-cell is NOT Reduced

==========

Unless for special reasons related to the structure/content, a unit-cell and structure is best reported with reference to the Niggli Reduced Cell. This ALERT may originate also from a failure to order the axes from small to large.

==========

ALERT_4_156 The Triclinic Axial System Input Cell is not Standard

==========

The axial order should be from small to large in the triclinic cell.

==========

ALERT_4_157 - Non-standard Monoclinic Beta Angle less than 90 Degrees

==========

By convention, the Monoclinic beta angle is always chosen to be larger than 90.0 Degrees. A trivial transformation (1 0 0/0 -1 0/0 0 -1) should be applied to the data.

==========

ALERT_4_158 - The Input Unit-cell is NOT Standard/Reduced

==========

Unless for special reasons related to the structure/content, a unit cell and structure is best reported with reference to the Niggli Reduced Cell.

==========

ALERT_4_161 - Missing or Zero su (esd) on x-coordinate

==========

Missing or Zero s.u .on x-coordinate.positional parameters for all non-hydrogen atoms in general positions are checked for the presence of a non-zero s.u. on them. This includes parameters fixed to fix the origin in polar space-groups which is no longer necessary when refinement is done with modern programs (e.g. SHELXL, XTAL).

==========

ALERT_4_162 - Missing or Zero s.u. on y-coordinate

==========

Missing or Zero s.u. on y-coordinate.positional parameters for all non-hydrogen atoms in general positions are checked for the presence of a non-zero s.u. on them. This includes parameters fixed to fix the origin in polar space-groups (e.g. P21) which is no longer necessary when refinement is done with modern programs (e.g. SHELXL, XTAL).

==========

ALERT_4_163 - Missing or Zero s.u. on z-coordinate

==========

Missing or Zero s.u. on z-coordinate.

Positional parameters for all non-hydrogen atoms in general positions are checked for the presence of a non-zero s.u. on them. This includes parameters fixed to fix the origin in polar space-groups (e.g. P41) which is no longer necessary when refinement is done with modern programs (e.g. SHELXL, XTAL).

==========

ALERT_4_164 C-H Hydrogen atoms in Heavy Atom Structure Refined

==========

Warning: Refined C-H H-atoms in heavy-atom structure (i.e. containing an element beyond element #18). Such H-atoms are in general better refined at calculated positions riding on the atoms they are attached to. A better data over parameter ratio will be achieved.

==========

ALERT_3_165 - Status R Flagged Non-Hydrogen Atoms

==========

Report on restrained (riding) Non-Hydrogen atoms. Note: This may lead to non meaningful

bond and angle s.u.'s (ALERTS _751, _752). R-flagged atoms may arise unintentional being caused by an "AFIX 0" line being missing in a shelxl.ins file (SHELXL-97 refinement). Alternatively, the number of refined parameters may have been limited deliberately (e.g. by refinement of C-F with fixed known geometry, similar to C-H) in order to keep the data/parameter ratio acceptable.

==========

ALERT_4_166 - S.u's Given on Coordinates for calc-flagged Atoms

==========

Calc-flagged atoms are not supposed to carry s.u.'s on their coordinates.

==========

ALERT_4_170 - Insufficient Data in Coordinate Loop

==========

Insufficient data encountered in coordinate loop. A possible cause might be the use of a SHELX style '=' continuation line.

==========

ALERT_4_180 Check Cell Parameter Rounding

==========

It is unusual that more cell parameters end with a zero and the s.u. is 10. This problem might be caused by the specification of insufficient 'meaningful' digits as compared to the reported s.u..

see also: W. Clegg, Acta Cryst. (2003) E59, e2-e5.

==========

ALERT_1_193 - Cell Determination and Data Collection Temperatures differ

==========

The reported _cell_measurement_temperature deviates from the reported *_diffrn_ambient_temperature* values.

==========

ALERT_1_194 - Missing *_cell_measurement_reflns_used* Datum

==========

Please supply value for *_cell_measurement_reflns_used*

==========

ALERT_1_195 - Missing *_cell_measurement_theta_max* Datum

==========

Please supply value for *_cell_measurement_theta_max*

==========

ALERT_1_196 - Missing *_cell_measurement_theta_min* Datum

==========

Please supply value for *_cell_measurement_theta_min*

==========

ALERT_1_197 - Missing _*cell_measurement_temperature*

==========

Please specify the temperature (Kelvin) at which the unit-cell was determined.

==========

ALERT_1_198 - Missing _*diffrn_ambient_temperature*

==========

Please specify the temperature (Kelvin) at which the intensity data were collected.

==========

ALERT_1_199 - Check the Reported _*cell_measurement_temperature*

==========

The unit-cell determination temperature is set in the CIF by SHELXL by default to 293 K if the TEMP instruction is not used. The actual temperature is likely either slightly or significantly (for a low temperature data collection) different. A reported temperature of 273 K is also likely to be erroneous.

==========

ALERT_1_200 - Check the Reported _*diffrn_ambient_temperature*

==========

The data collection temperature is set in the CIF by SHELXL by default to 293 K if the TEMP instruction is not used. The actual temperature is likely either slightly or significantly (for a low temperature data collection) different. A reported temperature of 273 is also likely to be erroneous.

==========

ALERT_2_201 - Isotropic non-H Atoms in Main Residue(s)

==========

This test reports on non-hydrogen atoms that were refined with isotropic displacement parameters only in the main residue. Such a practice is unusual by modern standards and only needed for minor disorder modeling.

==========

ALERT_3_202 - Isotropic non-H Atoms in Anion/Solvent

==========

This test reports on isotropically refined atoms in small moieties (usually anions or solvent).

==========

ALERT_3_210 - No Anisotropic ADP's Found in CIF

==========

No anisotropically refined atoms in CIF ?

==========

ALERT_2_211 Atom with Non-Positive Definite Displacement Parameter Values

==========

This test reports on non-positive definite (i.e. complex and unrealistic) or (nearly) flat (2D) anisotropic displacement parameters in the main residue. This may be due to data quality problems or model errors. Refinement with an ISOR or similar restraint might be considered.

==========

ALERT_2_212 Non-Positive-Definite ADP in Anion or Solvent Molecule

==========

This test reports on non-positive definite (i.e. complex and unrealistic) or nearly flat (2D) anisotropic displacement parameters in an anion or solvent residue. This may be due to data quality problems or model errors. Refinement with an ISOR or similar restraint might be considered.

==========

ALERT_2_213 Atom with Large Maximum and Minimum ADP-axes Ratio

==========

The maximum and minimum main axis ADP ratio (Angstrom Units) is tested for the main residue. Large values may indicate unresolved disorder. Splitting over two positions should be considered.

==========

ALERT_2_214 Solvent Atom with Large Maximum and Minimum ADP-axes Ratio

==========

The maximum and minimum main axis ADP ratio (Angstrom Units) is tested for the minor residue(s). Large values may indicate unresolved disorder. Splitting over two positions should be considered.

==========

ALERT_3_215 - Unusual Disordered Atom ADP in Major Residue

==========

The maximum and minimum main axis ADP ratio (Angstrom Units) is tested for the main residue. Large values may indicate unresolved disorder.

==========

ALERT_3_216 - Unusual Disordered Atom ADP in Minor Residue

==========

The maximum and minimum main axis ADP ratio (Angstrom Units) is tested for the minor residue(s). Large values may indicate unresolved disorder.

==========

ALERT_1_217 - Incomplete U(aniso) data

==========

Check & Correct U(aniso) data for completeness etc. Do not use a SHELX style '=' continuation line in a CIF.

==========

ALERT_2_220 Unusual Ueq(max)/Ueq(Min) range for non-H Atoms in Non-solvent

==========

This test reports on a larger than usual U(eq) range for the specified element type in the non-solvent/anion part of the structure. Too high or too low Ueq's may be an indication for incorrectly identified atomic species (i.e. O versus N).

==========

ALERT_2_221 - Unusual Ueq(max)/Ueq(Min) Range for non-H Atoms in Solvent

==========

This test reports on a larger than usual U(eq) range for the non-hydrogen atoms solvent/anion. Too high or too low Ueq's may be an indication for incorrectly identified atomic species (i.e. Br versus Ag).

==========

ALERT_3_222 Large Uiso(max)/Uiso(Min) Range for H atoms in Non-solvent Residue

==========

This test reports on a larger than usual range of Uiso values for hydrogen atoms in the non-solvent/anion part of the structure.

Possible causes are:

1 - disorder, e.g. in t-butyl moieties.
2 - poor data, not adequate for the refinement of individual displacement parameters.
3 - Misplaced hydrogen atoms (i.e. there is no density at the position where one of the H-atoms is positioned).

==========

ALERT_4_223 Large Uiso(max)/Uiso(Min) range for H atoms in the Solvent Molecules

==========

This test reports on a larger than usual range of Uiso values for hydrogen atoms in the solvent/anion part of the structure.

Possible causes are:

1 - disorder, e.g. in t-butyl moieties.
2 - poor data, not adequate for the refinement of individual displacement parameters.
3 - Misplaced hydrogen atoms (i.e. there i
s no density at the position where one of the H-atoms is positioned).

==========

ALERT_1_224 Large Difference Between Implicit and Explicit U(eq) Values

==========

This test reports on a large difference between Ueq in the CIF and the Ueq calculated from the 6 reported Uij values.

.

==========

ALERT_2_230 Hirshfeld Rigid-Bond Test Violation (Non-solvent)

==========

The components of the anisotropic displacement parameters along chemical bonds are assumed to be equal in magnitude. Large differences supposedly indicate contamination of these parameters with other (unresolved) effects such as (substitutional) disorder, model or data errors and/or over refinement. Atomic sites assigned the wrong scattering type (e.g. Ag versus Br) should generate 'problem signals' with this test. Data sets corrected for absorption

effects with DELREF techniques (e.g. DIFABS, SHELXA, XABS2) often show large DELU values for bonds involving the heaviest atom.

Note: The original 'Hirshfeld-test' was defined in absolute terms (see F.L. Hirshfeld, Acta Cryst. (1976). A32, 239-244). The current test is with reference to the associated standard uncertainty.

==========

ALERT_4_231 - Hirshfeld Rigid-Bond Test Violation (solvent)

==========

The components of the anisotropic displacement parameters along chemical bonds are assumed to be equal in magnitude. Large differences supposedly indicate contamination of these parameters with other (unresolved) effects such as (substitutional) disorder, model or data errors and/or over refinement. Atomic sites that have been assigned the wrong scattering type (e.g. Ag versus Br) should generate 'problem signals' with this test. Data sets corrected for absorption effects with DELREF techniques (e.g. DIFABS, SHELXA, XABS2) often show large DELU values for bonds involving the heaviest atom.

