Sample 2

The powder pattern of this sample, as indicated in the SDPDRR-2 text, is simulated from a structure determined from single crystal data.

Below is the .pcr file which was used for the simulation by the FULLPROF program ;

```
==============================================================================================
COMM  Sample 2 - SDPDRR-2
! Files => DAT-file: sample2,  PCR-file: sample2
!Job Npr Nph Nba Nex Nsc Nor Dum Iwg Ilo Ias Res Ste Nre Cry Uni Cor
   2   5   1   0   2   0   1   1   0   0   1   0   0   0   0   0
!
!Ipr Ppl Ioc Mat Pcr Ls1 Ls2 Ls3 Syo Prf Ins Rpa Sym Hkl Fou Sho Ana
   0   0   1   1   1   0   0   0   1   1   0   1   1   1   2   0   0
!
! lambda1 Lambda2    Ratio   Bkpos    Wdt    Cthm     muR   AsyLim   Rpolarz
 0.797640 0.797640  0.0000 90.0000 30.0000  0.0000  0.0000   80.00    0.0000
!
!NCY Eps R_at R_an R_pr R_gl     Thmin       Step       Thmax    PSD    Sent0
  1 0.01 0.20 0.20 0.20 0.60      1.5000     0.0050    80.0000   0.000   0.000
!
! Excluded regions (LowT  HighT)
        1.00        1.50
       80.00      170.00
!
!
       0    !Number of refined parameters
!
!  Zero    Code    Sycos    Code   Sysin    Code  Lambda     Code MORE
  0.0018    0.00  0.0000    0.00  0.0000    0.00 0.000000    0.00   0
!   Background coefficients/codes
  87.590     -61.150      245.65      357.98     -440.81     -764.50
       0.000       0.000       0.000       0.000       0.000       0.000
!
!  Data for PHASE number:   1  ==> Current R_Bragg:     0.00
  "Sample-2"
!
!Nat Dis Mom Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth     ATZ   Nvk Npr More
  30   0   0 1.0 0.0 0.0   0   0   0   0   0        0.00   0   5   0
!
P 21/C                   <--Space group symbol
!Atom Typ       X        Y        Z     Biso      Occ     In Fin N_t  /Codes
SR1  SR+2    0.50808  0.08346  0.64675  0.68280  0.04000   0   0   0
                0.00     0.00     0.00     0.00     0.00
SR2  SR+2    0.14985  0.08409  0.64701  0.72345  0.04000   0   0   0
                0.00     0.00     0.00     0.00     0.00
SR3  SR+2    0.25964  0.08831  0.01762  0.82543  0.04000   0   0   0
                0.00     0.00     0.00     0.00     0.00
SR4  SR+2    0.15658  0.15558  0.32478  0.71345  0.04000   0   0   0
                0.00     0.00     0.00     0.00     0.00
SR5  SR+2    0.83532  0.33432  0.67120  0.67245  0.04000   0   0   0
                0.00     0.00     0.00     0.00     0.00
V1   V+5     0.42345  0.08461  0.84049  0.65234  0.04000   0   0   0
                0.00     0.00     0.00     0.00     0.00
V2   V+3     0.76550  0.07753  0.52365  1.05050  0.04000   0   0   0
                0.00     0.00     0.00     0.00     0.00
V3   V+3     0.89983  0.08220  0.82697  0.88654  0.04000   0   0   0
                0.00     0.00     0.00     0.00     0.00
O    O-2     0.83439  0.07484  0.88855  1.23264  0.04000   0   0   0
                0.00     0.00     0.00     0.00     0.00
F1   F-1     0.98792  0.08608  0.74569  1.85342  0.04000   0   0   0
                0.00     0.00     0.00     0.00     0.00
F2   F-1     0.24014  0.09468  0.77629  1.20567  0.04000   0   0   0
                0.00     0.00     0.00     0.00     0.00
F3   F-1     0.70325  0.10733  0.60604  1.32759  0.04000   0   0   0
                0.00     0.00     0.00     0.00     0.00
F4   F-1     0.92263  0.07552  0.60714  1.41527  0.04000   0   0   0
                0.00     0.00     0.00     0.00     0.00
F5   F-1     0.79844  0.18601  0.03306  1.35367  0.04000   0   0   0
                0.00     0.00     0.00     0.00     0.00
F6   F-1     0.60511  0.35814  0.68391  1.22538  0.04000   0   0   0
                0.00     0.00     0.00     0.00     0.00
F7   F-1     0.22757  0.34713  0.95418  1.23647  0.04000   0   0   0
                0.00     0.00     0.00     0.00     0.00
F8   F-1     0.75877  0.08224  0.74505  1.21371  0.04000   0   0   0
```

```
                0.00      0.00      0.00      0.00      0.00
F9   F-1      0.07712   0.35193   0.68695   1.24753   0.04000    0    0    0
                0.00      0.00      0.00      0.00      0.00
F10  F-1      0.07414   0.41620   0.38172   1.36437   0.04000    0    0    0
                0.00      0.00      0.00      0.00      0.00
F11  F-1      0.91635   0.18479   0.31127   1.33241   0.04000    0    0    0
                0.00      0.00      0.00      0.00      0.00
F12  F-1      0.62240   0.06996   0.46549   1.72317   0.04000    0    0    0
                0.00      0.00      0.00      0.00      0.00
F13  F-1      0.32963   0.02888   0.90771   1.12635   0.04000    0    0    0
                0.00      0.00      0.00      0.00      0.00
F14  F-1      0.30917   0.22593   0.61519   1.32678   0.04000    0    0    0
                0.00      0.00      0.00      0.00      0.00
F15  F-1      0.38793   0.18802   0.35037   1.26435   0.04000    0    0    0
                0.00      0.00      0.00      0.00      0.00
F16  F-1      0.86596   0.06056   0.46350   1.44724   0.04000    0    0    0
                0.00      0.00      0.00      0.00      0.00
F17  F-1      0.43514   0.57330   0.59865   1.82641   0.04000    0    0    0
                0.00      0.00      0.00      0.00      0.00
F18  F-1      0.47569   0.12073   0.76147   1.64638   0.04000    0    0    0
                0.00      0.00      0.00      0.00      0.00
OW1  O-2      0.65843   0.12594   0.32889   1.34672   0.04000    0    0    0
                0.00      0.00      0.00      0.00      0.00
OW2  O-2      0.05101   0.21294   0.02730   1.46342   0.04000    0    0    0
                0.00      0.00      0.00      0.00      0.00
OW3  O-2      0.48195   0.27897   0.53084   1.63856   0.04000    0    0    0
                0.00      0.00      0.00      0.00      0.00
!  Scale       Shape1       Bov      Str1      Str2      Str3    Strain-Model
 0.85000E-02   0.5583   0.0000   0.0000    0.0000    0.0000       0
     0.00000     0.00     0.00     0.00      0.00      0.00
!      U         V         W          X         Y       GauSiz   LorSiz Size-Model
   0.00192   0.00092   0.00031   0.00212   0.00000   0.00000   0.00000   0
      0.00      0.00      0.00      0.00      0.00      0.00      0.00
!     a          b         c        alpha      beta       gamma
  11.243328   8.195712  19.949343  90.000000 106.728279  90.000000
    0.00000    0.00000    0.00000    0.00000    0.00000    0.00000
!  Pref1  Pref2   Asy1    Asy2    Asy3     Asy4
 1.00000 0.00000 0.01565 0.00262 0.00000 0.00000
    0.00    0.00    0.00    0.00    0.00    0.00
==============================================================================
```

Below is the result of a refinement by FULLPROF limited to the scale factor and the zeropoint. That .sum file gives the minimum R values attainable with the exact starting atomic coordinates and cell and profile parameters (the simulated profile contains some added statistical error, so that the fit is not exact) :

```
        ******************************************************
        *** PROGRAM FULLPROF (Version 3.3  - Aug97-LLB JRC) ***
        ******************************************************
           Rietveld, Profile Matching & Integrated Intensity
                Refinement of X-ray and/or Neutron Data


    Date: 08/23/02  Time: 19:35:18.45

 => PCR file code: sample2
 => DAT file code: sample2
 => Title:  Smple 2 - SDPDRR-2

 ==> CONDITIONS OF THIS RUN:

 => Global Refinement of X-ray powder diffraction data
    Bragg-Brentano or Debye-Scherrer geometry
 => The    5th default profile function was selected
 => Data supplied in free format
 => Wavelengths:  0.79764 0.79764
 => Base of peaks: 2.0*HW*   10.00
 => Cos(Monochromator angle)=   0.0000
 => Absorption correction (muR-eff):   0.0000
 ==> Angular range, step and number of points:
     2Thmin:   1.5000  2Thmax:  80.0000  Step:   0.0050  No. of points:  15701
 => Crystal Structure Refinement for phase: 1
 => Scor: 1.1745
```

==> RESULTS OF REFINEMENT:

=> No. of fitted parameters: 2

=> Phase No. 1 "Sample-2" P 21/C

=> No. of reflections: 7710

==> ATOM PARAMETERS:

