CheckCif alerts are listed according to Alert Level for each compound. Responses are in bold.

COMPOUND 1

ALERT LEVEL A

PLAT027_ALERT_3_A _diffrn_reflns_theta_full (too) Low ..... 23.26 Deg.

A full set of data was collected, however the very high angle data was dominated by noise [I/sigma(I) < 1.0] and was omitted. This arbitrary theta limit is inappropriate for highly disordered structures. It would rule out all macromolecular structures. A limit on data / parameter ratio's that properly takes into account the number of restraints / constraints and the redundancy of the measurements would be more appropriate. Unfortunately the cifcheck routine does not do this.

PLAT113_ALERT_2_A ADDSYM Suggests Possible Pseudo/New Spacegroup . P-1

Our compound is chiral (L-Leu-L-Leu-L-Leu was used) and cannot crystallize in a centrosymmetric space group (i.e. P-1)

PLAT213_ALERT_2_A Atom C1A has ADP max/min Ratio ..... 5.90 oblat
PLAT220_ALERT_2_A Large Non-Solvent C Ueq(max)/Ueq(min) ... 6.32 Ratio
PLAT220_ALERT_2_A Large Non-Solvent C Ueq(max)/Ueq(min) ... 5.21 Ratio
PLAT222_ALERT_3_A Large Non-Solvent H Ueq(max)/Ueq(min) ... 10.00 Ratio
PLAT222_ALERT_3_A Large Non-Solvent H Ueq(max)/Ueq(min) ... 6.17 Ratio
PLAT413_ALERT_2_A Short Inter XH3 .. XHn H5PA .. H33E .. 1.86 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C14 .. C12P .. 2.23 Ang.
PLAT432_ALERT_2_A Short Inter X...Y Contact C14 .. C11P .. 2.28 Ang.

These alerts are generated because there is a large amount of disorder in the structure. In particular the disordered side-chains are very dynamic and may be considered as a solvent. Short contacts between disordered fragments are to be expected.

ALERT LEVEL B

THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575
Calculated sin(theta_max)/wavelength = 0.5556

See PLAT027_ALERT_3_A, from above

PLAT024_ALERT_4_B Merging of Friedel Pairs is STRONGLY Indicated . !

It may be indicated this would only serves to speed up calculations and artificially improve the redundancy. Failure to merge the data ill not compromise the analysis. Mathematically there should be no difference in the derived results.

PLAT111_ALERT_2_B ADDSYM Detects (Pseudo) Centre of Symmetry ..... 100 PerFi

See PLAT113_ALERT_2_A, from above

PLAT213_ALERT_2_B Atom C16A has ADP max/min Ratio ..... 4.10 prola

PLAT301_ALERT_3_B Main Residue Disorder ..... 50.00 Perc.
PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds (x 1000) Ang ... 12

These alerts are generated because there is a large amount of disorder in the structure

ALERT LEVEL C

REFNR01_ALERT_3_C Ratio of reflections to parameters is < 8 for a
non-centrosymmetric structure, where ZMAX < 18
sine(theta)/lambda 0.5556
Proportion of unique data used 1.0000
Ratio reflections to parameters 6.3713

See above response (PLAT 027 ALERT 3A) Checkcif does not properly account for restraints / constraints. The proper data / parameter ratio (including restraints) is > 9.0.

PLAT066_ALERT_1_C Predicted and Reported Transmissions Identical . ?

PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax .LT. 18) 6.37

See REFNR01_ALERT_3_C

PLAT154_ALERT_1_C The su's on the Cell Angles are Equal (x 10000) 400 Deg.

The su's are the true values

PLAT213_ALERT_2_C Atom O2A has ADP max/min Ratio ..... 3.10 prola
PLAT213_ALERT_2_C Atom O22A has ADP max/min Ratio ..... 3.90 prola
PLAT220_ALERT_2_C Large Non-Solvent O Ueq(max)/Ueq(min) ... 2.80 Ratio
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C15
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C5
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C6
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C15A
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C32
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C36A
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors for C23P
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors for C14P
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors for C2P
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors for C4P
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors for N21P
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors for C21P
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors for N1P
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors for C3P
PLAT302_ALERT_4_C Anion/Solvent Disorder ..... 33.00 Perc.
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O .GT. 1.3 Ang) O22A
PLAT420_ALERT_2_C D-H Without Acceptor >N21 - >H21C ... ?