Note: The original 'Hirshfeld-test' was defined in absolute terms (see F.L. Hirshfeld, Acta Cryst. (1976). A32, 239-244). The current test is with reference to the associated standard uncertainty.

==========

ALERT_2_232 - Hirshfeld Rigid-Bond Test (Metal-X) Violation

==========

The components of the anisotropic displacement parameters along chemical bonds are assumed to be equal in magnitude. Large differences supposedly indicate contamination of these parameters with other (unresolved) effects such as (substitutional) disorder, model or data errors and/or over-refinement. Atomic sites that have been assigned the wrong scattering type (e.g. Ag versus Br) should generate 'problem signals' with this test. Data sets corrected for absorption effects with DELREF techniques (e.g. DIFABS, SHELXA, XABS2) often show large DELU values for bonds involving the heaviest atom.

A special case are M-C=O type of systems that generally show significant differences for the M-C bond. See D.Braga & T.F. Koetzle (1988), Acta Cryst. B44, 151-155).

Note: The original 'Hirshfeld-test' was defined in absolute terms (see F.L. Hirshfeld, Acta Cryst. (1976). A32, 239-244). The current test is with reference to the associated standard uncertainty.

==========

ALERT_4_233 - Hirshfeld Rigid-Bond Test (Metal-X) Violation (Solvent)

==========

The components of the anisotropic displacement parameters along chemical bonds are assumed to be equal in magnitude. Large differences supposedly indicate contamination of these parameters with other (unresolved) effects such as (substitutional) disorder, model or data errors and/or over refinement. Atomic sites assigned the wrong scattering type (e.g. Ag versus Br) should generate 'problem signals' with this test. Data sets corrected for absorption effects with DELREF techniques (e.g. DIFABS, SHELXA, XABS2) often show large DELU values for bonds involving the heaviest atom.

Note: The original 'Hirshfeld-test' was defined in absolute terms (see F.L. Hirshfeld, Acta Cryst. (1976). A32, 239-244). The current test is with reference to the associated standard uncertainty.

==========

ALERT_4_234 - Hirshfeld Rigid-Bond Test (Large Absolute Difference)

==========

The components of the anisotropic displacement parameters along chemical bonds are assumed to be equal in magnitude. Large differences supposedly indicate contamination of these parameters with other (unresolved) effects such as (substitutional) disorder, model or data errors and/or over refinement. Atomic sites assigned the wrong scattering type (e.g. Ag versus Br) should generate 'problem signals' with this test. Data sets corrected for absorption effects with DELREF techniques (e.g. DIFABS, SHELXA, XABS2) often show large DELU values for bonds involving the heaviest atom.

Note: The original 'Hirshfeld-test' was defined in absolute terms (see F.L. Hirshfeld, Acta Cryst. (1976). A32, 239-244).

==========

ALERT_2_241 Atom with Unusually high Ueq as Compared with Neighbors

==========

The Ueq value of an atom is compared with the average Ueq for to non-hydrogen atoms bonded to it. Large differences may indicate that the wrong atom type was assigned (e.g. N instead of O).

==========

ALERT_2_242 Atom with Unusually Low Ueq as Compared with Neighbors

==========

The Ueq value of an atom is compared with the average Ueq for non-hydrogen atoms bonded to it. Large differences may indicate that the wrong atom type was assigned (e.g. N instead of O). False alarms may occur for terminal groups such as the t-butyl moiety.

==========

ALERT_4_243 - High Solvent Atom Ueq as Compared to Neighbors

==========

The Ueq value of an atom in the solvent or ion is compared with the average Ueq for non-hydrogen atoms bonded to it. Large differences may indicate that the wrong atom type was assigned (e.g. N instead of O).

==========

ALERT_4_244 - Low Solvent Atom Ueq as Compared to Neighbors

==========

The Ueq value of an atom in the solvent or ion is compared with the average Ueq for non-hydrogen atoms bonded to it. Large differences may indicate that the wrong atom type was assigned (e.g. N instead of O). False alarms may occur for terminal groups such as the t-butyl moiety.

==========

ALERT_2_245 - Unusually low H-Uiso as Compared with the Ueq of the Bonded Atom

==========

The Uiso of a hydrogen atom is generally expected to be greater than the Ueq of the non-hydrogen atom it is attached to.

==========

ALERT_2_250 - Large U3/U1 Ratio for Average U(i,j) Tensor

==========

An average value of the U(i,j) tensor of the asymmetric unit of a residue is calculated. An ALERT is generated when the corresponding U3/U1 ratio deviates significantly from 1.0. Large values of this ratio should be taken as an indication of possible systematic errors in the data or errors in the model. Visual inspection of an ORTEP plot will show that many displacement ellipsoids have their major axis pointing in the same direction.

==========

ALERT_3_301 - Main Residue Disorder

==========

Atom sites that are not fully occupied are counted. A large fraction of disordered atoms may be both a signal for serious structure analysis problems or less reliable/interesting results.

==========

ALERT_4_302 - Anion/Solvent Disorder

==========

Atom sites that are not fully occupied are counted. A large fraction of disordered atoms may be both a signal for serious structure analysis problems or less reliable/interesting results.

==========

ALERT_2_303 - Full Occupancy H-Atom with more than one Connected Atom

==========

Hydrogen atoms are generally connected to only one other atom. A hydrogen atom between two oxygen atoms is a special case. Investigate whether this hydrogen atom is better described with a disorder model with two partially occupied sites. A difference map might show a double-well density.

==========

ALERT_2_305 - Isolated Hydrogen Atom (Outside Bonding Range ??)

==========

This test reports on hydrogen atoms that are not on bonding distance to any atom. This ALERT may indicate that the hydrogen atom refined to a non-bonding position or needs a symmetry operation to bring it to bonding distance. It also may indicate a problem with incompatible population parameters (e.g. C - H with population 0.8 and 0.9 respectively).

==========

ALERT_2_306 - Isolated Oxygen Atom (H-atoms Missing ?) .

==========

This test reports on oxygen atoms that are not within bonding distance to any other atom in the structure. A common reason may be that no hydrogen atoms are given for a water molecule.

Attempts should be made to locate those hydrogen atoms from a difference map.

==========

ALERT_2_307 - Isolated Metal Atom (Unusual !)

==========

This test reports on metal atoms that are not bonded or at coordination distance of other atoms. Isolated ions are very unusual (or non-existent ?)

==========

ALERT_2_308 - Single Bonded Metal Atom (Unusual !)

==========

This test reports on single bonded (coordinated) metal atoms/ions. This represents a very unusual situation. There are literature examples where such a 'single bonded metal' was shown to be a halogen.

==========

ALERT_2_309 - Single Bonded Oxygen (C-O .GT. 1.3 Angstrom)

==========

Single bonded Oxygen with C-O .GT. 1.3 Angstrom. Missing H-Atom ?

==========

ALERT_2_310 Atom (Symmetry Related) too Close to Full Weight Atom

==========

This test identifies (very) short contacts between atoms that only becomes apparent after the application of symmetry on the primary coordinate set.

==========

ALERT_2_311 - Isolated Disordered Oxygen Atom (No H's ?)

==========

This test reports on oxygen atoms (not full weight) that are not within bonding distance to any other atom in the structure. A common reason may be that no hydrogen atoms are given for a water molecule.

==========

ALERT_2_312 - Strange C=O-H Geometry (C-O .LT. 1.25 Angstrom)

==========

Strange C-O-H geometry with C-O .LT. 1.25 Angstrom detected. Misplaced H-Atom ?

==========

ALERT_2_313 - Oxygen Atom with Three Covalent Bonds (Rare)

==========

Oxygen atom with three covalent bonds detected. Check for correct atom type assignment (e.g. N rather than O)

Note: Exceptions are H3O+ (Oximium or Hydroxonium) and H5O2+ (Hydronium or aqua-hydroxonium) species.

==========

ALERT_2_314 Small Metal-O-H Angle of H2O

==========

A water molecule coordinated to a metal is detected with an unusually small value of the Metal-Oxygen-Hydrogen Angle.

==========

ALERT_2_316 - Too many H on C in C=N Moiety in Main Residue

==========

An sp3 hybridized C was detected as part of a C=N moiety. Only one attached H atom in sp2 configuration is expected and not two. In SHELXL terms this corresponds with an erroneous AFIX 23 rather than an AFIX 43 type of H atom position generation and refinement.

==========

ALERT_2_317 - Too many H on C in C=N Moiety in Solvent/Ion

==========

An sp3 hybridized C was detected as part of a C=N moiety. Only one attached H atom in sp2 configuration is expected and not two. In SHELXL terms this corresponds with an erroneous AFIX 23 rather than an AFIX 43 type of H atom position generation and refinement.

==========

ALERT_2_318 - Check Hybridization of N in Main Residue

==========

The test attempts to assign one of three hybridization's to N atoms in main residue: sp, sp2 or sp3 on the basis of the angles around N. This ALERT may indicate a mis-assigned H atom position (e.g. an atom placed in a sp2 position instead of sp3).

==========

ALERT_2_319 - Check Hybridization of N in Solvent/Ion

==========

The test attempts to assign one of three hybridization's to N atoms in main residue: sp, sp2 or sp3 on the basis of the angles around N. This ALERT may indicate a mis-assigned H atom position (e.g. an atom placed in a sp2 position instead of sp3).

==========

ALERT_2_320 - Hybridization Problem on C in Main Residue

==========

The test attempts to assign one of three hybridization's to C atoms in main residue: sp, sp2 or sp3 on the basis of the angles around C. In this way, missing H atoms or too many H-atoms on a carbon atom should be detected.

==========

ALERT_2_321 - Hybridization Problem on C in Solvent/Ion

==========

The test attempts to assign one of three hybridization's to C atoms in solvent/anion: sp, sp2 or sp3 on the basis of the angles around C. In this way missing H atoms or too many H-atoms on a carbon atom should be detected.

==========

ALERT_2_322 - Hybridization Problem on non-C in main residue

==========

The test attempts to assign one of three hybridization's to a non-C atom in the main residue: sp, sp2 or sp3 on the basis of the angles around the non-C atom. In this way, missing H atoms or too many H-atoms should be detected.

==========

ALERT_2_323 - Hybridization Problem on non-C in Solvent/Ion

==========

The test attempts to assign one of three hybridization's to a non-C atom in the solvent/anion: sp, sp2 or sp3 on the basis of the angles around the non-C atom. In this way, missing H atoms or too many H-atoms should be detected.