Name	x	sx	y	sy	z	sz	B	sB	occ.	socc.
SR1	0.50808	0	0.08346	0	0.64675	0	0.683	0	0.040	0
SR2	0.14985	0	0.08409	0	0.64701	0	0.723	0	0.040	0
SR3	0.25964	0	0.08831	0	0.01762	0	0.825	0	0.040	0
SR4	0.15658	0	0.15558	0	0.32478	0	0.713	0	0.040	0
SR5	0.83532	0	0.33432	0	0.67120	0	0.672	0	0.040	0
V1	0.42345	0	0.08461	0	0.84049	0	0.652	0	0.040	0
V2	0.76550	0	0.07753	0	0.52365	0	1.051	0	0.040	0
V3	0.89983	0	0.08220	0	0.82697	0	0.887	0	0.040	0
O	0.83439	0	0.07484	0	0.88855	0	1.233	0	0.040	0
F1	0.98792	0	0.08608	0	0.74569	0	1.853	0	0.040	0
F2	0.24014	0	0.09468	0	0.77629	0	1.206	0	0.040	0
F3	0.70325	0	0.10733	0	0.60604	0	1.328	0	0.040	0
F4	0.92263	0	0.07552	0	0.60714	0	1.415	0	0.040	0
F5	0.79844	0	0.18601	0	0.03306	0	1.354	0	0.040	0
F6	0.60511	0	0.35814	0	0.68391	0	1.225	0	0.040	0
F7	0.22757	0	0.34713	0	0.95418	0	1.236	0	0.040	0
F8	0.75877	0	0.08224	0	0.74505	0	1.214	0	0.040	0
F9	0.07712	0	0.35193	0	0.68695	0	1.248	0	0.040	0
F10	0.07414	0	0.41620	0	0.38172	0	1.364	0	0.040	0
F11	0.91635	0	0.18479	0	0.31127	0	1.332	0	0.040	0
F12	0.62240	0	0.06996	0	0.46549	0	1.723	0	0.040	0
F13	0.32963	0	0.02888	0	0.90771	0	1.126	0	0.040	0
F14	0.30917	0	0.22593	0	0.61519	0	1.327	0	0.040	0
F15	0.38793	0	0.18802	0	0.35037	0	1.264	0	0.040	0
F16	0.86596	0	0.06056	0	0.46350	0	1.447	0	0.040	0
F17	0.43514	0	0.57330	0	0.59865	0	1.826	0	0.040	0
F18	0.47569	0	0.12073	0	0.76147	0	1.646	0	0.040	0
OW1	0.65843	0	0.12594	0	0.32889	0	1.347	0	0.040	0
OW2	0.05101	0	0.21294	0	0.02730	0	1.463	0	0.040	0
OW3	0.48195	0	0.27897	0	0.53084	0	1.639	0	0.040	0

==> PROFILE PARAMETERS:

=> Cell parameters	:	11.24333 0.00000
		8.19571 0.00000
		19.94934 0.00000
		90.00000 0.00000
		106.72829 0.00000
		90.00000 0.00000
=> Overall scale factor	:	0.008513615 0.000006415
=> ETA(p-V) or M(P-VII)	:	0.55830 0.00000
=> Overall Tem. factor	:	0.00000 0.00000
=> Halfwidth parameters	:	0.00192 0.00000
		0.00092 0.00000
		0.00031 0.00000
=> Preferred orientation:		1.00000 0.00000
		0.00000 0.00000
=> Asymmetry parameters	:	0.01565 0.00000
		0.00262 0.00000
		0.00000 0.00000
		0.00000 0.00000
=> X and Y parameters	:	0.00212 0.00000
		0.00000 0.00000
=> Strain parameters	:	0.00000 0.00000
		0.00000 0.00000
		0.00000 0.00000
=> Size parameters	:	0.00000 0.00000
		0.00000 0.00000

==> GLOBAL PARAMETERS:

=> Zero-point: 0.0018 0.0000
=> Background Polynomial Parameters ==>

```
                              87.5900    0.000000
                             -61.1500    0.000000
                              245.650    0.000000
                              357.980    0.000000
                             -440.810    0.000000
                             -764.500    0.000000

 => Cos( theta)-shift parameter :   0.0000  0.0000
 => Sin(2theta)-shift parameter :   0.0000  0.0000

 ==> RELIABILITY FACTORS WITH ALL NON-EXCLUDED POINTS:

 => Cycle:  2 => MaxCycle:  2
 => N-P+C: 15698
 => Rp: 4.10     Rwp: 5.59     Rexp:    5.52 Chi2:  1.03      L.S. refinement
 => Conventional Rietveld R-factors ==>
 => Rp: 7.71     Rwp: 9.08     Rexp:    8.97 Chi2:  1.03
 => Deviance: 0.162E+05     Dev*  :  1.033
 => DW-Stat.:    1.9253     DW-exp:     1.9508
 => N-sigma of the GoF:    2.252

 ==> RELIABILITY FACTORS FOR POINTS WITH BRAGG CONTRIBUTIONS:

 => N-P+C: 14778
 => Rp: 4.08     Rwp: 5.58     Rexp:    5.50 Chi2:  1.03      L.S. refinement
 => Conventional Rietveld R-factors ==>
 => Rp: 7.26     Rwp: 8.83     Rexp:    8.70 Chi2:  1.03
 => Deviance: 0.153E+05     Dev*  :  1.036
 => DW-Stat.:    2.0371     DW-exp:     1.9493
 => N-sigma of the GoF:        2.529
 => Phase:  1
 => Bragg R-factor:  1.87       Vol:    1760.479   Fract(%):     0.00
 => Rf-factor= 1.83             ATZ:       0.000   Brindley:   1.0000
```

Slightly smaller R values are obtained if all parameters are refined :

```
        ******************************************************
        *** PROGRAM FULLPROF (Version 3.3  - Aug97-LLB JRC) ***
        ******************************************************
           Rietveld, Profile Matching & Integrated Intensity
                Refinement of X-ray and/or Neutron Data


    Date: 11/15/02  Time: 15:22:12.71

 => PCR file code: sample3
 => DAT file code: sample3
 => Title:  Sample 2 - SDPDRR-2

 ==> CONDITIONS OF THIS RUN:

 => Global Refinement of X-ray powder diffraction data
    Bragg-Brentano or Debye-Scherrer geometry
 => The    5th default profile function was selected
 => Data supplied in free format
 => Wavelengths:  0.79764 0.79764
 => Base of peaks: 2.0*HW*   10.00
 => Cos(Monochromator angle)=   0.0000
 => Absorption correction (muR-eff):   0.0000
 ==> Angular range, step and number of points:
     2Thmin:   1.5000  2Thmax:  80.0000  Step:   0.0050  No. of points:  15701
 => Crystal Structure Refinement for phase: 1
 => Scor: 1.1491

 ==> RESULTS OF REFINEMENT:


 => No. of fitted parameters:  139


------------------------------------------------------------------------------
 => Phase No.  1   "Sample-2"                            P 21/C
------------------------------------------------------------------------------

 =>  No. of reflections:   7710


 ==> ATOM PARAMETERS:
```

Name	x	sx	y	sy	z	sz	B	sB	occ.	socc.
SR1	0.50806(	9)	0.08347(	0)	0.64668(	5)	0.685(	21)	0.040(	0)
SR2	0.14981(	9)	0.08422(	16)	0.64696(	5)	0.723(	21)	0.040(	0)
SR3	0.25968(	9)	0.08832(	16)	0.01769(	5)	0.816(	21)	0.040(	0)
SR4	0.15641(	11)	0.15564(	13)	0.32480(	6)	0.711(	25)	0.040(	0)
SR5	0.83522(	12)	0.33436(	13)	0.67117(	6)	0.664(	25)	0.040(	0)
V1	0.42343(	18)	0.08487(	31)	0.84034(	9)	0.682(	35)	0.040(	0)
V2	0.76549(	19)	0.07740(	29)	0.52372(	10)	1.024(	38)	0.040(	0)
V3	0.89992(	18)	0.08225(	30)	0.82686(	10)	0.918(	39)	0.040(	0)
O	0.83369(	55)	0.07331(	96)	0.88874(	31)	1.319(	161)	0.040(	0)
F1	0.98786(	52)	0.08572(	83)	0.74564(	30)	2.153(	143)	0.040(	0)
F2	0.24018(	47)	0.09375(	84)	0.77643(	27)	1.126(	128)	0.040(	0)
F3	0.70258(	49)	0.10560(	80)	0.60624(	25)	1.254(	133)	0.040(	0)
F4	0.92266(	50)	0.07540(	87)	0.60680(	27)	1.519(	139)	0.040(	0)
F5	0.79808(	53)	0.18672(	68)	0.03243(	32)	1.310(	154)	0.040(	0)
F6	0.60521(	56)	0.35773(	68)	0.68404(	30)	1.154(	142)	0.040(	0)
F7	0.22851(	57)	0.34691(	67)	0.95425(	30)	1.221(	149)	0.040(	0)
F8	0.75893(	45)	0.08294(	90)	0.74511(	27)	1.198(	132)	0.040(	0)
F9	0.07687(	58)	0.35162(	69)	0.68739(	31)	1.165(	151)	0.040(	0)
F10	0.07420(	49)	0.41633(	90)	0.38128(	28)	1.205(	129)	0.040(	0)
F11	0.91628(	60)	0.18503(	71)	0.31181(	33)	1.090(	148)	0.040(	0)
F12	0.62279(	50)	0.07011(	87)	0.46581(	28)	1.845(	151)	0.040(	0)
F13	0.32967(	49)	0.02989(	70)	0.90741(	29)	1.108(	143)	0.040(	0)
F14	0.30927(	56)	0.22692(	66)	0.61525(	30)	1.325(	149)	0.040(	0)
F15	0.38789(	56)	0.18820(	73)	0.35029(	30)	1.405(	155)	0.040(	0)
F16	0.86550(	48)	0.06178(	82)	0.46373(	27)	1.564(	146)	0.040(	0)
F17	0.43510(	51)	0.57258(	92)	0.59879(	28)	1.993(	151)	0.040(	0)
F18	0.47566(	50)	0.12277(	72)	0.76177(	30)	1.472(	154)	0.040(	0)
OW1	0.65869(	62)	0.12539(	75)	0.32914(	34)	1.336(	169)	0.040(	0)
OW2	0.05067(	65)	0.21337(	82)	0.02690(	36)	1.540(	184)	0.040(	0)
OW3	0.48120(	67)	0.27974(	81)	0.53076(	36)	1.610(	190)	0.040(	0)

==> PROFILE PARAMETERS:

=> Cell parameters :

11.24330	0.00003
8.19570	0.00002
19.94933	0.00005
90.00000	0.00000
106.72833	0.00013
90.00000	0.00000

=> Overall scale factor :	0.008524861	0.000012423
=> ETA(p-V) or M(P-VII) :	0.55833	0.00675
=> Overall Tem. factor :	0.00000	0.00000
=> Halfwidth parameters :	0.00177	0.00013
	0.00097	0.00005
	0.00030	0.00000
=> Preferred orientation:	1.00000	0.00000
	0.00000	0.00000
=> Asymmetry parameters :	0.01461	0.00069
	0.00236	0.00016
	0.00000	0.00000
	0.00000	0.00000
=> X and Y parameters :	0.00239	0.00032
	0.00000	0.00000
=> Strain parameters :	0.00000	0.00000
	0.00000	0.00000
	0.00000	0.00000
=> Size parameters :	0.00000	0.00000
	0.00000	0.00000

==> GLOBAL PARAMETERS:

=> Zero-point: 0.0017 0.0001

=> Background Polynomial Parameters ==>

85.5361	1.75293
-74.0510	16.8662
208.984	55.8395
347.256	92.3947
-343.589	97.1404
-680.298	45.4950