These alerts are generated because there is a large amount of disorder in the structure. This disorder is greater on attached side-chains.

PLAT720_ALERT_4_C Number of Unusual/Non-Standard Label(s) 19

Not worthy of a response

COMPOUND 2

ALERT LEVEL A

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low 0.91

The completeness of data is less than the usual 99-100% for this compound, however it is only the very high angle data that is incomplete and above 0.75 angstroms we have 100% coverage. This will always be a problem with area detector data that is not truncated.

PLAT220_ALERT_2_A Large Non-Solvent C Ueq(max)/Ueq(min) ... 4.75 Ratio
PLAT220_ALERT_2_A Large Non-Solvent C Ueq(max)/Ueq(min) ... 7.25 Ratio
PLAT222_ALERT_3_A Large Non-Solvent H Ueq(max)/Ueq(min) ... 5.90 Ratio
PLAT222_ALERT_3_A Large Non-Solvent H Ueq(max)/Ueq(min) ... 8.30 Ratio

These alerts are generated because there is a large amount of disorder in the structure. Dynamically disordered side-chains (that are tethered to a relatively rigid backbone) may exhibit such unusual ratios.

ALERT LEVEL B

PLAT024_ALERT_4_B Merging of Friedel Pairs is STRONGLY Indicated . !

It may be indicated this would only serves to speed up calculations and artificially improve the redundancy. Failure to merge the data ill not compromise the analysis. Mathematically there should be no difference in the derived results.

PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C16

These alerts are generated because there is a large amount of disorder in the structure. Dynamically disordered side-chains (that are tethered to a relatively rigid backbone) may exhibit such unusual ratios.

ALERT LEVEL C

PLAT041_ALERT_1_C Calc. and Rep. SumFormula Strings Differ .... ?

This is because the H atoms from water are not included in the structure but are in the formula

PLAT063_ALERT_3_C Crystal Probably too Large for Beam Size ..... 0.80 mm

Long needle. SADABS will account for the resulting variation in exposed crystal volume.

PLAT066_ALERT_1_C Predicted and Reported Transmissions Identical . ?

PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... ?

This is because the H atoms from water are not included in the structure but are in the formula

PLAT077_ALERT_4_C Unitcell contains non-integer number of atoms .. ?
There are partially occupied water molecules

PLAT213_ALERT_2_C Atom O3 has ADP max/min Ratio ..... 3.10 prola
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C36
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.41
PLAT301_ALERT_3_C Main Residue Disorder ..... 7.00 Perc.
PLAT302_ALERT_4_C Anion/Solvent Disorder ..... 2.00 Perc.
PLAT311_ALERT_2_C Isolated Disordered Oxygen Atom (No H's ?) ..... <O1W
PLAT380_ALERT_4_C Check Incorrectly? Oriented X(sp2)-Methyl Moiety C16P
PLAT380_ALERT_4_C Check Incorrectly? Oriented X(sp2)-Methyl Moiety C26P
PLAT480_ALERT_4_C Long H...A H-Bond Reported H21B .. O23 .. 2.63 Ang.

These alerts are generated because there is a large amount of disorder in the structure

COMPOUND 3

ALERT LEVEL A

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.5262
PLAT027_ALERT_3_A _diffrn_reflns_theta_full (too) Low ..... 21.96 Deg.

A full set of data was collected, however the very high angle data was poor and was omitted A full set of data was collected, however the very high angle data was dominated by noise [I/sigma(I) < 1.0] and was omitted. This arbitrary theta limit is inappropriate for highly disordered structures. It would rule out all macromolecular structures. A limit on data / parameter ratio's that properly takes into account the number of restraints / constraints and the redundancy of the measurements would be more appropriate. Unfortunately the cifcheck routine does not do this.