==========

ALERT_2_324 - Possibly Missing H on Coordinating X-N-X in Main Residue

==========

Check for possibly missing Hydrogen atom on Nitrogen coordinating to a metal in the main residue.

==========

ALERT_2_325 - Possibly Missing H on Coordinating X-N-X in Solvent/Ion

==========

Check for possibly missing Hydrogen atom on Nitrogen coordinating to a metal in the solvent/anion.

==========

ALERT_2_326 - Possibly Missing H on Potentially sp3 Carbon Atom in Main Residue

==========

Check for possibly missing Hydrogen atom on Carbon with sp3-like geometry in the main residue.

==========

ALERT_2_327 - Possibly Missing H on potentially sp3 Carbon Atom in Solvent/Ion

==========

Check for possibly missing Hydrogen atom on Carbon with sp3-like geometry in the solvent/anion.

==========

ALERT_4_328 - Possibly Missing H on Potentially sp3 Phosphorus

==========

Check for a possibly missing Hydrogen atom on Phosphorus with sp3-like geometry.

==========

ALERT_2_330 - Large Average Phenyl C-C Distance

==========

The standard average C-C bond distance in a phenyl ring is 1.395 Angstrom. The actual average

ring distance may be larger than expected due to systematic errors in the cell dimensions (e.g. use of incorrect wavelength value for the determination of the cell parameters).

==========

ALERT_2_331 - Small Average Phenyl C-C Distance

==========

The standard average C-C bond distance in a phenyl ring is 1.395 Angstrom. The average ring distance may be smaller due to large thermal motion or incorrect cell dimensions.

==========

ALERT_2_332 - Large Phenyl C-C Bond Distance Range

==========

The standard average C-C in a phenyl ring is 1.395 Angstrom. Bond distances in the ring are expected to vary only slightly due to thermal motion or substituent effects.
Large deviations are likely due to data or likely due to data or model errors.

==========

ALERT_2_333 - Check Average in Multiple Substituted Benzene Type C-C

==========

The standard average C-C bond distance in a flat six carbon atom containing aromatic ring is 1.395 Angstrom. The actual average ring distance may be larger than expected due to substituents such as =O, single bonds or systematic errors in the cell dimensions (E.g. when the wrong wavelength is used in the derivation of the cell parameters).

==========

ALERT_2_334 - Check Average in Multiple Substituted Benzene Type C-C

==========

The standard average C-C bond distance in a benzene ring is 1.395 Angstrom. The average ring distance may be smaller due to large thermal motion, substituents such as =O or incorrect cell dimensions.

==========

ALERT_2_335 - Large Multiple Substituted Benzene Type C-C Range

==========

The standard average C-C bond distance in a benzene ring is 1.395 Angstrom. Bond distances in the ring are expected to vary only slightly when due to substituent effects (exceptions include =O substituents). Large deviations may indicate data or model errors.

==========

ALERT_4_338 - Small Average Tau Value in Cyclohexane Ring

==========

Cyclohexane moieties should have be significantly puckered as measured by the average torsion angle tau. Unresolved disorder generally results in flattened rings and elongated displacement ellipsoids. A disorder model should be included in the calculations.

==========

ALERT_3_340 Low Bond Precision for C-C in Light Atom Structures (Z(max) < 20)

==========

The average s.u. for X-Y bonds is tested (named bond-precision). X-Y will generally be C-C bonds, unless there are none. In the last case the s.u.'s of the lowest element numbers are considered (excluding hydrogen). There are three test ranges: one for structures with the largest element Z < 20, one for the largest Z in the range 20 to 39 and one for structures with Z(max) 40 or higher (_340, _341 and _342 respectively)

==========

ALERT_3_341 Low Bond Precision for C-C in Structures (19 < Z(max) < 40)

==========

The average su for X-Y bonds is tested (named bond-precision). X-Y will generally be C-C bonds, unless there are none. In the last case the s.u.'s of the lowest element numbers are considered (excluding hydrogen). There are three test ranges: one for structures with the largest element Z < 20, one for the largest Z in the range 20 to 39 and one for structures with Z(max) 40 or higher (_340, _341 and _342 respectively)

==========

ALERT_3_342 Low Bond Precision for C-C in Structures (Z(max) > 39)

==========

The average s.u. for X-Y bonds is tested (named bond-precision). X-Y will generally be C-C bonds, unless there are none. In the last case the s.u.'s of the lowest element numbers are considered (excluding hydrogen). There are three test ranges: one for structures with the largest element Z < 20, one for the largest Z in the range 20 to 39 and one for structures with Z(max) 40 or higher (_340, _341 and _342 respectively)

==========

ALERT_2_343 - Angle Range Hybridization Problem on C in Main Residue

==========

The angle range is larger than usual for the tentatively assigned hybridization of the reported atom in the main residue.

==========

ALERT_2_344 - Angle Range Hybridization Problem on C in Solvent/Ion

==========

The angle range is larger than usual for the tentatively assigned hybridization of the reported atom in the solvent/anion.

==========

ALERT_3_350 - Short C - H Bond: Expected XRAY: 0.96

==========

Large deviations from generally accepted values may indicate model problems, over refinement etc. Default C-H = 0.96 Angstrom. (X-Ray) value from SHELXL.

==========

ALERT_3_351 - Long C - H Bond: Expected XRAY: 0.96

==========

Large deviations from generally accepted values may indicate model problems, over refinement etc. Default C-H = 0.96 Angstrom. (X-Ray) value from SHELXL.

==========

ALERT_3_352 - Short N - H Bond: Expected XRAY: 0.87

==========

Large deviations from generally accepted values may indicate model problems, over refinement etc. Default N-H = 0.87 Angstrom. (X-Ray) value from SHELXL.

==========

ALERT_3_353 - Long N - H Bond: Expected XRAY: 0.87

==========

Large deviations from generally accepted values may indicate model problems, over refinement etc. Default N-H = 0.87 Angstrom. (X-Ray) value from SHELXL.

==========

ALERT_3_354 - Long N - H Bond: Expected XRAY: 0.87

==========

Large deviations from generally accepted values may indicate model problems, over refinement etc. Default O-H = 0.82 Angstrom. (X-Ray) value from SHELXL.

==========

ALERT_3_355 - long O - H Bond: Expected XRAY: 0.82

==========

Large deviations from generally accepted values may indicate model problems, over refinement etc. Default O-H = 0.82 Angstrom. (X-Ray) value from SHELXL.

==========

ALERT_2_360 - Short C4 - C4 Bond: Expected XRAY: 1.54

==========

Large deviations from generally accepted values may indicate model problems, over refinement etc. Default C4-C4 = 1.54 Angstrom. (X-Ray) value from Ladd & Palmer, Structure Determination by Xray Crystallography (1985).
Note: - C4-C4 indicates a bond between atoms with 4 bonds each.

==========

ALERT_2_361 - Long C4 - C4 Bond: Expected XRAY: 1.54

==========

Large deviations from generally accepted values may indicate model problems, over refinement etc. Default C4-C4 = 1.54 Angstrom. (X-Ray) value from Ladd & Palmer, Structure Determination by Xray Crystallography (1985).
Note: C4-C4 indicates a bond between atoms with 4 bonds each.

==========

ALERT_2_362 - Short C4 - C3 Bond: Expected XRAY: 1.52

==========

A Large deviation of a bond distance from the generally accepted value may indicate model problems such as over refinement, wrong number of attached hydrogen atoms, disorder etc. Default C4-C3 = 1.52 Angstrom (X-Ray) value from Ladd & Palmer, Structure Determination by Xray Crystallography (1985).

Note:
- C4-C3 indicates a bond between an atom with 4 bonds and one with 3 bonds.
- Conjugated systems may cause some 'false alarm' messages.

==========

ALERT_2_363 - Long C4 - C3 Bond: Expected XRAY: 1.52

==========

A Large deviation of a bond distance from the generally accepted value may indicate model problems such as over refinement, wrong number of attached hydrogen atoms, disorder etc. Default C4-C3 = 1.52 Angstrom (X-Ray) value from Ladd & Palmer, Structure Determination by Xray Crystallography (1985).

Note:
- C4-C3 indicates a bond between an atom with 4 bonds and one with 3 bonds.
- Conjugated systems may cause some 'false alarm' messages.

==========

ALERT_2_364 - Short C4 - C2 Bond: Expected XRAY: 1.46

==========

Large deviations from generally accepted values may indicate model problems, over refinement etc. Default C4-C2 = 1.46 Angstrom. (X-Ray) value from Ladd & Palmer, Structure Determination by Xray Crystallography (1985).

Note:
- C4-C2 indicates a bond between an atom with 4 bonds and one with 2 bonds.
- Conjugated systems may cause some 'false alarm' messages.

==========

ALERT_2_365 - Long C4 - C2 Bond: Expected XRAY: 1.46

==========

Large deviations from generally accepted values may indicate model problems, over refinement etc. Default C4-C2 = 1.46 Angstrom. (X-Ray) value from Ladd & Palmer, Structure Determination by Xray Crystallography (1985).

Note:
- C4-C2 indicates a bond between an atom with 4 bonds and one with 2 bonds.
- Conjugated systems may cause some 'false alarm' messages.

==========

ALERT_2_366 - Short C? - C? (Angstrom Difference) XRAY: 1.50

==========

Large deviations from generally accepted values may indicate model problems, over refinement etc. Default C?-C? = 1.50 Angstrom. (X-Ray) value from Ladd & Palmer, Structure Determination by Xray Crystallography (1985). This ALERT may also arise when the hybridization at least one atom is not recognized.

==========

ALERT_2_367 - Long C? - C? Bond: Expected XRAY: 1.50

==========

Large deviations from generally accepted values may indicate model problems, over refinement etc. Default C?-C? = 1.50 Angstrom. (X-Ray) value from Ladd & Palmer, Structure

Determination by Xray Crystallography (1985).

==========

ALERT_2_368 - Short C3 - C3 Bond: Expected XRAY: 1.34

==========

Large deviations from generally accepted values may indicate model problems, over refinement etc. Default C3-C3 = 1.34 Angstrom. (X-Ray) value from Ladd & Palmer, Structure Determination by Xray Crystallography (1985).

Note:

- C3-C3 indicates a bond between atoms with 3 bonds each.
- Conjugated systems may cause some 'false alarm' messages.