=> Cos(theta)-shift parameter : 0.0000 0.0000
=> Sin(2theta)-shift parameter : 0.0000 0.0000

==> RELIABILITY FACTORS WITH ALL NON-EXCLUDED POINTS:

=> Cycle: 8 => MaxCycle: 8
=> N-P+C: 15561

```
=> Rp: 4.04     Rwp: 5.55     Rexp:    5.50 Chi2:  1.02      L.S. refinement
=> Conventional Rietveld R-factors ==>
=> Rp: 7.61     Rwp: 9.02     Rexp:    8.95 Chi2:  1.02
=> Deviance: 0.159E+05     Dev*  :  1.020
=> DW-Stat.:    1.9593     DW-exp:     1.9684
=> N-sigma of the GoF:    1.576

==> RELIABILITY FACTORS FOR POINTS WITH BRAGG CONTRIBUTIONS:

=> N-P+C: 14635
=> Rp: 4.01     Rwp: 5.54     Rexp:    5.48 Chi2:  1.02      L.S. refinement
=> Conventional Rietveld R-factors ==>
=> Rp: 7.16     Rwp: 8.77     Rexp:    8.68 Chi2:  1.02
=> Deviance: 0.150E+05     Dev*  :  1.024
=> DW-Stat.:    2.0748     DW-exp:     1.9680
=> N-sigma of the GoF:        1.882
=> Phase:  1
=> Bragg R-factor:  1.61       Vol:    1760.471   Fract(%):     0.00
=> Rf-factor= 1.80             ATZ:       0.000   Brindley:   1.0000
```

For the curious, more details are below

The compound is obtained by hydrothermal synthesis and appears as small and thin needles, systematically twinned (no exact spot overlap). the cell and the structure were not easy to solve (several years ago). The "single crystal" data, recorded on a conventional 4-circle diffractometer, has some problem due to peak overlap with reflections belonging to another twin domain. Moreover, there is a huge number of very weak intensities due to the "crystal" small size. Some intensities obviously affected by twinning were excluded manually of the refinement (see the OMIT below). The quality of the refined atomic coordinates is consequently not very high. The exact formulation is difficult to establish with certitude. Valence bond analysis suggests some V^{IV}/V^{III} mixing, the hypothetical formula being :

$$\mathbf{Sr_5(V^{IV}OF_5))(V^{III}F_6)_2F\bullet 3H_2O}$$

Below is the final SHEXL refinement result, remade recently with SHELXL97-2 :

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+  SHELXL-97 - CRYSTAL STRUCTURE REFINEMENT - W95/98/NT/2000 VERSION  +
+  Copyright(C) George M. Sheldrick 1993-2001           Release 97-2  +
+  sv108b                          started at 19:06:18 on 22-Aug-2002  +
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

TITL Sr/V/F PHASE AIGUILLES P21/C
CELL  0.71073 11.2433 8.1957 19.9493 90.0 106.728 90.0
ZERR 4 0.0001 0.0001 0.0002 0.0 0.001 0.0
LATT 1
SYMM -X,0.5+Y,0.5-Z
SFAC SR 18.0874 1.4907 8.1373 12.6963 2.5654 24.5651 -34.193 =
        -0.0138 41.4025 -1.657 3.264 12810. 1.18 87.63
SFAC VA 9.43141 6.39535 7.74190 0.383349 2.15343 15.1908 =
       0.016865 63.969 0.656565 0.267 0.53 2135. 0.65 50.95
SFAC FF 3.6322 5.27756 3.51057 14.7353 1.26064 0.442258 0.940706 =
        47.3437 0.653396 0.014 0.010 49.99 1.28 19.0
SFAC OX 4.758 7.831 3.637 30.05 0. 0. 0. 0. 1.594 =
        0.008 0.006 30.48 1.35 16.00
SFAC H
UNIT 20 12 72 16 24

V =     1760.47     F(000) =    1863.6     Mu =  16.24 mm-1      Cell Wt =     4012.19    Rho =  3.784

OMIT 6
OMIT  -6   4   7
OMIT  -9   4   4
OMIT   2   6  20
OMIT  -1   6   2
OMIT  -2  10   4
OMIT   7   4   5
OMIT   3   8   6
OMIT  -7  10   7
OMIT  -8   4   9
OMIT -11   0  10
```

```
OMIT  -5   5  10
OMIT   2   7  13
OMIT   4   2  16
OMIT  -9   4  16
OMIT  -3   5  18
OMIT  -7   1  19
OMIT  -8   1  21
OMIT   5   2  21
OMIT   1   4  22
OMIT   0   0  24
OMIT  -6   3  26
OMIT  12   0   0
OMIT   9   2   1
OMIT -11   2   3
OMIT   8   2   3
OMIT   0   0   6
OMIT  -3   4   6
OMIT  -6   1   7
OMIT   0   2   7
OMIT  12   2   7
OMIT  -6   5   7
OMIT  -7   4   9
OMIT  11   4   9
OMIT   7   0  10
OMIT  -8   1  11
OMIT  -9   4  11
OMIT   0   0  12
OMIT  -6   6  12
OMIT   3   5  13
OMIT -14   0  18
OMIT  -6   2  19
OMIT   0   2  19
OMIT  -9   2  23
OMIT  -3   2  25
OMIT   6   0   0
OMIT   3   4   1
OMIT  -4   8   1
OMIT   8   1   3
OMIT   8   4   3
OMIT  -9   0   6
OMIT  -9   6   6
OMIT -13   4   7
OMIT  -2   4  11
OMIT   2   8  15
OMIT  -9   6  18
OMIT -10   3  20
OMIT -10   6  20
OMIT  -1   4  21
OMIT  -8   4  23
OMIT   9   4   1
OMIT  -8   0   4
OMIT  -8   6   4
OMIT   9   6   6
OMIT   0   4   7
OMIT  -8   2   9
OMIT   1   3  10
OMIT  -3   2  11
OMIT  -3   4  11
OMIT  -8   5  11
OMIT  -6   0  12
OMIT  -6   2  12
OMIT   6   2  12
OMIT  -4   2  15
OMIT  -5   4  15
OMIT  -8   4  16
OMIT  -6   2  17
OMIT  -5   8  17
OMIT -13   2  21
OMIT  -2   4  23
OMIT  -1   0  26
OMIT   6   2   0
OMIT  -1   2   2
OMIT  -1   4   7
OMIT   6   4   7
OMIT  -5   2  10
OMIT  -6   3  10
OMIT  -5   4  10
OMIT  -5   7  10
OMIT   1  10  10
OMIT   4   2  11
OMIT   4   4  11
OMIT   6   0  12
OMIT   6   3  12
OMIT  -7   4  14
OMIT  -5   2  15
OMIT  -6   1  17
OMIT  -9   0  18
OMIT -10   0  20
OMIT -10   2  20
OMIT  -4   3  20
OMIT -10   2  25
BOND
FMAP 2
```

```
PLAN 20
L.S. 8
WGHT      0.0384    108.7821
FVAR       0.13803
SR1   1    0.508104    0.083607    0.646757    11.00000    0.00853    0.00910 =
         0.01655    0.00122    0.00346    0.00079
SR2   1    0.149841    0.083932    0.647043    11.00000    0.00941    0.00779 =
         0.01315    0.00135    0.00162   -0.00021
SR3   1    0.259690    0.088432    0.017615    11.00000    0.01272    0.00700 =
         0.01404   -0.00146    0.00201    0.00023
SR4   1    0.156535    0.155588    0.324811    11.00000    0.01026    0.00974 =
         0.01104    0.00033    0.00028   -0.00178
SR5   1    0.835260    0.334305    0.671185    11.00000    0.00962    0.00788 =
         0.01086   -0.00151    0.00022   -0.00089
V1    2    0.423408    0.084370    0.840480    11.00000    0.01052    0.00867 =
         0.01427   -0.00177    0.00176   -0.00126
V2    2    0.765536    0.077203    0.523621    11.00000    0.01457    0.00848 =
         0.01169    0.00044    0.00283   -0.00428
V3    2    0.899639    0.082333    0.827010    11.00000    0.01271    0.00677 =
         0.01029    0.00129    0.00381    0.00141
O     4    0.834741    0.074253    0.888358    11.00000    0.02141
F1    3    0.987526    0.085432    0.745485    11.00000    0.03533
F2    3    0.240566    0.093738    0.776216    11.00000    0.01521
F3    3    0.703790    0.106747    0.606188    11.00000    0.01902
F4    3    0.922671    0.074332    0.607018    11.00000    0.01920
F5    3    0.798040    0.185746    0.032871    11.00000    0.01909
F6    3    0.604938    0.358466    0.683887    11.00000    0.01616
F7    3    0.227746    0.346453    0.953883    11.00000    0.01569
F8    3    0.758695    0.082225    0.745351    11.00000    0.01637
F9    3    0.076877    0.351721    0.686907    11.00000    0.01656
F10   3    0.074135    0.416509    0.381759    11.00000    0.02393
F11   3    0.915243    0.184715    0.311079    11.00000    0.02062
F12   3    0.622220    0.071557    0.465288    11.00000    0.02741
F13   3    0.329335    0.028733    0.907831    11.00000    0.01167
F14   3    0.309860    0.225804    0.614913    11.00000    0.01687
F15   3    0.387303    0.188177    0.350291    11.00000    0.01492
F16   3    0.865979    0.059115    0.463398    11.00000    0.02049
F17   3    0.435242    0.572972    0.598826    11.00000    0.03158
F18   3    0.475347    0.119713    0.761504    11.00000    0.02617
OW1   4    0.657858    0.125156    0.328468    11.00000    0.01587
OW2   4    0.050752    0.212678    0.027267    11.00000    0.02118
OW3   4    0.481111    0.278119    0.531200    11.00000    0.01780
HKLF 4


