

Chapter 6.1.7.3

SHELXL-97

Atom Lists & Least-squares Constraints

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Atom instructions begin with an atom name (up to 4 characters that do not correspond to any of the SHELXL command names, and terminated by at least one blank) followed by a scattering factor number (which refers to the list defined by the SFAC instruction(s)), x, y, and z in fractional coordinates, and (optionally) a site occupation factor (s.o.f.) and an isotropic U or six anisotropic U_{ij} components (both in \AA^2). Note that different program systems may differ in their order of U_{ij} components; SHELXL uses the same order as SHELX-76. The exponential factor takes the form $\exp(-8\pi^2 U [\sin(\theta)/\lambda]^2)$ for an isotropic displacement parameter U and:

$$\exp (-2\pi^2 [h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + \dots + 2hka^*b^*U_{12}])$$

for anisotropic U_{ij} . An atom is specified as follows in the *.ins* file:

```
atomname sfac x y z sof [11] U [0.05] or U11 U22 U33 U23 U13 U12
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The atom name must be unique, except that atoms in different residues - see RESI - may have the same names; in contrast to SHELX-76 it is not necessary to pad out the atom name to 4 characters with blanks. To fix any atom parameter, add 10. Thus the site occupation factor is normally given as 11 (i.e. fixed at 1). The site occupation factor for an atom in a special position should be multiplied by the multiplicity of that position (as given in International Tables, Volume A) and divided by the multiplicity of the general position for that space group. This is the same definition as in SHELX-76 and is retained for upwards compatibility; it might have been less confusing to keep the multiplicity and occupation factor separate. An atom on a fourfold axis for example will usually have s.o.f. = 10.25.

If any atom parameter is given as $(10 \cdot m + p)$, where $\text{abs}(p)$ is less than 5 and m is an integer, it is interpreted as $p \cdot f_{v_m}$, where f_{v_m} is the m th 'free variable' (see FVAR). Note that there is no f_{v_1} , since this position on an FVAR instruction is occupied by the overall scale factor, and $m=1$ corresponds to fixing an atom by adding 10. If m is negative, the parameter is interpreted as $p \cdot (f_{v_{-m}} - 1)$. Thus to constrain two occupation factors to add up to 0.25 (for two elements occupying the same fourfold special position) they could be given as 20.25 and -20.25, i.e. $0.25 \cdot f_{v_2}$ and $0.25 \cdot (1 - f_{v_2})$, which correspond to $p=0.25, m=2$ and $p=-0.25, m=-2$ respectively.

In SHELX-76, it was necessary to use free variables and coordinate fixing in this way to set up the appropriate constraints for refinement of atoms on special positions. In SHELXL, this is allowed (for upwards compatibility) but is NOT NECESSARY: the program will automatically work out and apply the appropriate positional, s.o.f. and U_{ij} constraints for any special position in any space group, in a conventional setting or otherwise. If the user applies (correct or incorrect) special position constraints using free variables etc., the program assumes that this has been done with intent, and reports but does not apply the correct constraints.

Thus the accidental application of a free variable to a U_{ij} term of an atom on a special position can lead to the refinement 'blowing up'! All that is necessary is to specify atomname, sfac, x, y and z, and leave the rest to the program; when the atom is (later) made anisotropic using the ANIS command, the appropriate U_{ij} constraints will be added by the program. For a well-behaved structure, the list of atom coordinates (from direct methods and/or difference electron density syntheses) suffices. If the multiplicity factor (s.o.f.) is left out, it will be fixed at the appropriate value of 1 for a general position and less than 1 for a special position. Since SHELXL automatically generates origin restraints for polar space groups, no atom coordinates should be fixed by the user for this purpose (in contrast to SHELX-76).

It may still be necessary to apply constraints by hand to handle disorder; a common case is when there are two possible positions for a group of atoms, in which the first set should all have s.o.f.'s of (say) 21, and the second set -21, with the result that the sum of the two occupation factors is fixed at 1, but the individual values may refine as fv_2 and $1-fv_2$. Similarly if a special position with 2/m symmetry is occupied by Ca^{2+} and Ba^{2+} , the two ions could be given the s.o.f.'s 30.25 and -30.25 respectively. In this case it would be desirable to use the EADP instruction to equate the Ca^{2+} and Ba^{2+} (anisotropic) displacement parameters.

If U is given as -T, where T is in the range $0.5 < T < 5$, it is fixed at T times the U_{eq} of the previous atom not constrained in this way. The resulting value is not refined independently but is updated after every least-squares cycle.

SPEC del[0.2]

All following atoms (until the next SPEC instruction) are considered to lie on special positions (for the purpose of automatic constraint generation) if they lie within del (Å) of a special position. The coordinates of such an atom are also adjusted so that it lies exactly on the special position.

RESI class[] number[0] alias