==========

ALERT_2_369 - Long C3 C3 Bond: Expected XRAY: 1.34

==========

Large deviations from generally accepted values may indicate model problems, over refinement etc. Default C3-C3 = 1.34 Angstrom. (X-Ray) value from Ladd & Palmer, Structure Determination by Xray Crystallography (1985).

Note:

- C3-C3 indicates a bond between atoms with 4 with 3 bonds each.
- Conjugated systems may cause some 'false alarm' messages.
- A notable exception is the C-C bond in -C(=O)-C(=O)- systems with an observed mean value of 1.54 Angstrom.

==========

ALERT_2_370 - Short C3 - C2 Bond: Expected XRAY: 1.31

==========

Large deviations from generally accepted values may indicate model problems, over refinement etc. Default C3-C2 = 1.31 Angstrom. (X-Ray) value from Ladd & Palmer, Structure Determination by X-ray Crystallography (1985).

Note:

- C3-C2 indicates a bond between an atom with 3 bonds and one with 2 bonds.
- Conjugated systems may cause some 'false alarm' messages.

==========

ALERT_2_371 - Long C3 - C2 Bond: Expected XRAY: 1.31

==========

Large deviations from generally accepted values may indicate model problems, over refinement etc. Default C3-C2 = 1.31 Angstrom. (X-Ray) value from Ladd & Palmer, Structure Determination by X-ray Crystallography (1985).

Note:

- C3-C2 indicates a bond between an atom with 3 bonds and one with 2 bonds.
- Conjugated systems may cause some 'false alarm' messages.

==========

ALERT_2_372 - Short C2 - C2 Bond: Expected XRAY: 1.25

==========

Large deviations from generally accepted values may indicate model problems, over refinement

etc. Default C2-C2 = 1.25 Angstrom. (X-Ray) value from Ladd & Palmer, Structure Determination by X-ray Crystallography (1985).
Note:
- C2-C2 indicates a bond between atoms with 2 bonds each.
- Conjugated systems may cause some 'false alarm' messages.

==========

ALERT_2_373 - Long C2 - C2 Bond: Expected XRAY: 1.25

==========

Large deviations from generally accepted values may indicate model problems, over refinement etc. Default C2-C2 = 1.25 Angstrom. (X-Ray) value from Ladd & Palmer, Structure Determination by X-ray Crystallography (1985).
Note:
- C2-C2 indicates a bond between atoms with 2 bonds each.
- Conjugated systems may cause some 'false alarm' messages.

==========

ALERT_2_374 - Long N - N Bond (> 1.45 Angstrom)

==========

Large deviations from generally observed bond distances may indicate model problems, over-refinement etc. Check for wrong atom-type assignments. For an example see: Acta Cryst. (2003) E59, m710-m712.

==========

ALERT_4_380 - Incorrectly? Oriented X(sp2)-Methyl Moiety

==========

This test alerts for possible incorrectly oriented CH3 moieties. (E.g. AFIX 33 instead of AFIX 137 etc. within the SHELXL realm)

==========

ALERT_3_390 - Deviating Methyl Moiety X-C-H Bond Angle

==========

Unusual Methyl Moiety X-C-H Angle (Ideally 109 Degrees for 4-bonded C).

==========

ALERT_3_391 - Deviating Methyl Moiety H-C-H Bond Angle

==========

Unusual Methyl Moiety H-C-H Angle (ideally 109 Degrees).

==========

ALERT_2_395 - Deviating X-O-Y Angle from 120 Degrees

==========

The X-O-Y angle is significantly larger than the expected 120.0 Degrees.

==========

ALERT_2_396 - Deviating Si-O-Si Angle from 150 Degrees

==========

The Si-O-Si angle is significantly larger than the expected 150.0 Degrees.

==========

ALERT_2_410 - Short Non-bonding Intra H..H Contact

==========

Short intramolecular contacts may arise when H-atoms are in (false) calculated positions. Short intramolecular contacts may also be a sign for a false structure with the molecule sitting on a site with improper site symmetry (e.g. '2' instead of '-1') which may happen when a lattice translation is missed. Short contacts are defined using a van der Waals radius of 1.2 Angstrom. For intramolecular contacts alerts are generated for contacts less than 2.0 Angstrom.

==========

ALERT_2_411 - Short Non-bonding Inter H..H Contact

==========

Short intermolecular H..H contacts may indicate incorrectly determined structures (i.e. wrong symmetry, missed translation symmetry, wrong position with reference to the symmetry elements, hydrogen atoms on atoms where there should not be any etc..) Short intermolecular contacts may be indicative for inconsistent symmetry data (e.g. coordinates for space-group P43 and symmetry specified as P41 or P21/n & P21/c confusions). Short contacts are defined using a van der Waals radius of 1.2 Angstrom. For intermolecular contacts, an alert is generated for contacts less than 2.4 Angstrom.

==========

ALERT_2_412 - Short Non-bonding Intra H..H Contact (involving XH3 .. XHn)

==========

Short intramolecular contacts may arise when H-atoms are in (false) calculated positions. Short intramolecular contacts may also be a sign for a false structure with the molecule sitting on a site with improper site symmetry (e.g. '2' instead of '-1') which may happen when a lattice translation is missed. Short contacts are defined using a van der Waals radius of 1.2 Angstrom. Short H .. H contact involving CH3 H-atoms are often hampered by the fact that they involve H atoms at not optimal calculated positions.

==========

ALERT_2_413 - Short Non-bonding Inter H..H Contacts (involving XH3 .. XHn)

==========

Short intermolecular H..H contacts may indicate incorrectly determined structures (i.e. wrong symmetry, missed translation symmetry, wrong position with reference to the symmetry elements, hydrogen atoms on atoms where there should not be any etc..). Short intermolecular contacts may be indicative for inconsistent symmetry data (e.g. coordinates for space-group P43 and symmetry specified as P41 or P21/n & P21/c confusions). Short contacts are defined using a van der Waals radius of 1.2 Angstrom. Short H .. H contact involving CH3 H-atoms are often hampered by the fact that they involve H atoms at not optimal calculated positions.

==========

ALERT_2_414 - Short Non-bonding Intra D-H..H-X Contact

==========

Short non-bonding intra D-H..H-X contact.

==========

ALERT_2_415 - Short Non-bonding Inter D-H..H-X Contact

==========

Short non-bonding inter D-H..H-X contact.

==========

ALERT_2_416 - Short Non-bonding Intra D-H..H-D Contact

==========

Short non-bonding intra D-H..H-D contacts may be related to disordered or misplaced H-atoms.

==========

ALERT_2_417 - Short Non-bonding Inter D-H..H-D Contact

==========

Short non-bonding inter D-H..H-D contacts may be related to disordered or misplaced H-atoms. Experience has shown that any intermolecular H...H separation of less than 1.8 Angstroms between full-occupancy H atoms is a clear indicator that one or both of these H atoms may be wrongly placed. A contoured difference map might clarify the issue.

==========

ALERT_2_420 - D-H Without Acceptor

==========

Potential hydrogen bond donors such as -OH and -NH are checked for the presence of suitable acceptors using commonly used H-bond criteria (Jeffrey). As a general rule there should be an acceptor for each donor. Exceptions are very rare for -O-H and more common for -NH and -NH2. A common error is an -OH on a calculated position pointing in the wrong direction due to not taking the molecular environment into account.

==========

ALERT_2_430 - Short Non-bonding Inter D...A Contact

==========

This test alerts for possibly missed Hydrogen bonds as indicated by short (i.e. shorter than sum of the van der Waals radii - 0.2 Angstrom) Donor - Acceptor distances.

Note: Short C=O .. O=C are observed sometimes when part of three-center O-H, N-H or C-H O..O bridging.

==========

ALERT_2_431 - Short Non-bonding Inter HL...A Contact

==========

This test reports on short intermolecular Halogen .. Donor/Acceptor atom-type distances.

==========

ALERT_2_432 - Short Non-bonding Inter X...Y Contact

==========

This test raised an ALERT for short intermolecular contacts. In general, intermolecular contact distances should be not much smaller than the sum of the associated van der Waals Radii. More often than not, such short contacts can be a warning sign for errors. All short contacts should

therefore be examined in some detail. Interesting exceptions are carbonyl- carbonyl interactions that often feature short O...C contacts (see F.H.. Allen et al. (1998) B54, 320-329, short NO2 O...O interactions and BF4(-) to (aromatic) carbon contacts.

ALERT_4_433 - Short Non-bonding Minor..Minor Inter X...Y Contact

==========

This test raised an ALERT for short intermolecular contacts between minor disorder components. In general, intermolecular contact distances should be not much smaller than the sum of the associated van der Waals Radii. More often than not, such short contacts can be a warning sign for errors. All short contacts should therefore examined in some detail. Interesting exceptions are carbonyl-carbonyl interactions that often feature short O...C contacts (see F.H. Allen et al. (1998) B54, 320-329.

==========

ALERT_4_480 - Long H...A H-Bond Reported

==========

Check this (unrealistically) long reported H..A contact. Jeffrey criterion: Contact .LT. vdWR(H) + vdWR(A) - 0.12 Angstrom.

==========

ALERT_4_481 - Long D...A H-Bond Reported

==========

Check this (unrealistically) long reported D..A contact. Jeffrey criterion: Contact .LT. vdWR(D) + vdWR(A) + 0.50 Angstrom.

==========

ALERT_4_482 - Small D-H..A Angle Reported

==========

Check this unrealistically small reported D-H..A Angle. Jeffrey criterion: D-H..A Angle .GT. 100 degrees.

==========

ALERT_4_484 - Round Reported D-H..A Angle to Integer Value

==========

D-H..A angles without s.u. should be rounded to integer values for publication purposes (Required for Acta Crystallographica).

==========

ALERT_2_601 - Structure Contains Solvent Accessible VOIDS

==========

Crystal structures in general do not contain large solvent accessible voids in the lattice. Most structures lose their long-range ordering when solvent molecules leave the crystal. Only when the remaining network is strongly bonded (e.g. zeolites and some hydrogen bonded network systems) the crystal structure may survive. Residual voids in a structure may indicate the omission of (disordered) density from the model. Disordered density may go undetected when smeared since peak search programs are not designed to locate maxima on density ridges. The presence or absence of residual density in the void may be verified on a printed/plotted

difference Fourier map or with PLATON/SQUEEZE. Voids of 40 Ang**3 may accommodate H2O. In such a case, hydrogen bond acceptors are expected at hydrogen bonding distance. Small molecules such as Tetrahydrofuran have typical volumes in the 100 to 200 Ang**3 range. This test reports the volume of the largest solvent accessible void in the structure only. PLATON/SOLV will give the complete list.A paper reporting a crystal structure with a significant solvent accessible void should at the least report and discuss the issue.