Covalent radii and connectivity table for  Sr/V/F PHASE AIGUILLES P21/C

SR   1.180
VA   0.650
FF   1.280
OX   1.350
H    0.320

Sr1 - F14 F18 F15_$1 F6 F3 F12_$1 OW1_$1 OW3 F8
Sr2 - F14 F4_$7 F16_$1 F2 F11_$1 F9 OW1_$1 OW2_$6
Sr3 - F14_$3 F7_$14 F5_$5 F17_$3 F13_$14 OW2 OW3_$3 O_$1 F10_$3
Sr4 - F7_$3 F15 F2_$3 F4_$1 F9_$3 F11_$7 F1_$1 F10 F8_$1 F3_$1
Sr5 - F3 F13_$10 F2_$10 F10_$8 F9_$2 F5_$6 F11_$6 F6 F1 F4 F8
V1 - F17_$9 F18 F6_$9 F15_$6 F13 F2
V2 - F12 F16 F7_$9 F5_$6 F3 F4
V3 - O F8 F9_$9 F10_$17 F11_$6 F1
O - V3 F9_$9 F8 F10_$17 Sr3_$1 F11_$6 OW2_$1 F17_$9 OW1_$6
F1 - V3 F11_$6 F9_$9 F8 F10_$17 F4 Sr4_$1 F2_$2 F9_$2 Sr5 F11_$12
F2 - V1 Sr2 F6_$9 Sr4_$6 F13 F15_$6 Sr5_$9 F1_$7 F18 F9
F3 - V2 F4 Sr5 Sr1 F5_$6 F7_$9 F8 F12 Sr4_$1 F15_$1 OW3 F6
F4 - V2 Sr2_$2 F3 F7_$9 F5_$6 Sr4_$1 F1 F16 Sr5 F11_$12 OW2_$17 F9_$2
F5 - V2_$3 Sr3_$5 F4_$3 F3_$3 Sr5_$3 F16_$3 F13_$1 F12_$3 OW2_$2 F10_$16
F6 - V1_$10 Sr1 F2_$10 F13_$10 F18_$10 Sr5 OW1_$6 F17 F8 F3 OW3
F7 - V2_$10 Sr3_$4 Sr4_$6 F4_$10 F3_$10 F12_$10 F16_$10 F10_$6 OW2_$4 OW3_$6
F8 - V3 F1 F11_$6 F3 F9_$9 Sr4_$1 O Sr5 F6 Sr1
F9 - V3_$10 Sr2 F1_$10 Sr4_$6 Sr5_$7 F10_$15 F8_$10 O_$10 F1_$7 F4_$7 F2
F10 - V3_$11 F1_$11 Sr5_$8 F9_$15 Sr4 F11_$7 O_$11 F13_$3 F7_$3 F5_$13 Sr3_$6
F11 - V3_$3 Sr2_$1 F1_$3 Sr4_$2 F8_$3 Sr5_$3 F10_$2 O_$3 F1_$12 F4_$12 OW1
F12 - V2 Sr1_$1 F7_$9 F3 F16 F5_$6 OW3 OW1 OW3_$1
F13 - V1 F6_$9 Sr3_$4 F2 Sr5_$9 F17_$9 F5_$1 F15_$6 F10_$6 OW3_$9 OW3_$6
F14 - Sr2 Sr3_$6 Sr1 OW3 OW2_$6 OW1_$1
F15 - V1_$3 Sr4 Sr1_$1 F2_$3 F13_$3 F18_$3 F17_$8 F3_$1
F16 - V2 Sr2_$1 F5_$6 F4 F12 F7_$9 OW2_$17 OW2_$16 OW1
F17 - V1_$10 Sr3_$6 F18_$10 F13_$10 F15_$8 F6 OW3 O_$10
F18 - V1 Sr1 F6_$9 F17_$9 F2 F15_$6 OW1_$1 OW1_$6
OW1 - Sr1_$1 Sr2_$1 F6_$3 F18_$1 F12 F18_$3 F11 F16 F14_$1 O_$3
OW2 - Sr3 F16_$11 Sr2_$3 F5_$7 O_$1 F14_$3 F16_$13 F4_$11 F7_$14
OW3 - Sr3_$6 Sr1 F12 F3 F17 F14 F13_$10 F7_$3 F13_$3 F6 F12_$1


Operators for generating equivalent atoms:

$1   -x+1, -y, -z+1
$2   x+1, y, z
$3   x, -y+1/2, z-1/2
$4   x, y, z+1
$5   -x+1, -y, -z
$6   x, -y+1/2, z+1/2
```

```
$7   x-1, y, z
$8   -x+1, -y+1, -z+1
$9   -x+1, y-1/2, -z+3/2
$10  -x+1, y+1/2, -z+3/2
$11  x-1, -y+1/2, z-1/2
$12  -x+2, -y, -z+1
$13  -x+1, y+1/2, -z+1/2
$14  x, y, z-1
$15  -x, -y+1, -z+1
$16  -x+1, y-1/2, -z+1/2
$17  x+1, -y+1/2, z+1/2


   3805  Reflections read, of which     5  rejected

-15 =< h =< 15,      0 =< k =< 11,      0 =< l =< 28,   Max. 2-theta =   60.04

      0  Systematic absence violations

      0  Inconsistent equivalents

   3800  Unique reflections, of which   2287  suppressed

R(int) = 0.0000     R(sigma) = 0.1588      Friedel opposites merged

Maximum memory for data reduction =  7416 /   40828


  ** Cell contents from UNIT instruction and atom list do not agree **


Unit-cell contents from UNIT instruction and atom list resp.

SR       20.00     20.00
VA       12.00     12.00
FF       72.00     72.00
OX       16.00     16.00
H        24.00      0.00


Least-squares cycle   1      Maximum vector length =  511      Memory required =   7502 /  201922

wR2 =  0.1145 before cycle   1 for   1513 data and   161 /   161 parameters

GooF = S =     1.067;     Restrained GooF =      1.067  for      0 restraints

Weight = 1 / [ sigma^2(Fo^2) + ( 0.0384 * P )^2 + 108.78 * P ]   where  P = ( Max ( Fo^2, 0 ) + 2 * Fc^2 ) / 3

    N      value        esd    shift/esd  parameter

    1     0.13730     0.00042    -1.728    OSF

Mean shift/esd =   0.192    Maximum =  -1.728 for  OSF

Max. shift = 0.011 A for OW3      Max. dU = 0.001 for F17


Least-squares cycle   8      Maximum vector length =  511      Memory required =   7502 /  201922

wR2 =  0.1138 before cycle   8 for   1513 data and   161 /   161 parameters

GooF = S =     1.059;     Restrained GooF =      1.059  for      0 restraints

Weight = 1 / [ sigma^2(Fo^2) + ( 0.0384 * P )^2 + 108.78 * P ]   where  P = ( Max ( Fo^2, 0 ) + 2 * Fc^2 ) / 3

    N      value        esd    shift/esd  parameter

    1     0.13722     0.00042     0.000    OSF

Mean shift/esd =   0.000    Maximum =   0.000 for   y  F1

Max. shift = 0.000 A for F1      Max. dU = 0.000 for F1

Largest correlation matrix elements

    0.506 z Sr5 / z Sr4


 Sr/V/F PHASE AIGUILLES P21/C

ATOM           x         y         z          sof         U11       U22       U33       U23       U13       U12        Ueq

Sr1         0.50808   0.08346   0.64675     1.00000     0.00809   0.00915   0.01627   0.00151   0.00327   0.00057    0.01122
  0.00365   0.00015   0.00029   0.00009     0.00000     0.00073   0.00077   0.00085   0.00098   0.00064   0.00091    0.00035