Until the next RESI instruction, all atoms are considered to be in the specified 'residue', which may be defined by a class (up to four characters, beginning with a letter) or number (up to four digits) or both. The same atom names may be employed in different residues, enabling them to be referenced globally or selectively. The residue number should be unique to a particular residue, but the class may be used to refer to a class of similar residues, e.g. a particular type of amino acid in a polypeptide.

Residues may be referenced by any instruction that allows atom names; the reference takes the form of the character '_' followed by either the residue class or number without intervening spaces. If an instruction codeword is followed immediately by a residue number, all atom names referred to in the instruction

are assumed to belong to that residue unless they are themselves immediately followed by '_' and a residue number, which is then used instead. Thus:

RTAB_4 Ang N H0 O_11

would cause the calculation of an angle N_4 - H0_4 - O_11, where the first two atoms are in residue 4 and the third is in residue 11.

If the instruction codeword is followed immediately by a residue class, the instruction is effectively duplicated for all residues of that class. '_'* ' may be used to match all residue classes; this includes the default class ' ' (residue number 0) which applies until the first RESI instruction is encountered. Thus:

MPLA_phe CB > CZ

would calculate least-squares planes through atoms CB to CZ inclusive of all residues of class 'phe' (phenylalanine). In the special case of HFIX, only the FIRST instruction which applies to a given atom is applied. Thus:

HFIX_1 33 N

HFIX_* 43 N

would add hydrogens to the N-terminal nitrogen (residue 1) of a polypeptide to generate a (protonated) -NH_3^+ group, but all other (amide) nitrogens would become -NH- .

Individual atom names in an instruction may be followed by '_' and a residue number, but not by '_'* or '_' and a residue class. If an atom name is not followed by a residue number, the current residue is assumed (unless overridden by a global residue number or class appended to the instruction codeword). The symbols '_+' meaning 'the next residue' and '_-' meaning 'the preceding residue'(i.e. residues number n+1 and n-1 if the current residue number is n) may be appended to atom names but not to instruction codenames. Thus the instruction:

RTAB_* Omeg CA_+ N_+ C CA

could be used to calculate all the peptide \square torsion angles in a protein or polypeptide. If (as at the C-terminus in this example) some or all of the named atoms cannot be found for a particular residue, the instruction is simply ignored for that residue.

'_\$_n' does not refer to a residue; it uses the symmetry operation \$n defined by a preceding 'EQIV \$n' instruction to generate an equivalent of the named atom (see EQIV). alias specifies an alternative value of the residue number so that cyclic chains of residues may be created; for a cyclic pentapeptide (residue numbers

2,3,..6) it could be set to 1 for residue 6 and to 7 for residue 2. If more than one RESI instruction refers to the same number, alias only needs to be specified once. alias is referenced only by the `_+` and `_-` operations (see above), and a value used for alias may not be used as a residue number on a RESI instruction. Note that if there is more than one cyclic peptide in the asymmetric unit, it is a good idea to leave a gap of TWO residue numbers between them. E.g. a cyclic pentapeptide with two molecules in the asymmetric unit would be numbered 2 to 6 and 9 to 13, with aliases 7 on RESI 2, 1 on RESI 6, 14 on RESI 9 and 8 on RESI 13. It will generally be found convenient for applying restraints etc. to use the same names for atoms in identical residues. Since SHELXL does not recognize chain ID's (used in PDB format) it is normal to add a constant to the residue numbers to denote a different chain (e.g. chain A could be 1001 to 1234 and chain B 2001 to 2234). The auxiliary program SHELXPRO provides extensive facilities for handling residues.

MOVE dx[0] dy[0] dz[0] sign[1]

The coordinates of the atoms that follow this instruction are changed to: $x = dx + \text{sign} * x$, $y = dy + \text{sign} * y$, $z = dz + \text{sign} * z$ until superseded by a further MOVE. MOVE should not be used at the same time as the specification of zero coordinates to indicate that an atom should not be used in fitting a fragment of known geometry (e.g. AFIX 66), because after the move the coordinates will no longer be zero!

ANIS n

The next n isotropic non-hydrogen atoms are made anisotropic, generating appropriate special position constraints for the U_{ij} if required. Intervening atoms which are already anisotropic are not counted. A negative n has the same effect.

ANIS names

The named atoms are made anisotropic (if not already), generating the appropriate constraints for special positions. Note that names may include '\$' followed by a scattering factor name (see SFAC); 'ANIS \$CL' would make all chlorine atoms anisotropic. Since ANIS, like other instructions, applies to the current residue unless otherwise specified, ANIS_* \$\$ would be required to make the sulfur atoms in all residues anisotropic (for example). ANIS MUST precede the atoms to which it is to be applied. ANIS on its own, with neither a number nor names as parameters, makes all FOLLOWING non-hydrogen atoms (in all residues) anisotropic. The L.S. and CGLS instructions provide the option of delaying the conversion to anisotropic of all atoms specified by ANIS until a given number of least-squares cycles has been performed.