==========

ALERT_2_602 - VERY LARGE Solvent Accessible VOID(S) in Structure

==========

This test reports on a solvent accessible void in the structure, too large or too time consuming for the current PLATON version for a more detailed analysis as part of the validation run. Use the SOLV option for more details. Such a warning might also indicate that the symmetry is incomplete e.g. should have been specified as P-1 and not P1, leaving out half of the unit cell content.

==========

ALERT_4_603 - Unit-Cell TOO large for VOID SEARCH in Structure

==========

No search for solvent accessible VOIDS done as part of VALIDATION in view of large unit-cell.

==========

ALERT_4_604 - Too Many VOIDS Detected in Structure

==========

Too many solvent accessible VOIDS.

==========

ALERT_4_605 - Structure Contains Solvent Accessible VOIDS

==========

Crystal structures in general do not contain large solvent accessible voids in the lattice. Most structures lose their long-range ordering when solvent molecules leave the crystal. Only when the remaining network is strongly bonded (e.g. zeolites and some hydrogen bonded networks) the crystal structure may survive. Residual voids in a structure may indicate the omission of (disordered) density from the model. Disordered density may go undetected when smeared since peak search programs are not designed to locate maxima on density ridges. The presence or absence of residual density in the void may be veryfied on a printed/plotted difference Fourier map or with PLATON/SQUEEZE. Voids of 40 Ang**3 may accommodate H2O. Small molecules such as Tetrahydrofuran have typical volumes in the 100 to 200 Ang**3 range. This test reports the volume of the largest solvent accessible void in the structure. A paper reporting a crystal structure with a significant solvent accessible void should at the least discuss the issue.

Note: The use of PLATON/SQUEEZE was reported in the CIF

==========

ALERT_4_606 - VERY LARGE Solvent Accessible VOID(S) in Structure

==========

This test reports on a solvent accessible void in the structure, too large or too time consuming for the current PLATON version for a more detailed analysis as part of the validation run. Use the SOLV option for more details. Such a warning might also indicate that the symmetry is incomplete e.g. should have been specified as P-1 and not P1, leaving out half of the unit cell content.

==========

ALERT_1_701 Check the Consistency of the Bond Distances and Coordinates

==========

Bond distances given in the CIF are cross-checked with corresponding values calculated from the coordinates. Alerts are set at 1,2 and 3 sigma deviation levels.
Note: Default s.u.'s are used where no su given (e.g. for C-H) In general, all differences should be within the associated s.u. Small differences may arise from rounding. Very large deviation (or zero distance) normally indicate incorrectly specified symmetry operations on the associated atoms, or 'cut-and-pasting' of incompatible CIF's.

==========

ALERT_1_702 Check the Consistency of the Bond Angles and Coordinates

==========

Bond Angles given in the CIF are cross-checked with corresponding values calculated from the coordinates. Alerts are set at 1,2 and 3 sigma deviation levels. In general, all differences should be within the associated s.u. Small differences may arise from rounding. Very large deviations normally indicate incorrectly specified symmetry operations on the associated atoms, or 'cut-and-pasting' of incompatible CIF's.

==========

ALERT_1_703 Check the Consistency of the Torsion Angles and the Coordinates

==========

Torsion angles given in the CIF are cross-checked with corresponding values calculated from the coordinates. Alerts are set at 1,2 and 3 sigma deviation levels. In general, all differences should be within the associated s.u. Small differences may arise from rounding. Very large deviations normally indicate incorrectly specified symmetry operations on the associated atoms, or 'cut-and-pasting' of incompatible CIF's.

==========

ALERT_1_704 Check the Consistency of the Contact Distances and Coordinates

==========

Intermolecular contacts listed in the CIF are checked against the coordinates in the CIF. Alerts are set at 1,2 and 3 sigma deviation levels.

==========

ALERT_1_705 Check the Consistency of H-Bond D-H Distance with Coordinates

==========

Hydrogen-Bond D-H listed in the CIF is checked. Alerts are set at 1,2 and 3 sigma deviation levels.

==========

ALERT_1_706 - Check the Consistency of H-Bond H...A Distance with Coordinates

==========

Hydrogen-Bond H..A listed in the CIF is checked. Alerts are set at 1,2 and 3 sigma deviation levels.

This ALERT is generally related to incorrect symmetry codes. The symmetry number s in the symmetry code s_pqr should correspond to the expression for s in the CIF. Those expressions can be different for different software packages. E.g. pasting H-bond table data generated with PLATON into a CIF generated with SHELXL may raise this ALERT. Manual correction of the symmetry code should be trivial.

==========

ALERT_1_707 - Check the Consistency of H-Bond D...A Distance with Coordinates

==========

Hydrogen-Bond D..A listed in the CIF is checked. Alerts are set at 1,2 and 3 sigma deviation levels.

This ALERT is generally related to incorrect symmetry codes. The symmetry number s in the symmetry code s_pqr should correspond to the expression for s in the CIF. Those expressions can be different for different software packages. E.g. pasting H-bond table data generated with PLATON into a CIF generated with SHELXL may raise this ALERT. Manual correction of the symmetry code should be trivial.

==========

ALERT_1_708 - Check the Consistency of H-Bond D-H...A Angle with Coordinates

==========

Hydrogen-Bond Angle D-H..A listed in the CIF is checked. Alerts are set at 1,2 and 3 sigma deviation levels.

This ALERT is generally related to incorrect symmetry codes. The symmetry number s in the symmetry code s_pqr should correspond to the expression for s in the CIF. Those expressions can be different for different software packages. E.g. pasting H-bond table data generated with PLATON into a CIF generated with SHELXL may raise this ALERT. Manual correction of the symmetry code should be trivial.

==========

ALERT_4_710 Delete Meaningless Linear Torsion Angle from CIF

==========

Torsion angles specified in the CIF are checked for the 'linear variety' where one or both of the 1-2-3 and 2-3-4 bond angles are close to 180 Deg. SHELXL97 will generate those 'torsions' for molecules containing linear moieties (E.g. Metal-C=O).

==========

ALERT_1_711 Unknown or Inconsistent Atom Label in BOND CIF Item

==========

When labels are found on geometry items (bonds, angles etc.) that are not in the coordinate list,

and alert _71n is issued, related to alert _70n.

==========

ALERT_1_712 - Unknown or Inconsistent Atom Label in ANGLE CIF Item

==========

When labels are found on geometry items (bonds, angles etc.) that are not in the coordinate list, and alert _71n is issued, related to alert _70n.

==========

ALERT_1_713 - Unknown or Inconsistent Atom Label in TORSION CIF Item

==========

When labels are found on geometry items (bonds, angles etc.) that are not in the coordinate list, and alert _71n is issued, related to alert _70n.

==========

ALERT_1_714 - Unknown or Inconsistent Atom Label in CONTACT CIF Item

==========

When labels are found on geometry items (bonds, angles etc.) that are not in the coordinate list, and alert _71n is issued, related to alert _70n.

==========

ALERT_1_715 - Unknown or Inconsistent Atom Label in D-H CIF Item

==========

When labels are found on geometry items (bonds, angles etc.) that are not in the coordinate list, and alert _71n is issued, related to alert _70n.

==========

ALERT_1_716 - Unknown or Inconsistent Atom Label in H..A CIF Item

==========

When labels are found on geometry items (bonds, angles etc.) that are not in the coordinate list, and alert _71n is issued, related to alert _70n.

==========

ALERT_1_717 - Unknown or Inconsistent Atom Label in D...A CIF Item

==========

When labels are found on geometry items (bonds, angles etc.) that are not in the coordinate list, and alert _71n is issued, related to alert _70n.

==========

ALERT_1_718 - Unknown or Inconsistent Atom Label in D-H..A CIF Item

==========

When labels are found on geometry items (bonds, angles etc.) that are not in the coordinate list, and alert _71n is issued, related to alert _70n.

==========

ALERT_4_720 Unusual and/or Non-Standard Labels

==========

Up to 4 Character Labels of the type C11, H101, N10A, i.e. chemical symbol + number + optional letter are to be preferred.

==========

ALERT_1_721 - Consistency of Bonds and Coordinates in the CIF

==========

Same as 701 but for distance without s.u. The difference is tested in terms of Angstroms.

==========

ALERT_1_722 - Consistency of Angles and Coordinates in the CIF

==========

Same as 702 but for angle without s.u. The difference is tested in terms of Degrees.

==========

ALERT_1_723 - Consistency of Torsions and Coordinates in the CIF

==========

Same as 703 but for torsion without s.u. The difference is tested in terms of Degrees.

==========

ALERT_2_724 - Consistency of Contact Distances and Coordinates in the CIF

==========

Same as 704, but for distance without s.u. Difference is tested in terms of Angstroms.

==========

ALERT_2_725 - Consistency of H-Bond D-H distances and Coordinates in the CIF

==========

Same as 705 but for distance without s.u. Differences are tested in terms of Angstrom.

==========

ALERT_2_726 - Consistency of H-Bond H..A Distances and Coordinates in the CIF

==========

Same as 706 but for distance without s.u. (esd). Differences are tested in terms of Angstrom.

==========

ALERT_1_727 - Consistency of H-Bond D..A Distances and Coordinates in the CIF

==========

Same as 707 but for distance without s.u. Differences are tested in terms of Angstrom.

==========

ALERT_1_728 - Consistency of H-Bond D-H..A Angles and Coordinates in the CIF

==========

Same as 708 but for angle without s.u. Differences are tested in terms of Degrees.

==========

ALERT_1_731 - Consistency of Bond su's and Coordinate s.u.'s in the CIF

==========

A large ratio of the reported and calculated bond s.u.'s is found. The use of a DFIX instruction

might cause such a warning since calculated s.u.'s are based on reported variances only.
Note_1: s.u.'s on the unit-cell dimensions are taken into account in the calculation of expected s.u.'s. This may result in large differences between expected and reported s.u.'s when this contribution is not included in the reported s.u.'s, in particular for inaccurate unit-cells.
Note_2: Another source for the discrepancy between calculated and reported s.u.'s can be that the validation software has access only to the variances of the refined parameters as opposed to the full co-variance matrix used by e.g. SHELXL for the calculation of derived parameters with associated s.u.'s. Constrained/restrained refinement may cause large co-variances.