PLAT213_ALERT_2_A Atom O4 has ADP max/min Ratio ..... 5.80 oblat
PLAT220_ALERT_2_A Large Non-Solvent C Ueq(max)/Ueq(min) ... 7.60 Ratio
PLAT222_ALERT_3_A Large Non-Solvent H Ueq(max)/Ueq(min) ... 10.00 Ratio
PLAT413_ALERT_2_A Short Inter XH3 .. XHn H6PB .. H33E .. 1.70 Ang.
PLAT413_ALERT_2_A Short Inter XH3 .. XHn H6PC .. H37D .. 1.58 Ang.

These alerts are generated because there is a large amount of disorder in the structure (see response to similar alerts above).

ALERT LEVEL B

RFACR01_ALERT_3_B The value of the weighted R factor is > 0.35
Weighted R factor given 0.367

We made several attempts to obtain better quality data for this structure however, due to twinning, disorder, poor crystal quality etc. the R2 value is high. This structure was included for comparison with the other 3 similar compounds. We are confidant the structural characterization is valid.

PLAT024_ALERT_4_B Merging of Friedel Pairs is STRONGLY Indicated . !

See response to this alert above.

PLAT084_ALERT_2_B High R2 Value 0.37

See RFACR01_ALERT_3_B, from above

PLAT213_ALERT_2_B Atom O1 has ADP max/min Ratio ..... 4.70 oblat
PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C12
PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C16
PLAT301_ALERT_3_B Main Residue Disorder ..... 50.00 Perc.
PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds (x 1000) Ang ... 19
PLAT413_ALERT_2_B Short Inter XH3 .. XHn H6PC .. H37B .. 2.08 Ang.
PLAT413_ALERT_2_B Short Inter XH3 .. XHn H23C .. H38E .. 1.98 Ang.
PLAT413_ALERT_2_B Short Inter XH3 .. XHn H24A .. H29E .. 2.03 Ang

These alerts are generated because there is a large amount of disorder in the structure (as above)

ALERT LEVEL C

REFNR01_ALERT_3_C Ratio of reflections to parameters is < 8 for a
non-centrosymmetric structure, where ZMAX < 18
sine(theta)/lambda 0.5262
Proportion of unique data used 1.0000
Ratio reflections to parameters 7.8968

See REFNR01_ALERT_3_C, for compound 1

RFACG01_ALERT_3_C The value of the R factor is > 0.10
R factor given 0.129

See RFACR01_ALERT_3_B, above

PLAT041_ALERT_1_C Calc. and Rep. SumFormula Strings Differ .... ?

This is because the H atoms from water are not included in the structure but are in the formula

PLAT045_ALERT_1_C Calculated and Reported Z Differ by ..... 0.50 Ratio

Our reported value of Z should be consistent with the

PLAT066_ALERT_1_C Predicted and Reported Transmissions Identical . ?

PLAT082_ALERT_2_C High R1 Value 0.13

See RFACR01_ALERT_3_B, above

PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax .LT. 18) 7.90

See REFNR01_ALERT_3_C, for compound 1

PLAT213_ALERT_2_C Atom O3 has ADP max/min Ratio ..... 3.50 oblat
PLAT213_ALERT_2_C Atom O21 has ADP max/min Ratio ..... 3.60 oblat
PLAT213_ALERT_2_C Atom C1 has ADP max/min Ratio ..... 3.40 oblat
PLAT213_ALERT_2_C Atom C2 has ADP max/min Ratio ..... 3.70 oblat
PLAT213_ALERT_2_C Atom C15 has ADP max/min Ratio ..... 3.30 prola
PLAT214_ALERT_2_C Atom C26P (Anion/Solvent) ADP max/min Ratio 4.50 oblat
PLAT220_ALERT_2_C Large Non-Solvent O Ueq(max)/Ueq(min) ... 3.05 Ratio
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C28
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C36
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C32A
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C36A
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors for C4P
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors for C24P
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors for N1P
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors for C2P
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors for C3P
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors for C5P
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors for N21P
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors for C22P
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.86
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.65
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 3.66
PLAT318_ALERT_2_C Check Hybridisation of >N23 in Main Residue . ?
PLAT380_ALERT_4_C Check Incorrectly? Oriented X(sp2)-Methyl Moiety C26P
PLAT411_ALERT_2_C Short Inter H...H Contact H1PB .. H32B .. 2.11 Ang.