AFIX mn d[#] sof[11] U[10.08]

AFIX applies constraints and/or generates idealized coordinates for all atoms until the next AFIX instruction is read. The digits mn of the AFIX code control two logically quite separate operations. Although this is confusing for new users, it has been retained for upwards compatibility with SHELX-76, and because it provides a

very concise notation. *m* refers to geometrical operations which are performed before the first refinement cycle (hydrogen atoms are idealized before every cycle), and *n* sets up constraints which are applied throughout the least-squares refinement. *n* is always a single digit; *m* may be two, one or zero digits (the last corresponds to *m* = 0).

The options for idealizing hydrogen atom positions depend on the connectivity table that is set up using CONN, BIND, FREE and PART; with experience, this can also be used to generate hydrogen atoms attached to disordered groups and to atoms on special positions. *d* determines the bond lengths in the idealized groups, and *sof* and *U OVERRIDE* the values in the atom list for all atoms until the next AFIX instruction. *U* is not applied if the atom is already anisotropic, but is used if an isotropic atom is to be made anisotropic using ANIS. Any legal *U* value may be used, e.g. 31 (a free variable reference) or -1.2 (1.2 times *U_{eq}* of the preceding normal atom). Each AFIX instruction must be followed by the required number of hydrogen or other atoms. The individual AFIX options are as follows; the default X-H distances depend on both the chemical environment and the temperature (to allow for librational effects) which is specified by means of the TEMP instruction.

m = 0 No action.

m = 1 Idealized tertiary C-H with all X-C-H angles equal. There must be three and only three other bonds in the connectivity table to the immediately preceding atom, which is assumed to be carbon. *m* = 1 is often combined with a riding model refinement (*n* = 3).

m = 2 Idealized secondary CH₂ with all X-C-H and Y-C-H angles equal, and H-C-H determined by X-C-Y (i.e. approximately tetrahedral, but widened if X-C-Y is much less than tetrahedral). This option is also suitable for riding refinement (*n* = 3).

m = 3 Idealized CH₃ group with tetrahedral angles. The group is staggered with respect to the shortest other bond to the atom to which the -CH₃ is attached. If there is no such bond (e.g. an acetonitrile solvent molecule) this method cannot be used (but *m* = 13 is still viable).

m = 4 Aromatic C-H or amide N-H with the hydrogen atom on the external bisector of the X-C-Y or X-N-Y angle. *m* = 4 is suitable for a riding model refinement, i.e. AFIX 43 before the H atom.

m = 5 Next five non-hydrogen atoms are fitted to a regular pentagon, default *d* = 1.42 Å.

m = 6 Next six non-hydrogen atoms are fitted to a regular hexagon, default *d* = 1.39 Å.

- m = 7** Identical to m = 6 (included for upwards compatibility from SHELX-76). In SHELX-76 only the first, third and fifth atoms of the six-membered ring were used as target atoms; in SHELXL this will still be the case if the other three are given zero coordinates, but the procedure is more general because any one, two or three atoms may be left out by giving them zero coordinates.
- m = 8** Idealized OH group, with X-O-H angle tetrahedral. If the oxygen is attached to a saturated carbon, all three staggered positions are considered for the hydrogen. If it is attached to an aromatic ring, both positions in the plane are considered. The final choice is based on forming the 'best' hydrogen bond to a nitrogen, oxygen, chlorine or fluorine atom. The algorithm involves generating a potential position for such an atom by extrapolating the O-H vector, then finding the nearest N, O, F or Cl atom to this position, taking symmetry equivalents into account. If another atom that (according to the connectivity table) is bonded to the N, O, F or Cl atom, is nearer to the ideal position, the N, O, F or Cl atom is not considered. Note that m = 8 had a different effect in SHELX-76 (but was rarely employed).
- m = 9** Idealized terminal X=CH₂ or X=NH₂⁺ with the hydrogen atoms in the plane of the nearest substituent on the atom X. Suitable for riding model refinement (AFIX 93 before the two H atoms).
- m = 10** Idealized pentamethylcyclopentadienyl (Cp*). This AFIX must be followed by the 5 ring carbons and then the 5 methyl carbons in cyclic order, so that the first methyl group (atom 6) is attached to the first carbon (atom 1). The default d is 1.42 Å, with the C-CH₃ distance set to 1.063d. A variable-metric rigid group refinement (AFIX 109) would be appropriate, and would allow for librational shortening of the bonds. Hydrogen atoms (e.g. with AFIX 37 or 127) may be included after the corresponding carbon atoms, in which case AFIX 0 or 5 (in the case of a rigid group refinement) must be inserted before the next carbon atom.
- m = 11** Idealized naphthalene group with equal bonds (default d = 1.39 Å). The atoms should be numbered as a symmetrical figure of eight, starting with the alpha C and followed by the beta, so that the first six atoms (and also the last six) describe a hexagon in cyclic order. m = 11 is also appropriate for rigid group refinement (AFIX 116).