Sr2         0.14985   0.08410   0.64701     1.00000     0.00920   0.00807   0.01300   0.00137   0.00191  -0.00024    0.01036
  0.00361   0.00015   0.00030   0.00009     0.00000     0.00075   0.00074   0.00080   0.00094   0.00062   0.00088    0.00035
```

Sr3	0.25965	0.08832	0.01762	1.00000	0.01243	0.00722	0.01375	-0.00133	0.00183	0.00030	0.01154
	0.00372	0.00015	0.00030	0.00009	0.00000	0.00076	0.00072	0.00083	0.00104	0.00062	0.00095	0.00035
Sr4	0.15658	0.15559	0.32478	1.00000	0.01000	0.00958	0.01085	0.00047	0.00011	-0.00185	0.01075
	0.00422	0.00020	0.00026	0.00012	0.00000	0.00087	0.00086	0.00095	0.00085	0.00081	0.00081	0.00041
Sr5	0.83533	0.33432	0.67120	1.00000	0.00938	0.00795	0.01064	-0.00147	0.00033	-0.00080	0.00986
	0.00422	0.00020	0.00024	0.00012	0.00000	0.00087	0.00091	0.00093	0.00085	0.00080	0.00080	0.00041
V1	0.42345	0.08462	0.84050	1.00000	0.00994	0.00825	0.01460	-0.00212	0.00187	-0.00186	0.01128
	0.00669	0.00027	0.00056	0.00017	0.00000	0.00138	0.00138	0.00149	0.00175	0.00115	0.00162	0.00061
V2	0.76551	0.07753	0.52365	1.00000	0.01503	0.00826	0.01188	0.00013	0.00305	-0.00483	0.01190
	0.00652	0.00029	0.00050	0.00017	0.00000	0.00143	0.00148	0.00152	0.00182	0.00120	0.00174	0.00063
V3	0.89983	0.08221	0.82698	1.00000	0.01252	0.00672	0.01036	0.00116	0.00345	0.00097	0.00983
	0.00669	0.00028	0.00051	0.00016	0.00000	0.00140	0.00131	0.00145	0.00180	0.00118	0.00168	0.00060
O	0.83440	0.07484	0.88856	1.00000	0.02103						
	0.02901	0.00125	0.00221	0.00073	0.00000	0.00317					
F1	0.98793	0.08609	0.74570	1.00000	0.03503						
	0.02885	0.00126	0.00219	0.00075	0.00000	0.00313					
F2	0.24014	0.09468	0.77629	1.00000	0.01414						
	0.02217	0.00094	0.00172	0.00056	0.00000	0.00223					
F3	0.70326	0.10733	0.60604	1.00000	0.01861						
	0.02306	0.00104	0.00166	0.00060	0.00000	0.00263					
F4	0.92264	0.07553	0.60714	1.00000	0.01949						
	0.02392	0.00102	0.00187	0.00059	0.00000	0.00258					
F5	0.79844	0.18602	0.03306	1.00000	0.01767						
	0.02416	0.00113	0.00155	0.00065	0.00000	0.00280					
F6	0.60512	0.35815	0.68391	1.00000	0.01617						
	0.02294	0.00107	0.00150	0.00062	0.00000	0.00259					
F7	0.22758	0.34714	0.95418	1.00000	0.01605						
	0.02335	0.00110	0.00157	0.00063	0.00000	0.00260					
F8	0.75877	0.08224	0.74505	1.00000	0.01631						
	0.02298	0.00094	0.00185	0.00056	0.00000	0.00232					
F9	0.07712	0.35194	0.68695	1.00000	0.01690						
	0.02593	0.00121	0.00161	0.00070	0.00000	0.00284					
F10	0.07414	0.41621	0.38172	1.00000	0.02351						
	0.02546	0.00108	0.00200	0.00062	0.00000	0.00261					
F11	0.91636	0.18479	0.31127	1.00000	0.02071						
	0.02679	0.00130	0.00163	0.00073	0.00000	0.00308					
F12	0.62240	0.06996	0.46549	1.00000	0.02765						
	0.02563	0.00113	0.00191	0.00065	0.00000	0.00305					
F13	0.32963	0.02888	0.90771	1.00000	0.01120						
	0.02049	0.00096	0.00141	0.00056	0.00000	0.00234					
F14	0.30918	0.22593	0.61520	1.00000	0.01619						
	0.02249	0.00106	0.00154	0.00060	0.00000	0.00249					
F15	0.38793	0.18803	0.35037	1.00000	0.01465						
	0.02224	0.00103	0.00148	0.00061	0.00000	0.00260					
F16	0.86597	0.06057	0.46350	1.00000	0.01952						
	0.02269	0.00104	0.00158	0.00060	0.00000	0.00277					
F17	0.43515	0.57330	0.59865	1.00000	0.03340						
	0.02799	0.00119	0.00218	0.00069	0.00000	0.00333					
F18	0.47570	0.12073	0.76148	1.00000	0.02553						
	0.02523	0.00116	0.00164	0.00068	0.00000	0.00309					
OW1	0.65843	0.12594	0.32889	1.00000	0.01614						
	0.02759	0.00129	0.00175	0.00076	0.00000	0.00313					
OW2	0.05102	0.21295	0.02730	1.00000	0.02088						
	0.02977	0.00140	0.00201	0.00079	0.00000	0.00338					
OW3	0.48196	0.27897	0.53085	1.00000	0.01894						
	0.02866	0.00137	0.00192	0.00076	0.00000	0.00322					

Final Structure Factor Calculation for Sr/V/F PHASE AIGUILLES P21/C

Total number of l.s. parameters = 161 Maximum vector length = 511 Memory required = 7341 / 24017

wR2 = 0.1665 before cycle 9 for 3800 data and 0 / 161 parameters

GooF = S = 0.965; Restrained GooF = 0.965 for 0 restraints

Weight = 1 / [sigma^2(Fo^2) + (0.0384 * P)^2 + 108.78 * P] where P = (Max (Fo^2, 0) + 2 * Fc^2) / 3

R1 = 0.0466 for 1513 Fo > 4sig(Fo) and 0.1659 for all 3800 data
wR2 = 0.1665, GooF = S = 0.965, Restrained GooF = 0.965 for all data

Occupancy sum of asymmetric unit = 30.00 for non-hydrogen and 0.00 for hydrogen atoms

Principal mean square atomic displacements U

0.0168	0.0090	0.0078	Sr1
0.0143	0.0091	0.0077	Sr2
0.0162	0.0115	0.0069	Sr3
0.0152	0.0096	0.0075	Sr4
0.0138	0.0092	0.0066	Sr5
0.0161	0.0111	0.0066	V1
0.0182	0.0119	0.0057	V2
0.0127	0.0105	0.0063	V3

Analysis of variance for reflections employed in refinement K = Mean[Fo^2] / Mean[Fc^2] for group

Fc/Fc(max)	0.000	0.138	0.183	0.247	1.000	0.000	0.000	0.000	0.000	0.000	0.000
Number in group	386.	382.	371.	374.	0.	0.	0.	0.	0.	0.	
GooF	1.026	1.037	1.085	0.946	0.000	0.000	0.000	0.000	0.000	0.000	
K	1.113	1.019	1.011	0.992	0.000	0.000	0.000	0.000	0.000	0.000	

Resolution(A)	0.71	0.86	1.06	1.37	0.00	0.00	0.00	0.00	0.00	0.00	inf
Number in group	383.	382.	374.	374.	0.	0.	0.	0.	0.	0.	
GooF	1.143	1.060	0.968	0.910	0.000	0.000	0.000	0.000	0.000	0.000	
K	1.022	1.009	0.997	1.005	0.000	0.000	0.000	0.000	0.000	0.000	
R1	0.062	0.054	0.042	0.033	0.000	0.000	0.000	0.000	0.000	0.000	

** Extinction (EXTI) or solvent water (SWAT) correction may be required **

Recommended weighting scheme: WGHT 0.0215 128.7603
Note that in most cases convergence will be faster if fixed weights (e.g. the default WGHT 0.1) are retained until the refinement is virtually complete, and only then should the above recommended values be used.

Most Disagreeable Reflections (* if suppressed or used for Rfree)

h	k	l	Fo^2	Fc^2	Delta(F^2)/esd	Fc/Fc(max)	Resolution(A)
-1	4	2	12107.09	7830.39	3.73	0.164	1.99
-15	0	6	17518.81	11808.97	3.67	0.201	0.75
-3	7	6	8817.75	5209.45	3.56	0.133	1.08
-12	2	19	15136.93	10158.26	3.56	0.186	0.78
-5	8	3	9945.28	6041.94	3.49	0.144	0.93
-9	4	6	25734.96	19206.64	3.49	0.256	1.06
4	8	11	13072.63	8098.91	3.48	0.166	0.80
-4	6	6	10407.80	15282.03	3.46	0.229	1.19
-3	8	11	15302.11	10520.41	3.46	0.190	0.89
6	6	12	12815.26	8192.49	3.40	0.167	0.83
-2	5	9	20143.68	14697.75	3.36	0.224	1.32
-2	8	11	12220.06	8023.95	3.34	0.166	0.89
-7	6	14	8363.22	4891.37	3.32	0.129	0.90
-3	9	6	8275.30	4776.01	3.31	0.128	0.87
6	6	0	32093.04	24729.42	3.28	0.291	1.09
6	8	7	12066.06	7485.68	3.26	0.160	0.81
13	2	5	15051.67	10414.56	3.24	0.189	0.75
-9	2	18	4644.40	1943.54	3.24	0.082	0.92
7	8	5	13357.18	8889.63	3.22	0.174	0.81
-5	10	10	11940.84	7576.06	3.21	0.161	0.74
6	7	7	21492.34	15836.67	3.21	0.233	0.88
0	8	7	21088.44	15511.24	3.21	0.230	0.96
3	8	1	19770.14	14381.32	3.19	0.222	0.98
-1	10	2	12443.33	8377.83	3.18	0.169	0.82
-2	1	16	3215.80	1165.10	3.18	0.063	1.23
-6	2	14	5934.98	9416.46	3.13	0.179	1.22
-6	7	7	19833.55	14780.39	3.11	0.225	0.97
0	5	5	8799.64	5768.36	3.10	0.140	1.51