==========

ALERT_1_732 - Consistency of Angles and Coordinates in the CIF s.u.'s

==========

A large ratio of the reported and calculated bond angle s.u.'s is found. This check should warn for erroneous rounding: E.g. 105.5(19) to 105.5(2) or 105.0(5) to 105(5) etc. Note: Large differences are possible when certain constraints/restraints were applied in the refinement (e.g. the FLAT option in SHELXL97).
Note: s.u.'s on the unit-cell dimensions are taken into account in the calculation of expected su's. This may result in large differences between expected and reported s.u.'s when this contribution is not included in the reported s.u.'s, in particular for inaccurate unitcells.
Note_2: Another source for the discrepancy between calculated and reported s.u.'s can be that the validation software has access only to the variances of the refined parameters as opposed to the full co-variance matrix used by e.g. SHELXL for the calculation of derived parameters with associated s.u.'s. Constrained/restrained refinement may cause large co-variances.

==========

ALERT_1_733 - Consistency of Torsions and Coordinates in the CIF s.u's

==========

A large ratio of the reported and calculated torsion angle s.u.'s is found. This check should warn for erroneous rounding: E.g. 105.5(19) to 105.5(2) or 105.0(5) to 105(5) etc.
Note: s.u.'s on the unit cell dimensions are taken into account in the calculation of expected s.u.'s. This may result in large differences between expected and reported s.u.'s when this contribution is not included in the reported su's, in particular for inaccurate unit-cells.
Note_2: Another source for the discrepancy between calculated and reported s.u.'s can be that the validation software has access only to the variances of the refined parameters as opposed to the full co-variance matrix used by e.g. SHELXL for the calculation of derived parameters with associated s.u.'s. Constrained/restrained refinement may cause large co-variances.

==========

ALERT_1_734 - Consistency of Contact Distance s.u. and Coordinate s.u. in the CIF

==========

A large ratio of the reported and calculated contact distance s.u.'s is found.
Note: s.u.'s on the unit-cell dimensions are taken into account in the calculation of expected su's. This may result in large differences between expected and reported s.u.'s when this contribution is not included in the reported s.u.'s, in particular for inaccurate unit-cells.

==========

ALERT_1_735 - Consistency of H-Bond D-H distance s.u. and Coordinate s.u in the CIF

==========

A large ratio of the reported and calculated H-bond D-H distance s.u.'s is found. The use of a DFIX instruction might cause such a warning since calculated s.u.'s are based on reported variances only.
Note: s.u.'s on the unit-cell dimensions are taken into account in the calculation of expected s.u.'s. This may result in large differences between expected and reported s.u.'s when this contribution is not included in the reported s.u.'s, in particular for inaccurate unit-cells.

==========

ALERT_1_736 - Consistency of H-Bond H..A Distance s.u. and Coordinates in the CIF

==========

A large ratio of the reported and calculated H-bond H..A distance s.u.'s is found.
Note: s.u.'s on the unit-cell dimensions are taken into account in the calculation of expected s.u.'s. This may result in large differences between expected and reported s.u.'s when this contribution is not included in the reported s.u.'s, in particular for inaccurate unit-cells.

==========

ALERT_1_737 - Consistency of H-Bond D..A Distance s.u. and Coordinates in the CIF

==========

A large ratio of the reported and calculated H-Bond D...A distance s.u.'s is found.

==========

ALERT_1_738 - Consistency of H-Bond D-H..A Angle and Coordinates in the CIF s.u.

==========

A large ratio of the reported and calculated H-Bond D-H..A angle s.u.'s is found.
Note: s.u's on the unit cell dimensions are taken into account in the calculation of expected s.u.'s. This may result in large differences between expected and reported su's when this contribution is not included in the reported s.u.'s, in particular for inaccurate unit-cells.

==========

ALERT_1_741 - Missing Bond s.u. in the CIF

==========

Likely missing s.u. on Bond in CIF.

==========

ALERT_1_742 - Missing Angle s.u. in the CIF

==========

Likely missing s.u. on Bond angle in CIF.

==========

ALERT_1_743 - Missing Torsion s.u. in the CIF

==========

Likely missing s.u. on Torsion angle in CIF.

==========

ALERT_1_744 - Missing Contact Distance s.u. in the CIF

==========

Likely missing s.u. on contact Distance in CIF.

==========

ALERT_1_745 - Missing H-Bond D-H distance s.u. in the CIF

==========

Likely missing s.u. on H-Bond D-H distance in CIF.

==========

ALERT_1_746 - Missing H-Bond H..A Distance s.u. in the CIF

==========

Likely missing s.u. on H-Bond H...A distance in CIF.

==========

ALERT_1_747 - Missing H-Bond D..A Distance s.u. in the CIF

==========

Likely missing s.u. on H-Bond D...A distance in CIF.

==========

ALERT_1_748 - Missing H-Bond D-H..A Angle s.u. in the CIF

==========

Likely missing s.u. on H-Bond D-H..A angle in CIF.

==========

ALERT_4_751 - Senseless Bond s.u. in the CIF

==========

An s.u. should not be given in the CIF for constrained distances. Please check for proper refinement status flags (e.g. R)

==========

ALERT_4_752 - Senseless Angle s.u. in the CIF

==========

An s.u. should not be given in the CIF for constrained angles. Please check for proper refinement status flags (e.g. R)

==========

ALERT_4_753 - Senseless Torsion s.u. in the CIF

==========

An s.u. should not be given in the CIF for constrained torsion angles. Please check for proper refinement status flags (e.g. R)

==========

ALERT_4_754 - Senseless Contact Distance s.u. in the CIF

==========

An s.u. should not be given in the CIF for constrained contact distances. Please check for proper refinement status flags (e.g. R)

==========

ALERT_4_755 - Senseless H-Bond D-H distance s.u. in the CIF

==========

An s.u. should not be given in the CIF for constrained distances. Please check for proper refinement status flags (e.g. R)

==========

ALERT_4_756 - Senseless H-Bond H..A Distance s.u. in the CIF

==========

An s.u. should not be given in the CIF for constrained distances. Please check for proper refinement status flags (e.g. R).

==========

ALERT_4_757 - Senseless H-Bond D..A Distance s.u. in the CIF

==========

An s.u. should not be given in the CIF for constrained distances. Please check for proper refinement status flags (e.g. R)

==========

ALERT_4_758 - Senseless H-Bond D-H..A Angle s.u. in the CIF

==========

An s.u. should not be given in the CIF for constrained angles. Please check for proper refinement status flags (e.g. R)

==========

ALERT_1_760 - CIF Contains no Torsion Angles

==========

The CIF contains no torsion angle entries. Torsion angles may be included with the SHELXL instruction CONF. Inclusion is encouraged for Acta Crystallographica submissions but not necessarily so by other journals.

==========

ALERT_1_761 - CIF Contains no X-H Bonds

==========

The CIF contains no X-H Bonds. This might be caused by not using the SHELXL instruction BOND $H Inclusion is required by Acta Cryst. but not necessarily so by other journals.

==========

ALERT_1_762 - CIF Contains no X-Y-H or H-Y-H Angles

==========

The CIF contains no X-Y-H or H-Y-H bond angles. This might be caused by not using the SHELXL instruction BOND $H. Those data should also be supplied when H-atoms are introduced on calculated positions and/or refined riding on their carrier atom. Inclusion is required by Acta Cryst. but not necessarily so by other journals.

==========

ALERT_1_763 - Incomplete CIF Bond list Detected (Reported/Expected)

==========

Bond list in CIF likely incomplete.

==========

ALERT_4_764 Over complete CIF Bond List Detected (Reported/Expected)

==========

The CIF contains more bonds than the unique set, indicating redundancy. An example is redundancy due to the inclusion of symmetry related bonds.

==========

ALERT_2_770 - Suspect C-H bonds in CIF (Not caught otherwise)

==========

Report on unusual C-H bonds not caught in other tests.

==========

ALERT_2_771 - Suspect N-H bonds in CIF (Not caught otherwise)

==========

Report on unusual N-H bonds not caught in other tests.

==========

ALERT_2_772 - Suspect O-H bonds in CIF (Not caught otherwise)

==========

Report on unusual O-H bonds not caught in other tests.
Note: Exceptions can be H-atoms in acid O..H..O bridges or in H5O2+ (Hydronium) species.

==========

ALERT_2_773 - Suspect C-C bonds in CIF (Not caught otherwise)

==========

Report on unusual C-C bonds, possibly not caught in other tests. Exceptions include C-C distances of around 1.75 Ang. in e.g. 1,2-dicarba-closo-dodecaborane.

==========

ALERT_1_774 - Too Large / Erroneous Bond Distance

==========

Likely erroneous bond distance entry

==========

ALERT_1_775 - Too Large / Erroneous Contact Distance

==========

too large / erroneous contact distance entry

==========

ALERT_1_776 - Likely Erroneous Contact Entry

==========

Likely Erroneous D-H Entry

==========

ALERT_4_779 - Suspect or Irrelevant (Bond) Angle in CIF

==========

Possibly erroneous (Bond)angle less than 45 degree. The angle might be considered for elimination from the CIF when irrelevant. This ALERT can also be triggered when the assigned occupancy factors are incorrect.

==========

ALERT_1_780 - Coordinates do not Form a Properly Connected Set

==========

Atoms given in a CIF should form a 'connected set', i.e. no symmetry operations are needed to get atoms in a bonding position. A connected set of atoms is not needed for the least squares refinement (unless hydrogen atoms are to be added at calculated positions). Geometry listings (bonds, angles, torsions & H-bonds) become unwieldy for non-connected atom sets.

==========

ALERT_1_781 - Flack Parameter is given for Centro-symmetric Space-group

==========

A Flack parameter value is erroneously given for a structure reported in a centro-symmetric space-group.

==========

ALERT_2_782 - Unusual C-NO2 an C-CO2 Moiety Geometry

==========

The geometry of the reported moiety appears to be unusual/inconsistent. The C-O bond distances in C-CO2 are expected to add up to about 2.5
The N-O bond distances in C-NO2 are expected to add up to about 2.4

==========

ALERT_4_790 The Center of Gravity of a Residue is not Within the Unit Cell Bounds

==========

Unless for a good reason, molecular species should be transformed (by symmetry and/or translation) so that their centers of gravity are close to or within the unit-cell bounds. This is a strict and easy to accomplish rule for the main species. Deviations from this general rule are for smaller additional species when relevant for the convenient description of their intermolecular interactions with the main species.

==========

ALERT_4_791 - Check the absolute configuration of chiral atom in 'chiral' Space-group

==========

This test addresses the consistency of the absolute configuration assignment in non-centro-symmetric structures with proper symmetry operations (i.e. all matrices with determinant = 1) only.