- m = 12** Idealized disordered methyl group; as m = 3 but with two positions rotated from each other by 60 degrees. The corresponding occupation factors should normally be set to add up to one, e.g. by giving them as 21 (i.e. 1*f_v(2)) and -21 (1*(1-f_v(2))). If HFIX is used to generate an AFIX

instruction with $m=12$, the occupation factors are fixed at 0.5. AFIX 12n is suitable for a *para* methyl on a phenyl group with no *meta* substituents, and should be followed by 6 half hydrogen atoms (first the three belonging to one $-CH_3$ component, then the three belonging to the other, so that hydrogens n and $n+3$ are opposite one another). The six hydrogens should have the same PART number as the carbon to which they are attached (e.g. PART 0).

m = 13 Idealized CH_3 group with tetrahedral angles. If the coordinates of the first hydrogen atom are non-zero, they define the torsion angle of the methyl group. Otherwise (or if the AFIX instruction is being generated via HFIX) a structure-factor calculation is performed (of course only once, even if many hydrogens are involved) and the torsion angle is set that maximizes the sum of the electron density at the three calculated hydrogen positions. Since even this is not an infallible method of getting the correct torsion angle, it should normally be combined with a rigid or rotating group refinement for the methyl group (e.g. $mn = 137$ before the first H). In subsequent least-squares cycles the group is re-idealized retaining the current torsion angle

m = 14 Idealized OH group, with X-O-H angle tetrahedral. If the coordinates of the hydrogen atom are non-zero, they are used to define the torsion angle. Otherwise (or if HFIX was used to set up the AFIX instruction) the torsion angle is chosen which maximizes the electron density (see $m = 13$). Since this torsion angle is unlikely to be very accurate, the use of a rotating group refinement is recommended (i.e. AFIX 147 before the H atom).

m = 15 BH group in which the boron atom is bonded to either four or five other atoms as part of an polyhedral fragment. The hydrogen atom is placed on the vector that represents the negative sum of the unit vectors along the four or five other bonds to the boron atom.

m = 16 Acetylenic C-H, with X-C-H linear. Usually refined with the riding model, i.e. AFIX 163.

m > 16 A group defined in a FRAG...FEND section with code = m is fitted, usually as a preliminary to rigid group refinement. The FRAG...FEND section MUST precede the corresponding AFIX instruction in the *.ins* file, but there may be any number of AFIX instructions with the same m corresponding to a single FRAG...FEND section.

When a group is fitted ($m = 5, 6, 10$ or 11 , or $m > 16$), atoms with non-zero coordinates are used as target atoms with equal weight. Atoms with all three coordinates zero are ignored. Any three or more non-colinear atoms may be used as target atoms.

'Riding' (n = 3, 4) and 'rotating' (n = 7, 8) hydrogen atoms, but not other idealized groups, are re-idealized (if m is 1, 2, 3, 4, 8, 9, 12, 13, 14, 15 or 16) before each refinement cycle (after the first cycle, the coordinates of the first hydrogen of a group are always non-zero, so the torsion angle is retained on re-idealizing). For n = 4 and 8, the angles are re-idealized but the (refined) X-H bond length is retained, unless the hydrogen coordinates are all zero, in which case d (on the AFIX instruction) or (if d is not given) a standard value which depends on the chemical environment and temperature (TEMP) is used instead.

n = 0 No action.

n = 1 The coordinates, s.o.f. and U or U_{ij} are fixed.

n = 2 The s.o.f. and U (or U_{ij}) are fixed, but the coordinates are free to refine.

n = 3 The coordinates, but not the s.o.f. or U (or U_{ij}) 'ride' on the coordinates of the previous atom with n not equal to 3. The same shifts are applied to the coordinates of both atoms, and both contribute to the derivative calculation. The atom on which riding is performed may not itself be a riding atom, but it may be in a rigid group (m = 5, 6 or 9).

n = 4 This constraint is the same as n = 3 except that the X-H distance is free to refine. The X-H vector direction does not change. This constraint requires better quality reflection data than n = 3, but allows for variations in apparent X-H distances caused by libration and bonding effects. If there is more than one equivalent hydrogen, the same shift is applied to each equivalent X-H distance (e.g. to all three C-H bonds in a methyl group). n = 4 may be combined with DFIX or SADI restraints (to restrain chemically equivalent X-H distances to be equal) or embedded inside a rigid (n = 6) group, in which case the next atom (if any) in the same rigid group must follow an explicit AFIX instruction with n = 5. Note that n = 4 had a different effect in SHELX-76.

n = 5 The next atom(s) are 'dependent' atoms in a rigid group. Note that this is automatically generated for the atoms following an n = 6 or n = 9 atom, so does not need to be included specifically unless m has to be changed (e.g. AFIX 35 before the first hydrogen of a rigid methyl group with AFIX 6 or 9 before the preceding carbon).

n = 6 The next atom is the 'pivot atom' of a NEW rigid group, i.e. the other atoms in the rigid group rotate about this atom, and the same translational shifts are applied to all atoms in the rigid group.