1	4	5	37074.21	29591.41	3.10	0.318	1.74
-14	2	4	18659.13	13739.40	3.09	0.217	0.78
8	0	8	17845.45	12950.52	3.08	0.210	1.05
5	6	14	7533.56	4247.89	3.08	0.121	0.82
-5	4	12	12251.50	16819.33	3.05	0.240	1.21

9	3	6	10492.53	7106.95	3.00	0.156	0.96
4	4	4	71262.45	60194.21	2.98	0.454	1.47
-10	1	20	5085.07	2358.51	2.97	0.090	0.84
-1	4	9	10164.82	7027.16	2.97	0.155	1.50
-11	1	15	3757.19	1413.28	2.96	0.070	0.91
-11	4	17	25723.24	19701.17	2.95	0.260	0.80
5	10	7	21254.69	15629.61	2.94	0.231	0.72
-7	5	19	4712.61	2063.72	2.88	0.084	0.84
-4	7	1	6897.86	4262.75	2.87	0.121	1.08
3	5	1	27451.30	21462.19	2.85	0.271	1.47
7	1	5	4278.33	2222.09	2.85	0.087	1.29
-14	3	14	3560.03	6815.67	2.85	0.153	0.74
-9	2	25	8401.59	5034.25	2.84	0.131	0.74
-4	0	24	4709.41	2218.04	2.83	0.087	0.83
6	4	12	4828.77	2241.42	2.82	0.088	0.93
-4	0	20	9302.12	6269.05	2.79	0.146	1.00
12	4	0	22241.01	17367.79	2.79	0.244	0.82

Bond lengths and angles

Sr1 -	Distance	Angles						
F14	2.4394 (0.0119)							
F18	2.4379 (0.0132)	78.98 (0.40)						
F15_$1	2.5065 (0.0123)	144.86 (0.40)	106.53 (0.42)					
F6	2.5184 (0.0126)	86.30 (0.40)	77.34 (0.42)	128.84 (0.37)				
F3	2.5572 (0.0115)	133.49 (0.41)	131.47 (0.41)	68.77 (0.41)	71.73 (0.41)			
F12_$1	2.6185 (0.0134)	76.28 (0.41)	131.66 (0.42)	74.70 (0.41)	140.32 (0.42)	94.93 (0.39)		
OW1_$1	2.6852 (0.0145)	73.59 (0.42)	67.04 (0.45)	76.90 (0.40)	141.59 (0.42)	144.40 (0.44)	66.40 (0.43)	
OW3	2.7585 (0.0152)	68.72 (0.43)	134.87 (0.46)	118.12 (0.41)	70.13 (0.42)	65.38 (0.42)	70.36 (0.44)	127.69 (0.44)
F8	2.9340 (0.0105)	143.82 (0.39)	75.36 (0.37)	68.26 (0.39)	63.57 (0.40)	57.69 (0.34)	139.81 (0.40)	117.55 (0.41)
	Sr1 -	F14	F18	F15_$1	F6	F3	F12_$1	OW1_$1

Sr2 -	Distance	Angles						
F14	2.3701 (0.0121)							
F4_$7	2.4483 (0.0112)	136.51 (0.42)						
F16_$1	2.4642 (0.0121)	82.06 (0.40)	84.01 (0.40)					
F2	2.4865 (0.0106)	98.41 (0.39)	114.47 (0.37)	147.95 (0.42)				
F11_$1	2.5416 (0.0138)	145.90 (0.45)	72.84 (0.47)	85.60 (0.44)	76.19 (0.44)			
F9	2.5490 (0.0136)	89.80 (0.43)	74.19 (0.45)	138.33 (0.42)	73.60 (0.43)	119.59 (0.36)		
OW1_$1	2.6915 (0.0143)	74.53 (0.42)	138.31 (0.47)	72.54 (0.41)	76.71 (0.42)	71.45 (0.43)	143.85 (0.44)	
OW2_$6	2.8596 (0.0157)	68.47 (0.43)	68.10 (0.44)	67.79 (0.43)	142.23 (0.46)	134.25 (0.47)	71.19 (0.44)	128.31 (0.45)
	Sr2 -	F14	F4_$7	F16_$1	F2	F11_$1	F9	OW1_$1

Sr3 -	Distance	Angles						
F14_$3	2.4068 (0.0121)							
F7_$14	2.4430 (0.0130)	80.51 (0.41)						
F5_$5	2.4747 (0.0129)	151.35 (0.43)	126.51 (0.38)					
F17_$3	2.5348 (0.0146)	81.86 (0.45)	139.10 (0.46)	81.44 (0.47)				
F13_$14	2.5802 (0.0109)	138.64 (0.38)	76.07 (0.40)	65.82 (0.38)	94.10 (0.40)			
OW2	2.6160 (0.0157)	72.36 (0.44)	72.39 (0.47)	104.37 (0.45)	134.99 (0.46)	129.47 (0.41)		
OW3_$3	2.6684 (0.0152)	70.74 (0.44)	72.04 (0.43)	122.70 (0.44)	67.35 (0.47)	69.81 (0.39)	131.90 (0.48)	
O_$1	2.7475 (0.0154)	78.56 (0.44)	138.34 (0.45)	74.22 (0.46)	72.11 (0.43)	139.32 (0.46)	67.09 (0.47)	131.62 (0.42)
F10_$3	2.9062 (0.0118)	134.38 (0.41)	64.44 (0.41)	64.73 (0.43)	143.72 (0.49)	61.14 (0.33)	69.87 (0.42)	119.85 (0.41)
	Sr3 -	F14_$3	F7_$14	F5_$5	F17_$3	F13_$14	OW2	OW3_$3

Sr4 -	Distance	Angles						
F7_$3	2.4729 (0.0121)							
F15	2.5165 (0.0115)	77.58 (0.40)						
F2_$3	2.5555 (0.0134)	111.04 (0.39)	61.38 (0.36)					
F4_$1	2.6309 (0.0139)	60.67 (0.39)	117.07 (0.38)	171.11 (0.38)				
F9_$3	2.6360 (0.0136)	177.92 (0.43)	103.55 (0.41)	71.04 (0.37)	117.27 (0.40)			
F11_$7	2.6469 (0.0144)	96.92 (0.42)	167.41 (0.41)	111.38 (0.38)	68.32 (0.39)	82.32 (0.41)		
F1_$1	2.6879 (0.0163)	120.29 (0.44)	128.16 (0.43)	128.67 (0.41)	59.74 (0.42)	57.64 (0.43)	64.40 (0.43)	
F10	2.7051 (0.0152)	67.38 (0.40)	106.89 (0.39)	74.59 (0.40)	98.27 (0.42)	113.72 (0.39)	60.56 (0.39)	124.95 (0.43)
F8_$1	2.7220 (0.0134)	118.20 (0.40)	71.71 (0.36)	99.15 (0.39)	88.21 (0.40)	60.84 (0.38)	120.63 (0.39)	56.79 (0.40)
F3_$1	2.7891 (0.0129)	60.65 (0.38)	65.00 (0.36)	126.10 (0.35)	54.22 (0.36)	118.14 (0.39)	122.34 (0.39)	81.95 (0.43)
	Sr4 -	F7_$3	F15	F2_$3	F4_$1	F9_$3	F11_$7	F1_$1

Sr5 -	Distance	Angles						
F3	2.4989 (0.0129)							
F13_$10	2.6038 (0.0109)	85.88 (0.39)						
F2_$10	2.6233 (0.0133)	126.96 (0.37)	59.16 (0.34)					
F10_$8	2.6362 (0.0153)	127.53 (0.39)	64.71 (0.36)	74.67 (0.40)				
F9_$2	2.6493 (0.0135)	122.55 (0.40)	124.50 (0.39)	110.31 (0.38)	60.26 (0.40)			
F5_$6	2.6714 (0.0128)	61.60 (0.38)	62.77 (0.36)	119.38 (0.38)	66.32 (0.39)	88.57 (0.40)		
F11_$6	2.6828 (0.0142)	118.11 (0.41)	129.40 (0.39)	71.55 (0.38)	114.07 (0.41)	81.40 (0.42)	167.47 (0.40)	
F6	2.6794 (0.0120)	70.00 (0.38)	58.21 (0.36)	58.04 (0.36)	118.44 (0.39)	166.18 (0.39)	103.58 (0.38)	87.33 (0.40)
F1	2.7971 (0.0163)	85.22 (0.43)	171.08 (0.42)	126.79 (0.40)	121.90 (0.42)	61.64 (0.42)	113.08 (0.42)	55.36 (0.43)
F4	2.7960 (0.0142)	55.37 (0.37)	118.09 (0.36)	174.86 (0.38)	100.28 (0.41)	67.19 (0.38)	56.76 (0.37)	111.91 (0.38)
F8	2.8124 (0.0137)	60.00 (0.37)	119.63 (0.34)	101.85 (0.37)	172.39 (0.36)	115.86 (0.37)	120.97 (0.38)	58.32 (0.38)
	Sr5 -	F3	F13_$10	F2_$10	F10_$8	F9_$2	F5_$6	F11_$6

V1 -	Distance	Angles						
F17_$9	1.7026 (0.0133)							
F18	1.8577 (0.0135)	98.93 (0.62)						
F6_$9	1.9223 (0.0129)	100.47 (0.72)	90.54 (0.58)					
F15_$6	1.9276 (0.0132)	99.10 (0.72)	93.33 (0.58)	159.20 (0.50)				
F13	1.9833 (0.0112)	94.28 (0.57)	165.94 (0.53)	82.31 (0.52)	89.28 (0.50)			
F2	2.0917 (0.0106)	172.75 (0.57)	88.32 (0.51)	79.61 (0.55)	80.09 (0.52)	78.52 (0.44)		
	V1 -	F17_$9	F18	F6_$9	F15_$6	F13		

V2 -	Distance	Angles											
F12	1.6924 (0.0126)												
F16	1.8749 (0.0123)	100.81 (0.56)											
F7_$9	1.9358 (0.0137)	95.08 (0.66)	94.70 (0.58)										
F5_$6	1.9717 (0.0135)	102.52 (0.67)	90.15 (0.57)	160.54 (0.48)									
F3	1.9781 (0.0119)	94.60 (0.56)	164.43 (0.50)	86.05 (0.55)	84.33 (0.57)								
F4	2.0498 (0.0113)	169.66 (0.60)	88.99 (0.50)	80.68 (0.56)	80.57 (0.57)	75.77 (0.48)							
	V2 -	F12	F16	F7_$9	F5_$6	F3							

V3 -	Distance	Angles											
O	1.6045 (0.0144)												
F8	1.9220 (0.0109)	101.72 (0.60)											
F9_$9	1.9358 (0.0140)	100.55 (0.80)	89.42 (0.62)										
F10_$17	1.9498 (0.0121)	100.36 (0.63)	157.92 (0.51)	86.13 (0.65)									
F11_$6	1.9526 (0.0143)	104.21 (0.81)	87.52 (0.63)	155.17 (0.49)	87.51 (0.65)								
F1	2.1297 (0.0149)	178.64 (0.82)	78.66 (0.49)	78.14 (0.64)	79.26 (0.52)	77.10 (0.66)							
	V3 -	O	F8	F9_$9	F10_$17	F11_$6							

O -	Distance	Angles											
V3	1.6045 (0.0144)												
F9_$9	2.7311 (0.0208)	44.17 (0.54)											
F8	2.7424 (0.0180)	43.33 (0.43)	59.45 (0.51)										
F10_$17	2.7389 (0.0184)	44.45 (0.44)	58.03 (0.52)	87.78 (0.53)									
Sr3_$1	2.7475 (0.0154)	153.01 (1.00)	108.84 (0.67)	131.10 (0.64)	128.62 (0.63)								
F11_$6	2.8151 (0.0216)	42.25 (0.54)	86.41 (0.52)	57.64 (0.51)	58.13 (0.52)	164.69 (0.74)							
OW2_$1	2.9658 (0.0227)	104.07 (0.79)	67.19 (0.56)	124.20 (0.76)	77.06 (0.58)	54.34 (0.43)	135.17 (0.67)						