Verify the (R/S) absolute configuration assignment of this atom and the consistency of the absolute configuration implicit in the CIF data with that in the 'ORTEP' illustration. Torsion angles should have the correct sign.

The absolute structure assignment should also be consistent with the lowest value of the Flack parameter and/or know absolute configuration.

==========

ALERT_1_792 - Check the absolute configuration of chiral atom in 'non-chiral' spgr

==========

This test addresses the consistency of the absolute structure assignment (i.e. polarity etc.) in

non-centrosymmetric structures in space groups that include improper symmetry operations (e.g. mirror planes).

Check the (R/S) absolute configuration assignment of this atom and the consistency of the absolute configuration implicit in the CIF data with that in the 'ORTEP' illustration.

==========

ALERT_4_793 - Absolute Configuration of Chiral Atom in Centrosymmetric Space-group

==========

This test addresses the consistency of the absolute configuration assignment of molecules in the reported asymmetric unit among coordinates, molecular presentations and chemical diagrams. Check the (R/S) absolute configuration assignment of this atom and the consistency of the absolute configuration implicit in the CIF data with that in the 'ORTEP' illustration.

==========

ALERT_5_794 - Check Predicted Bond Valency

==========

This test reports the valency of an atom as predicted by the Valence Bond Model. See:
N.E. Brese & M. O'Keeffe (1991) Acta Cryst. B47, 192-197.
I.D. Brown (2002). The Chemical Bond in Inorganic Chemistry:
The Bond Valence Model. Oxford University Press.

More explicit info on the calculations can be obtained by running the calculations explicitly with the PLATON option BondValence.

Note: The underlying theory is empirical and might not apply to the
case at hand (e.g. charged species).

==========

ALERT_4_795 - C-Atom in CIF Coordinate List out of Sequence

==========

The atoms in the CIF are not given in logical order (i.e. C1, C2 etc.).The recommended procedure is to sort the atom list in some logical order before the final refinement cycles. Hydrogen atoms associated with their carrier atom are recommended to directly follow them.

==========

ALERT_4_796 - O-Atom in CIF Coordinate List out of Sequence

==========

The atoms in the CIF are not given in logical order (i.e. O1, O2 etc.) The recommended procedure is to sort the atom list in some logical order before the final refinement cycles. Hydrogen atoms associated with their carrier atom are recommended to directly follow them.

==========

ALERT_4_797 - Test for N-atom Labels Ordered

==========

The atoms in the CIF are not given in logical order (i.e. N1, N2 etc.) The recommended procedure is to sort the atom list in some logical order before the final refinement cycles.

Hydrogen atoms associated with their carrier atom are recommended to directly follow them.

==========

ALERT_4_798 - Numeric Atom Label on Coordinate Parameter Record

==========

Atom labels are generally not a number (i.e. starting with one or two characters indicating the atom type). Labels can be erroneously numeric due to typing errors (e.g. 'Oxygen' typed as 'zero').

==========

ALERT_4_799 - Alphanumeric Label on Displacement Parameter Record

==========

Atom labels are generally not a number (i.e. starting with one or two characters indicating the atom type). Labels can be erroneously numeric due to typing errors (e.g. 'Oxygen' typed as 'zero').

==========

ALERT_4_801- Cell Data Missing, Incomplete or Out-of-Order

==========

PLATON has a problem with the Cell data. The possible reason can be that the cell data are missing, incomplete or out-of-sequence. PLATON/CHECK wishes to see the cell and symmetry data before any coordinates are given. PLATON expects the values of all six cell parameters.

==========

ALERT_4_802 - CIF Input Record(s) with more than 80 Characters

==========

The CIF contains records longer than 80 characters. Not all software will read beyond column 80. The CIF-1.1 definition specifies a maximum of 2048 character per record.

==========

ALERT_1_803 - Loop Problem in CIF-Reading (Too Many loop Items)

==========

Fatal Problem: Check loop data names and data for errors. There are likely too many or to few data in the loop.

==========

ALERT_5_804 - ARU-Pack Problem in PLATON Analysis

==========

Problem: ARU representations turn out to be needed outside the ORTEP style -5:5 unit cell translation range. The Analysis might be incomplete. The problem often occurs for structures with aliphatic chains stretching over many unit cells or network structures. Transformation of the unit cell content to a symmetry related position might solve the problem.

==========

ALERT_4_805 - Fatal Problem: Insufficient Data in Atom Loop

==========

Check Coordinate Data Loop.

==========

ALERT_4_806 - Fatal Problem: Insufficient Data in Uij Loop

==========

Check UIJ Data Loop.

==========

ALERT_5_807 - Fatal Problem: Maximum Number of Atoms Exceeded

==========

PLATON can handle up to 7000 atoms in the (expanded) ATOM list. This might happen with disordered or network structures in high symmetry space groups. Deletion of the symmetry information might solve part of the problem and provide a partial validation. Alternatively, clicking on 'NOSYMM' on the PLATON menu before invoking validation might address the problem.

==========

ALERT_5_808 - No Parseable SHELXL Style Weighting Scheme Found

==========

The software did not succeed in finding/analyzing a parseable weighting scheme.

SHELXL weight parameters are expected to be given in the format:

_refine_ls_weighting_details
'calc w=1/[\s^2^(Fo^2^)+(0.1000P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3'

The JANA weight is expected to be given as:

_refine_ls_weighting_details 'w=1/(\s^2^(I)+0.0016I^2^)'

Do not edit this string or make it into a text block between ';'.

==========

ALERT_1_809 - Can not Parse the SHELXL Weighting Scheme String

==========

The software did not succeed in Parsing SHELXL style weighting scheme. The string might have been edited.

ALERT_5_810 - Out-of-Memory Problem in PLATON/ASYM

==========

Analysis for missing reflections may be incomplete due to an out-of-memory problem.

==========

ALERT_5_811 - No ADDSYM Analysis: Too Many Excluded Atoms

==========

The ADDSYM test for missed symmetry is not executed for structures with too many disordered atoms.

ALERT_5_820 Report Read Problem in Routine PLATON/PLA230

==========

Internal PLATON Problem. Please refer problem to author at a.l.spek@uu.nl

==========

ALERT_4_850 Check the Exact Value 0.00 and s.u. of the Flack Parameter

==========

This G_ALERT can be ignored in the case that the so-called 'on-the-cheap' Flack parameter is reported as determined with SHELXL.

Exactly zero values are possible but may also be a software artifact.

The following should be checked:

Problem #1: Some SHELXL97 versions do not allow negative values of the Flack parameter when determined using the BASF/TWIN instructions. Negative values are set to 0.00001. Refinement may not converge completely.

Problem #2: Some SHELXL97 versions put meaningless values in the CIF for the Flack parameter when 'TWIN -1 0 0 0 -1 0 0 0 -1 2 / BASF' instructions (i.e. an explicit matrix is specified on the TWIN instruction) are used. Please check the value of BASF (in the list output) against the Flack parameter in the CIF.

==========

ALERT_3_860 Explain the Non-trivial Least-Squares Restraints

==========

The use of restraints used in the refinement should be explained in the write-up of a structure analysis. An exception are restraints for floating origins in space-groups such as $P2_1$.

ALERT_5_870 Twinning Related ALERTS Suppressed

ALERTS related to twinning effects that can not (yet) be accounted for as part of the VALIDATION algorithms have been suppressed.

ALERT_5_871 non AgKa, MoKa, CuKa ALERTS suppressed

ALERTS related to the use of radiation other than AgKa, MoKa or CuKa radiation have been suppressed. No f' and f'' data are available in PLATON for other radiation types (including Synchrotron).

==========

ALERT_1_900 No Matching Reflection File Found for Parameter CIF

==========

Likely cause: Data set names specified with *data_* in the CIF and FCF differ.

Note: FCF Validation is Skipped for this Entry.

==========

ALERT_1_901 The Cell Parameters in the CIF and FCF do not Match

==========

Likely causes: Wrong Data set, CIF or FCF Parameters Edited inconsistently.

Note: FCF Validation is Skipped for this Entry.

==========

ALERT_1_902 No (interpretable) Reflections found in FCF

==========

Either no reflections in the FCF or uninterpretable due to unknown format or editing.

Note: FCF Validation is Skipped for this Entry.

==========

ALERT_2_908 Maximum Percentage of Observed Data of the Lowest Resolution Shell

==========

A low maximum percentage of reflections with I .gt. 2*σ(I) may indicate:
1 - Missed translation symmetry. E.g. all reflections hkl weak for l = 2n +1
2 - Pseudo-merohedral twinning, index .gt. 1. (e.g. non-space-group extinctions.
3 - Very weak observed data.

==========

ALERT_3_909 Significant Percentage of Observed data at Θ (Max)

==========

This ALERT Reports on whether there is still a significant level of observed data beyond the Theta cutoff of the data set. There should be a good reason for a cutoff below sin(Θ)/λ = 0.6.

==========

ALERT_3_910 Missing Reflections Below Θ(min)

==========

Possible causes: The beam-stop theta-min limit set too high, large unit-cell etc. A possible technical solution on CCD based equipment involves the collection of additional images with the detector at a larger distance from the crystal with the beam-stop setting changed accordingly.

==========

ALERT_3_911 Missing Reflections Between ?(min) and sin(Θ) / λ = 0.6 in the FCF

==========

Possible causes: Missing cusp of data (due to rotation about one axis only), deleted (overflow) reflections or improper strategy (orthorhombic for monoclinic crystal etc.)
A data set is expected to be essentially complete up to **sin(Θ) / λ =** 0.6**.** Exceptions can be data sets collected using a high pressure cell due to physical restrictions.

==========

ALERT_4_912 Missing Reflections Above sin(Θ) / λ = 0.6 in the FCF

==========

Possible causes: Missing cusp of data (due to rotation about one axis), deleted (overflow) reflections or improper strategy (orthorhombic for monoclinic crystal etc.)

==========

ALERT_3_913 A number of Very Strong Reflections are Missing from the FCF

==========

This ALERT reports the number of missing reflections with Fcalc**2 values greater than the largest Fcalc**2 value in the FCF. Possible causes: Missing cusp of data (due to rotation about one axis), deleted (overflow) reflections or improper strategy (orthorhombic for monoclinic crystal etc.) or behind the beam stop.

==========

ALERT_3_914 No Bijvoet Pairs in FCF for Non-centrosymmetric Structure

==========

This ALERT reflects the notion that a data set should contain a sufficient number of Bijvoet (Friedel) pairs for the reliable determination of the absolute structure of a non-centrosymmetric crystal structure.