- n = 7** The following (usually hydrogen) atoms (until the next AFIX with n not equal to 7) are allowed to ride on the immediately preceding atom X and rotate about the Y-X bond; X must be bonded to one and only one atom Y in the connectivity list, ignoring the n = 7 atoms (which, if they are F rather than H, may be present in the connectivity list). The motion of the atoms of this 'rotating group' is a combination of riding motion (c.f. n = 3) on the atom X plus a tangential component perpendicular to the Y-X and X-H bonds, so that the X-H distances, Y-X-H and H-X-H angles remain unchanged. This constraint is intended for -OH, -CH₃ and possibly -CF₃ groups. X may be part of a rigid group, which may be resumed with an AFIX n = 5 following the n = 7 atoms.
- n = 8** This constraint is similar to n = 7 except that the X-H distances may also vary, the same shifts being applied along all the X-H bonds. Thus only the Y-X-H and H-X-H angles are held constant; the relationship of n = 8 to n = 7 corresponds to that of n = 4 to n = 3. DFIX and SADI restraints may be useful for the X-H distances. This constraint is useful for -CF₃ groups or for -CH₃ groups with good data.
- n = 9** The first (pivot) atom of a new 'variable metric' rigid group. Such a group retains its 'shape' but may shrink or expand uniformly. It is useful for C₅H₅ and BF₄ groups, which may show appreciable librational shortening of the bond lengths. Subsequent atoms of this type of rigid group should have n = 5, which is generated automatically by the program if no other AFIX instruction is inserted between the atoms. Riding atoms are not permitted inside this type of rigid group. Only the pivot atom coordinates may be fixed (by adding 10) or tied to free variables, and only the pivot atom may lie on a special position (for the automatic generation of special position constraints).

Although there are many possible combinations of m and n, in practice only a small number is used extensively, as discussed in the section on hydrogen atoms. Rigid group fitting and refinement (e.g. AFIX 66 followed by six atoms of a phenyl ring or AFIX 109 in front of a Cp* group) is particularly useful in the initial stages of refinement; atoms not found in the structure solution may be given zero coordinates, in which case they will be generated from the rigid group fit.

A rigid group or set of dependent hydrogens must ALWAYS be followed by 'AFIX 0' (or another AFIX instruction). Leaving out 'AFIX 0' by mistake is a common cause of error; the program is able to detect and correct some obvious cases, but in many cases this is not logically possible.

HFIX mn U[#] d[#] atomnames

HFIX generates AFIX instructions and dummy hydrogen atoms bonded to the named atoms, the AFIX parameters being as specified on the HFIX instruction. This is

exactly equivalent to the corresponding editing of the atom list. The atom names may reference residues (by appending '_n' to the name, where n is the residue number), or SFAC names (preceded by a '\$' sign). U may be any legal value for the isotropic temperature factor, e.g. 21 to tie a group of hydrogen U value to free variable 2, or -1.5 to fix U at 1.5 times U(eq) of the preceding normal atom. HFIX MUST precede the atoms to which it is to be applied. If more than one HFIX instruction references a given atom, only the FIRST is applied. 'HFIX 0' is legal, and may be used to switch off following HFIX instructions for a given atom (which is useful if they involve '_' or a global reference to a residue class).

FRAG code[17] a[1] b[1] c[1] α [90] β [90] γ [90]

Enables a fragment to be input using a cell and coordinates taken from the literature. Orthogonal coordinates may also be input in this way. Such a fragment may be fitted to the set of atoms following an AFIX instruction with m = code (code must be greater than 16); there must be the same number of atoms in this set as there are following FRAG, and they must be in the same order. Only the coordinates of the FRAG fragment are actually used; atom names, sfac numbers, sof and U_{ij} are IGNORED. A FRAG fragment may be given anywhere between UNIT and HKLF or END, and must be terminated by a FEND instruction, but must precede any AFIX instruction which refers to it. This 'rigid fit' is often a preliminary to a rigid group refinement (AFIX with n = 6 or 9).

FEND

This must immediately follow the last atom of a FRAG fragment.

EXYZ atomnames

The same x, y and z parameters are used for all the named atoms. This is useful when atoms of different elements share the same site, e.g. in minerals (in which case EADP will probably be used as well). The coordinates (and possibly free variable references) are taken from the named atom which precedes the others in the atom list, and the actual values, free variable references etc. given for the x, y and z of the other atoms are ignored. An atom should not appear in more than one EXYZ instruction.

EADP atomnames

The same isotropic or anisotropic displacement parameters are used for all the named atoms. The displacement parameters (and possibly free variable references) are taken from the named atom which precedes the others in the atom list, and the actual values, free variable references etc. given for the U_{ij} of the other atoms are ignored. The atoms involved must either be all isotropic or all anisotropic. An atom should not appear in more than one EADP instruction. 'Opposite' fluorines of PF_6 or disordered $-CF_3$ groups are good candidates for EADP, e.g.