F17_$9	3.1136 (0.0183)	137.27 (0.73)	124.07 (0.70)	93.96 (0.50)	177.80 (0.75)	50.78 (0.38)	121.84 (0.68)	103.00 (0.66)					
OW1_$6	3.1605 (0.0217)	93.31 (0.72)	126.81 (0.62)	67.50 (0.51)	118.61 (0.71)	108.20 (0.53)	61.24 (0.51)	162.38 (0.68)					
	O -	V3	F9_$9	F8	F10_$17	Sr3_$1	F11_$6	OW2_$1					

F1 -	Distance	Angles											
V3	2.1297 (0.0148)												
F11_$6	2.5478 (0.0216)	48.34 (0.47)											
F9_$9	2.5668 (0.0211)	47.57 (0.45)	95.89 (0.61)										
F8	2.5730 (0.0175)	47.09 (0.38)	63.11 (0.57)	63.75 (0.56)									
F10_$17	2.6057 (0.0185)	47.32 (0.39)	63.15 (0.58)	61.71 (0.57)	94.41 (0.59)								
F4	2.6492 (0.0183)	138.07 (0.66)	121.75 (0.77)	119.12 (0.76)	91.03 (0.55)	174.07 (0.76)							
Sr4_$1	2.6879 (0.0162)	92.50 (0.55)	125.38 (0.64)	60.16 (0.47)	62.27 (0.46)	121.81 (0.72)	59.06 (0.45)						
F2_$2	2.7244 (0.0170)	120.80 (0.62)	109.15 (0.68)	109.70 (0.67)	167.86 (0.71)	73.48 (0.50)	101.10 (0.58)	124.73 (0.67)					
F9_$2	2.7934 (0.0213)	129.26 (0.81)	81.09 (0.64)	173.49 (0.63)	119.17 (0.73)	111.82 (0.71)	67.23 (0.56)	126.25 (0.61)					
Sr5	2.7971 (0.0163)	93.83 (0.55)	60.04 (0.48)	126.75 (0.61)	63.00 (0.46)	123.09 (0.71)	61.71 (0.45)	94.13 (0.42)					
F11_$12	2.8430 (0.0212)	127.24 (0.80)	173.05 (0.66)	79.81 (0.62)	118.83 (0.73)	109.91 (0.70)	65.20 (0.54)	57.10 (0.45)					
	F1 -	V3	F11_$6	F9_$9	F8	F10_$17	F4	Sr4_$1					

F2 -	Distance	Angles											
V1	2.0917 (0.0105)												
Sr2	2.4865 (0.0106)	132.06 (0.50)											
F6_$9	2.5730 (0.0175)	47.30 (0.37)	109.37 (0.53)										
Sr4_$6	2.5555 (0.0133)	101.81 (0.48)	109.62 (0.46)	140.92 (0.51)									
F13	2.5803 (0.0150)	48.87 (0.33)	165.92 (0.70)	59.85 (0.45)	82.02 (0.42)								
F15_$6	2.5890 (0.0168)	47.17 (0.37)	128.27 (0.58)	94.37 (0.49)	58.57 (0.39)	64.23 (0.45)							
Sr5_$9	2.6233 (0.0133)	95.64 (0.46)	107.66 (0.46)	62.07 (0.41)	107.69 (0.38)	60.04 (0.37)	124.04 (0.49)						
F1_$7	2.7244 (0.0170)	156.17 (0.60)	71.27 (0.40)	128.13 (0.68)	68.48 (0.44)	107.37 (0.53)	126.96 (0.63)	68.47 (0.45)					
F18	2.7564 (0.0160)	42.35 (0.35)	90.54 (0.43)	60.41 (0.45)	116.60 (0.56)	91.11 (0.46)	61.92 (0.45)	122.48 (0.55)					
F9	3.0167 (0.0173)	135.51 (0.64)	54.15 (0.34)	161.94 (0.55)	55.73 (0.37)	137.67 (0.59)	92.15 (0.55)	126.37 (0.44)					
	F2 -	V1	Sr2	F6_$9	Sr4_$6	F13	F15_$6	Sr5_$9					

F3 -	Distance	Angles											
V2	1.9781 (0.0119)												
F4	2.4741 (0.0162)	53.43 (0.39)											
Sr5	2.4989 (0.0127)	102.99 (0.50)	68.42 (0.45)										
Sr1	2.5572 (0.0115)	142.71 (0.57)	159.00 (0.61)	109.11 (0.45)									
F5_$6	2.6514 (0.0179)	47.73 (0.40)	60.87 (0.50)	62.41 (0.40)	137.91 (0.60)								
F7_$9	2.6708 (0.0181)	46.31 (0.39)	60.09 (0.51)	128.47 (0.52)	117.99 (0.55)	92.71 (0.53)							
F8	2.6695 (0.0160)	145.17 (0.63)	92.77 (0.51)	65.84 (0.42)	68.26 (0.36)	127.52 (0.62)	113.24 (0.63)						
F12	2.7045 (0.0171)	38.59 (0.35)	91.95 (0.53)	126.56 (0.59)	104.92 (0.47)	64.62 (0.49)	59.85 (0.49)	167.58 (0.72)					
Sr4_$1	2.7891 (0.0129)	91.78 (0.46)	59.63 (0.43)	98.70 (0.37)	101.42 (0.42)	120.35 (0.50)	53.81 (0.36)	59.78 (0.40)					
F15_$1	2.8601 (0.0177)	113.06 (0.60)	110.60 (0.63)	133.10 (0.51)	54.77 (0.34)	160.77 (0.61)	68.73 (0.47)	67.42 (0.47)					
OW3	2.8760 (0.0191)	94.98 (0.52)	140.07 (0.65)	101.68 (0.55)	60.69 (0.39)	80.01 (0.53)	118.43 (0.57)	119.21 (0.58)					
F6	2.9738 (0.0177)	142.43 (0.65)	125.95 (0.62)	57.85 (0.35)	53.53 (0.34)	96.57 (0.54)	170.67 (0.61)	61.41 (0.46)					
	F3 -	V2	F4	Sr5	Sr1	F5_$6	F7_$9	F8					

F4 -	Distance	Angles											
V2	2.0498 (0.0113)												
Sr2_$2	2.4483 (0.0111)	146.98 (0.58)											
F3	2.4741 (0.0162)	50.81 (0.37)	160.78 (0.62)										
F7_$9	2.5814 (0.0184)	47.73 (0.41)	130.84 (0.65)	63.74 (0.51)									
F5_$6	2.6010 (0.0183)	48.40 (0.40)	120.16 (0.60)	62.93 (0.50)	96.00 (0.50)								
Sr4_$1	2.6309 (0.0139)	94.85 (0.48)	109.24 (0.47)	66.15 (0.43)	56.63 (0.40)	128.91 (0.51)							
F1	2.6492 (0.0183)	139.70 (0.62)	73.16 (0.42)	88.97 (0.55)	117.72 (0.69)	120.70 (0.70)	61.20 (0.46)						
F16	2.7534 (0.0168)	42.91 (0.33)	104.28 (0.47)	93.67 (0.49)	63.30 (0.48)	61.09 (0.47)	119.59 (0.57)	177.33 (0.63)					
Sr5	2.7960 (0.0142)	91.80 (0.47)	107.49 (0.47)	56.21 (0.41)	119.92 (0.51)	59.21 (0.40)	95.43 (0.37)	61.75 (0.46)					
F11_$12	2.9634 (0.0189)	134.38 (0.71)	55.03 (0.36)	122.04 (0.65)	87.20 (0.57)	174.99 (0.63)	56.10 (0.39)	60.56 (0.52)					
OW2_$17	2.9915 (0.0206)	89.87 (0.52)	62.49 (0.40)	124.53 (0.66)	121.20 (0.60)	61.61 (0.48)	168.23 (0.61)	120.35 (0.65)					
F9_$2	3.0153 (0.0185)	130.83 (0.68)	54.43 (0.35)	110.29 (0.62)	173.68 (0.59)	82.47 (0.54)	119.83 (0.45)	58.67 (0.51)					
	F4 -	V2	Sr2_$2	F3	F7_$9	F5_$6	Sr4_$1	F1					

F5 -	Distance	Angles											
V2_$3	1.9717 (0.0134)												
Sr3_$5	2.4746 (0.0129)	146.49 (0.62)											
F4_$3	2.6010 (0.0183)	51.03 (0.41)	161.84 (0.60)										
F3_$3	2.6514 (0.0179)	47.94 (0.40)	134.74 (0.58)	56.19 (0.44)									
Sr5_$3	2.6714 (0.0128)	97.39 (0.49)	108.01 (0.46)	64.04 (0.39)	56.00 (0.36)								

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F16_$3    2.7243 (0.0183)   43.49 (0.39) 124.33 (0.56)  62.22 (0.47)  90.48 (0.55) 126.14 (0.55)
F13_$1    2.7479 (0.0166)  124.30 (0.60)  58.94 (0.36) 119.96 (0.57)  80.16 (0.49)  57.41 (0.34) 164.79 (0.59)
F12_$3    2.8633 (0.0184)   35.24 (0.37) 112.14 (0.52)  85.87 (0.53)  58.59 (0.44) 114.22 (0.50)  58.93 (0.45) 105.86 (0.52)
OW2_$2    2.8835 (0.0193)   94.65 (0.58) 101.56 (0.53)  65.88 (0.50) 122.06 (0.62) 100.58 (0.49)  59.95 (0.47) 135.25 (0.61)
F10_$16   2.9035 (0.0190)  148.40 (0.65)  64.85 (0.40)  98.39 (0.54) 111.97 (0.56)  56.26 (0.36) 135.72 (0.56)  59.43 (0.41)
              F5 -          V2_$3         Sr3_$5        F4_$3         F3_$3         Sr5_$3        F16_$3        F13_$1

F6 -        Distance       Angles
V1_$10    1.9223 (0.0128)
Sr1       2.5184 (0.0125)  139.63 (0.58)
F2_$10    2.5730 (0.0176)   53.10 (0.42) 164.05 (0.58)
F13_$10   2.5708 (0.0164)   49.87 (0.39) 117.74 (0.53)  60.22 (0.44)
F18_$10   2.6859 (0.0174)   43.76 (0.40) 131.85 (0.53)  63.18 (0.47)  92.95 (0.54)
Sr5       2.6794 (0.0120)   98.16 (0.48) 104.80 (0.43)  59.89 (0.36)  59.42 (0.35) 123.06 (0.52)
OW1_$6    2.7827 (0.0188)  100.86 (0.58) 107.05 (0.53)  73.73 (0.49) 133.89 (0.63)  62.46 (0.49) 100.18 (0.48)
F17       2.7898 (0.0190)   36.88 (0.40) 102.88 (0.51)  89.75 (0.57)  60.53 (0.44)  59.24 (0.48) 119.95 (0.51) 120.59 (0.60)
F8        2.8935 (0.0179)  153.80 (0.62)  65.23 (0.38) 100.96 (0.51) 117.85 (0.52) 133.30 (0.57)  60.47 (0.33)  71.01 (0.47)
F3        2.9738 (0.0177)  126.53 (0.60)  54.74 (0.34) 111.25 (0.53)  77.30 (0.47) 170.23 (0.60)  52.15 (0.32) 125.03 (0.57)
OW3       3.0379 (0.0186)   87.54 (0.51)  58.65 (0.39) 122.90 (0.58)  62.77 (0.46) 117.99 (0.57)  93.59 (0.46) 162.60 (0.63)
              F6 -          V1_$10        Sr1           F2_$10        F13_$10       F18_$10       Sr5           OW1_$6