This test is invoked when a Flack parameter value is specified.
Note: SHELXL97 will calculate/report a Flack parameter value even for refinement against Friedel merged data. Remove the Flack entry from the CIF.

==========

ALERT_3_915 Low Friedel Pair coverage

==========

This ALERT reflects the notion that a data set should contain a sufficient number of Bijvoet (Friedel) pairs for the reliable determination of the absolute structure of a non-centrosymmetric crystal structure.

A Friedel coverage that deviates significantly from 100 percent may bias/invalidate the value of the Flack parameter.

==========

ALERT_2_916 The Flack x and Hooft y Parameters Differ

==========

The Hooft y Parameter is calculated independently from the Bijvoet differences and should have a value similar (observing the su's) to that of the Flack x Parameter.
See:
Hooft, R.W.W, Straver, L.H. & Spek,A.L. (2008). J. Appl, Cryst. 41, 96-103.
Thompson,A.L. & Watkin, D.J. (2009). Tetrahedron: Asymmetry,
doi:10.1016/j.tetasy.2009.02.025

Large differences may arise in cases where the Flack parameter was not done with BASF/TWIN or with essentially centros-symmetric data.
See:
Flack, H.D., Bernardinelli, G., Clemente, D.A., Linden, A.,. Spek, A.L. (2006) Acta Cryst. B62,

695-701.

==========

ALERT_2_917 The FCF is Likely not Based on a BASF/TWIN Refinement

==========

The contribution of F(-h,-k,-l) to F(h,k,l) is likely not included in the FCF file. This usually indicates that the Flack parameter was NOT determined with a BASF/TWIN type of refinement.

==========

ALERT_3_918 Reflections with I(obs) << I(calc)

==========

This ALERT reports the number of reflections with $(Fobs^2 - Fcalc^2) / sigma(Fobs^2) < - 100.0$. Those reflections are better removed from the final refinement since they are in systematic error. Of course, a valid reason should be found for this problem. 'Behind the Beam stop' can be one of the possible reasons.

==========

ALERT_3_919 Reflections Likely Affected by the Beam stop Detected

==========

This ALERT reports the number of reflections with intensities seriously effected by the beam stop. Reflections are counted for which theta < 3 Degrees and $(Fobs^2 - Fcalc^2) / sqrt(weight) < -10.0$. Those reflections are better removed from the final refinement since they are in systematic error.

==========

ALERT_1_920 Theta(Max) in CI and FCF Differ

==========

Check reflection statistics of the data in the FCF for consistency with the data reported in the CIF.

A difference usually indicates an edited CIF or an FCF file that was not created in the same SHELXL run where the CIF was created.

==========

ALERT_1_921 Reported (CIF) and Calculated (From FCF/Fcalc)) R1 Values Differ

==========

Please check whether the supplied FCF corresponds with the CIF produced in the same least squares refinement job.

The test is based on the observed and calculated F**2 in the FCF and the weight parameters taken from the CIF.

==========

ALERT_1_922 Reported (CIF) and Calculated (From FCF/Fcalc) wR2 Values Differ

==========

Please check whether the supplied FCF corresponds with the CIF produced in the same least

squares refinement job.

The test is based on the observed and calculated F^2 in the FCF and the weight parameters taken from the CIF.

==========

ALERT_1_923 - Reported (CIF) and Calculated (From FCF/Fcalc) S Values Differ

==========

Please check whether the supplied FCF corresponds with the CIF produced in the same least squares refinement job.

The test is based on the observed and calculated F^2 in the FCF and the weight parameters taken from the CIF.

==========

ALERT_1_924 The Reported and Calculated Difference Map Rho(min) Values Differ

==========

Check & Explain why the Reported Rho(min) differs significantly from the value calculated on the basis of the reported structure.

Note: The Reported and Calculated values may differ slightly due to a differing peak interpolation algorithm.

==========

ALERT_1_925 The Reported and Calculated Difference Map Rho(max) Values Differ

==========

Check & Explain why the Reported Rho(max) differs significantly from the value calculated on the basis of the reported structure.

Note: The Reported and Calculated values may differ slightly due to a differing peak interpolation algorithm.

==========

ALERT_1_926 The Reported and Calculated R1 Values Differ

==========

Please check whether the R1 value that is reported in the CIF corresponds with the R1 value calculated from the parameters supplied in the CIF.

This test is based on the observed reflection data in the FCF and reflection data that are calculated with the parameters (i.e. coordinates, displacement and weight parameters) taken from the CIF.

==========

ALERT_1_927 The Reported and Calculated wR2 Values Differ

==========

Please check whether the wR2 value that is reported in the CIF corresponds with the wR2 value calculated from the parameters supplied in the CIF.

This test is based on the observed reflection data in the FCF and reflection data that are calculated with the parameters (i.e. coordinates, displacement and weight parameters) taken from the CIF.

==========

ALERT_1_928 The Reported and Calculated S Values Differ

==========

Please check whether the S value that is reported in the CIF corresponds with the S value calculated from the parameters supplied in the CIF.

This test is based on the observed reflection data in the FCF and reflection data that are calculated with the parameters (i.e. coordinates, displacement and weight parameters) taken from the CIF.

==========

ALERT_5_929 No Weight Parameters: No Comparison of Obs and Calc R1,wR2 & S

==========

R1, wR2 and S values for Fcalc data in the .fcf cannot be compared with the reported values because of the absence of (SHELXL) weight parameters.

SHELXL weight parameters are expected to be given in the format below:

_refine_ls_weighting_details
'calc w=1/[\s^2^(Fo^2^)+(0.1000P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3'

The JANA weight is expected to be given as:

_refine_ls_weighting_details 'w=1/(\s^2^(I)+0.0016I^2^)'

Do not edit this string or make it into a text block between ';'.

==========

ALERT_5_930 Twinning Detected

==========

Check the proposed Twin Law. The entry in () represents the proposed rotation axis in reciprocal space and the one in [] the corresponding rotation is direct space. The relevant Twin Matrix can be found in the file '.ckf'.

Note: This analysis is based on Fo/Fc differences with Fc data given in the .fcf file (i.e. Fobs, Fcalc listing).

ALERT_930 is expected to generate an related ALERT_931 as well.

==========

ALERT_5_931 Twinning Detected

==========

Check the proposed Twin Law. The entry in () represents the proposed rotation axis in reciprocal space and the one in [] the corresponding rotation is direct space. The relevant Twin Matrix can be found in the file '.ckf'.

Note: This test is based on F(calc) values calculated with the data in the CIF. This ALERT can be ignored when twinning has been addressed in the refinement (As indicated by the absence of ALERT_930).

Please check whether twinning is mentioned in the write-up of the paper.

ALERT_3_934 Report the number of outliers.

This ALERT reports on the number of reflections for which I(obs) and I(calc) differ by more than ten times SigmaW, where SigmaW is the square root of the weight for that reflection in the least-squares refinement. The reason for those deviations should be investigated. When shown to be systematic errors, those reflections are best removed from the refinement and their omission from the refinement reported in the experimental section of an associated report or paper.

==========

ALERT_5_935 Large Absolute Value of Pseudo Extinction Parameter

A pseudo extinction parameter is calculated. Both significantly positive and significantly negative values should invoke a search for a likely cause and a corrective action.

==========

ALERT_3_940 Refinement done with Observed Data Only

==========

Apparently, only data with I > n * σ(I) were used in the F**2 least squares refinement, rather than all data.

==========

ALERT_1_950 The Reported and Calculated Hmax Values Differ

==========

Reported and Calculated Max(Hmax,-Hmin) values differ by more than one unit. Check the consistency of wavelength and reported resolution data.

==========

ALERT_1_951 The Reported and Calculated Kmax Values Differ

==========

Reported and Calculated Max(Kmax,-Kmin) values differ by more than one unit. Check the consistency of wavelength and reported resolution data.

==========

ALERT_1_952 The Reported and Calculated Lmax Values Differ

==========

Reported and Calculated Max(Lmax,-Lmin) values differ by more than one unit. Check the1 consistency of wavelength and reported resolution data.

==========

ALERT_1_953 The Reported and Actual Hmax Values Differ

==========

Reported (in the CIF) and Actual (in the FCF) Max(Hmax,-Hmin) values differ by more than one unit. Check for data set truncation.

==========

ALERT_1_954 The Reported and Actual Kmax Values Differ

==========

Reported (in the CIF) and Actual (in the FCF) Max(Kmax,-Kmin) values differ by more than one unit. Check for data set truncation.

==========

ALERT_1_955 - The Reported and Actual Lmax Values Differ

==========

Reported (in the CIF) and Actual (in the FCF) Max(Lmax,-Lmin) values differ by more than one unit. Check for data set truncation.

==========

ALERT_3_960 Test for large number of reflections with I < - 2 * sigma(I)

==========

Multiple strongly negative intensities may be indicative for poor integration of diffraction images. Too many negative intensities may result in higher than usual wR2 values.

==========

ALERT_2_971 Large Positive Calculated Non-Heavy Atom Residual Density Peak

==========

A Larger than expected residual density maximum outside heavy atom locations. This might be caused by unaccounted for twinning, wrongly assigned atom types and other model errors.

==========

ALERT_2_972 Large Negative Calculated Non-Heavy Atom Residual Density Peak

==========

A larger than expected residual density minimum outside heavy atom locations. This might be caused by unaccounted for twinning, wrongly assigned atom types and other model errors.

==========

ALERT_2_973 Large Positive Calculated Residual Density on Heavy Atom Location

==========

A larger than expected residual density maximum on heavy atom location. This might be caused by unaccounted for twinning, wrongly assigned atom types and other model errors.
 Another cause may be a SHELXL 'DAMP 0 0' instruction for a non-converged refinement.

==========

ALERT_2_974 Large Negative Calculated Residual Density on Heavy Atom Location

A larger than expected residual density minimum found on heavy atom location. This might be caused by unaccounted for twinning, wrongly assigned atom types or other model errors. Another cause may be improper use of the SHELXL 'DAMP 0 0' instruction for a non-converged refinement.

ALERT_1_981 No non-zero f'' Anomalous Scattering Factor Values Found

Check for non-zero f'' anomalous scattering factor values in the CIF.
Note: Zero values are correct for SHELXL MERG 4 refinements.

ALERT_1_982 The reported f' Value Deviates from the International Tables Value

Check the anomalous scattering factor values. Note: Some software seems to truncate the published values to a limited number of decimals.

ALERT_1_983 The Reported f'' Value Deviates from the International Tables Value

Check the anomalous scattering factor values. Note: Some software seems to truncate the published values to a limited number of decimals.