```

EADP F11 F14
EADP F12 F15
EADP F13 F16
C1 .....
PART 1
F11 ..... 21 .....
F12 ..... 21 .....
F13 ..... 21 .....
PART 2
F14 ..... -21 .....
F15 ..... -21 .....
F16 ..... -21 .....
PART 0

```

EADP applies an (exact) *constraint*. The SIMU instruction *restrains* the Uij components of neighboring atoms to be approximately equal with an appropriate (usually fairly large) esd.

EQIV \$n symmetry operation

Defines symmetry operation \$n for referencing symmetry equivalent atoms on any instruction which allows atom names, by appending '_\$n' (where n is an integer between 1 and 511 inclusive) to the atom name. Such a symmetry operation must be defined before it is used; it does not have to be an allowed operation of the space group, but the same notation is used as on the SYMM instruction. The same \$n may not appear on two separate EQIV instructions. Thus:

```

EQIV $2 1-x, y, 1-z
CONF C1 C2 C2_$2 C1_$2

```

could be used to calculate a torsion angle across a crystallographic twofold axis (note that this may be required because CONF with no atom names only generates torsion angles automatically that involve the unique atom list and a one atom deep shell of symmetry equivalents). If the instruction codeword refers to a residue, this is applied to the named atoms before any symmetry operation specified with '_\$n'. Thus:

```

RTAB_23 O..O OG_12 O_$3

```

would calculate the (hydrogen bond) distance between OG_12 and (O_23)_\$3, i.e. between OG in residue 12 and the equivalent obtained by applying the symmetry operation defined by EQIV \$3 to the atom O in residue 23.

OMIT atomnames

The named atoms are retained in the atom list but ignored in the structure factor calculation and least-squares refinement. This instruction may be used, together

with L.S. 0 and FMAP 2, to create an 'OMIT map' to get a clearer picture of disordered regions of the structure; this concept will be familiar to macromolecular crystallographers. In particular, 'OMIT \$H' can be used to check the hydrogen atom assignment of -OH groups etc. If an actual peak is present within 0.31 Å of the calculated hydrogen atom position, the electron density appears in the 'Peak' column of the output created by PLAN with a negative first parameter. OMIT_* \$H must be used for this if residues are employed.