These alerts are generated because there is a large amount of disorder in the structure

PLAT720_ALERT_4_C Number of Unusual/Non-Standard Label(s) 20

PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 2
C6 H7 N
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 3
C6 H7 N

COMPOUND 4

ALERT LEVEL A

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low 0.87

This may occur with area detector data. The higher angle (less well determined) may not be complete but this alone is not sufficient reason to ignore the data. If we impose a more rigid (lower) high angle cutoff we will achieve 100% coverage. Merging of the Freidel pairs would also push this number well above the arbitrary 0.90 level that triggers this alert.

PLAT213_ALERT_2_A Atom O1 has ADP max/min Ratio ..... 5.10 prola
PLAT213_ALERT_2_A Atom O1A has ADP max/min Ratio ..... 5.10 prola
PLAT213_ALERT_2_A Atom O22 has ADP max/min Ratio ..... 5.20 prola
PLAT213_ALERT_2_A Atom O22A has ADP max/min Ratio ..... 5.20 prola
PLAT220_ALERT_2_A Large Non-Solvent C Ueq(max)/Ueq(min) ... 4.66 Ratio
PLAT220_ALERT_2_A Large Non-Solvent C Ueq(max)/Ueq(min) ... 4.77 Ratio
PLAT222_ALERT_3_A Large Non-Solvent H Ueq(max)/Ueq(min) ... 5.65 Ratio
PLAT222_ALERT_3_A Large Non-Solvent H Ueq(max)/Ueq(min) ... 5.50 Ratio

These alerts are generated because there is a large amount of disorder in the structure (see above responses to this alert)

ALERT LEVEL B

PLAT024_ALERT_4_B Merging of Friedel Pairs is STRONGLY Indicated . !

See response to this alert above.

PLAT301_ALERT_3_B Main Residue Disorder ..... 50.00 Perc.
PLAT432_ALERT_2_B Short Inter X...Y Contact C34 .. C4P .. 2.94 Ang.

These alerts are generated because there is a large amount of disorder in the structure

ALERT LEVEL C

PLAT041_ALERT_1_C Calc. and Rep. SumFormula Strings Differ .... ?

This is because the H atoms from water are not included in the structure but are in the formula

PLAT045_ALERT_1_C Calculated and Reported Z Differ by ..... 2.00 Ratio

Our reported Z refers to the number of tripeptide molecules in the unit cell.

PLAT066_ALERT_1_C Predicted and Reported Transmissions Identical . ?

PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... ?

See PLAT041_ALERT_1_C, above

PLAT077_ALERT_4_C Unitcell contains non-integer number of atoms .. ?

There are partial occupancy water molecules in the structure

PLAT213_ALERT_2_C Atom O23 has ADP max/min Ratio ..... 3.10 prola
PLAT302_ALERT_4_C Anion/Solvent Disorder ..... 49.00 Perc.
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O .GT. 1.3 Ang) O1
PLAT311_ALERT_2_C Isolated Disordered Oxygen Atom (No H's ?) ..... <O1W
PLAT420_ALERT_2_C D-H Without Acceptor >N1 - >H1B ... ?
PLAT420_ALERT_2_C D-H Without Acceptor >N1 - >H1C ... ?
PLAT432_ALERT_2_C Short Inter X...Y Contact C11P .. O1W .. 2.92 Ang.
PLAT432_ALERT_2_C Short Inter X...Y Contact C11P .. N1A .. 2.98 Ang.
PLAT432_ALERT_2_C Short Inter X...Y Contact C37 .. C10A .. 3.17 Ang.

These alerts are generated because there is a large amount of disorder in the structure(see similar responses above).

PLAT720_ALERT_4_C Number of Unusual/Non-Standard Label(s) 30