F7 -        Distance       Angles
V2_$10    1.9358 (0.0136)
Sr3_$4    2.4430 (0.0130)  137.59 (0.60)
Sr4_$6    2.4729 (0.0121)  103.12 (0.52) 119.22 (0.51)
F4_$10    2.5814 (0.0183)   51.59 (0.42) 148.65 (0.61)  62.69 (0.40)
F3_$10    2.6708 (0.0182)   47.64 (0.40) 155.18 (0.58)  65.54 (0.40)  56.17 (0.47)
F12_$10   2.6818 (0.0191)   38.95 (0.40) 107.94 (0.52) 126.05 (0.59)  90.15 (0.58)  60.70 (0.49)
F16_$10   2.8030 (0.0177)   41.81 (0.37) 105.23 (0.50) 123.67 (0.52)  61.35 (0.45)  88.41 (0.53)  60.17 (0.45)
F10_$6    2.8789 (0.0186)  145.57 (0.62)  65.60 (0.41)  60.16 (0.38)  95.16 (0.54) 125.64 (0.57) 173.44 (0.64) 119.36 (0.53)
OW2_$4    2.9908 (0.0206)  103.65 (0.59)  56.48 (0.41) 116.47 (0.53)  93.57 (0.55) 146.41 (0.62) 110.52 (0.58)  61.97 (0.48)
OW3_$6    3.0115 (0.0190)  104.41 (0.56)  57.45 (0.39) 120.07 (0.54) 152.34 (0.66)  98.37 (0.53)  65.68 (0.49) 112.23 (0.54)
              F7 -          V2_$10        Sr3_$4        Sr4_$6        F4_$10        F3_$10        F12_$10       F16_$10

F8 -        Distance       Angles
V3        1.9220 (0.0109)
F1        2.5730 (0.0175)   54.25 (0.42)
F11_$6    2.6800 (0.0190)   46.71 (0.42)  57.98 (0.54)
F3        2.6695 (0.0160)  140.56 (0.57)  86.48 (0.52) 112.39 (0.62)
F9_$9     2.7141 (0.0186)   45.50 (0.40)  58.01 (0.52)  89.50 (0.45) 119.66 (0.62)
Sr4_$1    2.7220 (0.0134)   96.35 (0.49)  60.94 (0.46) 118.92 (0.48)  62.29 (0.38)  58.01 (0.40)
O         2.7424 (0.0180)   34.95 (0.34)  89.19 (0.53)  62.54 (0.53) 174.68 (0.67)  60.07 (0.52) 118.00 (0.60)
Sr5       2.8124 (0.0136)   98.25 (0.49)  62.39 (0.46)  58.42 (0.41)  54.16 (0.37) 120.41 (0.46)  93.04 (0.32) 120.89 (0.60)
F6        2.8935 (0.0179)  127.23 (0.70) 117.91 (0.66)  83.16 (0.57)  64.48 (0.46) 172.60 (0.64) 126.74 (0.45) 115.18 (0.63)
Sr1       2.9340 (0.0104)  165.28 (0.53) 140.47 (0.54) 134.32 (0.63)  54.06 (0.32) 136.10 (0.62)  94.04 (0.36) 130.34 (0.48)
              F8 -          V3            F1            F11_$6        F3            F9_$9         Sr4_$1        O

F9 -        Distance       Angles
V3_$10    1.9358 (0.0139)
Sr2       2.5490 (0.0135)  136.59 (0.65)
F1_$10    2.5668 (0.0211)   54.29 (0.50) 166.62 (0.68)
Sr4_$6    2.6360 (0.0136)   98.82 (0.54) 105.25 (0.46)  62.20 (0.45)
Sr5_$7    2.6493 (0.0134)  102.20 (0.53) 109.06 (0.48)  70.46 (0.46)  98.66 (0.45)
F10_$15   2.6531 (0.0196)   47.16 (0.44) 132.15 (0.61)  59.86 (0.52) 121.99 (0.58)  59.63 (0.40)
F8_$10    2.7141 (0.0187)   45.08 (0.41) 121.47 (0.56)  58.24 (0.51)  61.15 (0.39) 128.61 (0.58)  90.14 (0.58)
O_$10     2.7311 (0.0209)   35.28 (0.43) 101.72 (0.56)  89.57 (0.65) 121.54 (0.58) 119.69 (0.56)  61.13 (0.52)  60.48 (0.49)
F1_$7     2.7934 (0.0213)  154.12 (0.74)  69.24 (0.47)  99.95 (0.44)  66.36 (0.43)  61.78 (0.41) 121.41 (0.63) 127.39 (0.64)
F4_$7     3.0153 (0.0185)  137.49 (0.64)  51.38 (0.34) 129.08 (0.62) 120.27 (0.51)  58.73 (0.35)  94.54 (0.54) 172.66 (0.61)
F2        3.0167 (0.0173)  133.04 (0.64)  52.25 (0.34) 115.43 (0.59)  53.24 (0.32) 117.40 (0.50) 174.75 (0.62)  88.90 (0.51)
              F9 -          V3_$10        Sr2           F1_$10        Sr4_$6        Sr5_$7        F10_$15       F8_$10

F10 -       Distance       Angles
V3_$11    1.9498 (0.0120)
F1_$11    2.6057 (0.0185)   53.42 (0.43)
Sr5_$8    2.6362 (0.0151)  102.25 (0.58)  70.08 (0.50)
F9_$15    2.6531 (0.0196)   46.72 (0.43)  58.42 (0.54)  60.11 (0.45)
Sr4       2.7051 (0.0151)  100.41 (0.57)  68.08 (0.49) 103.05 (0.41) 126.50 (0.55)
F11_$7    2.6989 (0.0195)   46.29 (0.44)  57.38 (0.55) 127.46 (0.54)  90.39 (0.48)  58.65 (0.44)
O_$11     2.7389 (0.0184)   35.19 (0.37)  88.60 (0.55) 119.88 (0.66)  60.84 (0.53) 120.21 (0.65)  62.35 (0.53)
F13_$3    2.8046 (0.0156)  155.98 (0.68) 104.35 (0.56)  57.08 (0.35) 116.79 (0.66)  75.39 (0.39) 133.93 (0.65) 163.11 (0.69)
F7_$3     2.8789 (0.0184)  130.29 (0.76) 120.47 (0.69) 122.54 (0.48) 177.01 (0.68)  52.46 (0.37)  86.77 (0.59) 116.82 (0.66)
F5_$13    2.9035 (0.0191)  124.74 (0.71) 126.03 (0.73)  57.42 (0.40)  83.79 (0.58) 132.55 (0.50) 168.43 (0.63) 106.10 (0.62)
Sr3_$6    2.9062 (0.0118)  149.13 (0.59) 157.42 (0.58)  97.32 (0.42) 132.23 (0.65)  98.11 (0.42) 131.64 (0.64) 113.97 (0.51)
              F10 -         V3_$11        F1_$11        Sr5_$8        F9_$15        Sr4           F11_$7        O_$11

F11 -       Distance       Angles
V3_$3     1.9526 (0.0142)
Sr2_$1    2.5416 (0.0137)  138.17 (0.69)
F1_$3     2.5478 (0.0216)   54.57 (0.51) 166.59 (0.72)
Sr4_$2    2.6469 (0.0143)  102.33 (0.56) 105.94 (0.48)  69.82 (0.47)
F8_$3     2.6800 (0.0189)   45.77 (0.41) 124.38 (0.61)  58.90 (0.51) 128.69 (0.59)
Sr5_$3    2.6828 (0.0142)  101.81 (0.55) 104.28 (0.48)  64.59 (0.47)  97.55 (0.46)  63.26 (0.40)
F10_$2    2.6989 (0.0195)   46.20 (0.43) 130.50 (0.62)  59.47 (0.52)  60.79 (0.41)  89.90 (0.57) 123.96 (0.58)
O_$3      2.8151 (0.0215)   33.54 (0.42) 104.75 (0.57)  88.11 (0.63) 119.53 (0.58)  59.82 (0.49) 123.01 (0.59)  59.52 (0.49)
F1_$12    2.8430 (0.0212)  153.16 (0.75)  68.53 (0.46)  99.12 (0.46)  58.50 (0.40) 129.19 (0.65)  65.93 (0.43) 119.29 (0.63)
F4_$12    2.9634 (0.0189)  133.42 (0.68)  52.13 (0.35) 125.41 (0.66)  55.59 (0.36) 175.08 (0.65) 120.04 (0.54)  90.80 (0.56)
OW1       3.0582 (0.0194)   89.92 (0.57)  56.55 (0.39) 128.71 (0.66) 161.37 (0.61)  69.80 (0.48)  93.53 (0.49) 123.64 (0.62)
              F11 -         V3_$3         Sr2_$1        F1_$3         Sr4_$2        F8_$3         Sr5_$3        F10_$2

F12 -       Distance       Angles
V2        1.6924 (0.0125)
Sr1_$1    2.6185 (0.0133)  142.37 (0.76)
F7_$9     2.6818 (0.0189)   45.97 (0.45) 106.57 (0.61)
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F3        2.7045 (0.0171)   46.81 (0.40) 151.56 (0.66)  59.45 (0.46)
F16       2.7512 (0.0169)   42.02 (0.38) 106.81 (0.53)  62.10 (0.47)  88.81 (0.49)
F5_$6     2.8633 (0.0185)   42.24 (0.45) 151.55 (0.59)  87.92 (0.48)  56.79 (0.46)  58.01 (0.45)
OW3       2.8832 (0.0201)  101.80 (0.65) 115.28 (0.52) 117.81 (0.59)  61.86 (0.48) 134.44 (0.67)  76.50 (0.53)
OW1       2.9045 (0.0192)  106.00 (0.62)  57.90 (0.38) 115.76 (0.60) 149.18 (0.64)  65.34 (0.45)  93.85 (0.55) 124.95 (0.66)
OW3_$1    3.0999 (0.0219)  108.02 (0.72)  56.94 (0.40)  62.29 (0.50)  95.54 (0.57) 111.08 (0.64) 148.03 (0.61) 106.09 (0.54)
              F12 -          V2            Sr1_$1        F7_$9         F3            F16           F5_$6         OW3

F13 -       Distance       Angles
V1        1.9833 (0.0112)
F6_$9     2.5708 (0.0164)   47.82 (0.38)
Sr3_$4    2.5802 (0.0109)  151.97 (0.57) 157.85 (0.58)
F2        2.5803 (0.0150)   52.60 (0.35)  59.93 (0.46) 134.33 (0.51)
Sr5_$9    2.6038 (0.0109)   99.04 (0.43)  62.37 (0.37) 106.92 (0.38)  60.80 (0.38)
F17_$9    2.7085 (0.0171)   38.82 (0.35)  63.74 (0.49) 123.72 (0.51)  91.42 (0.50) 126.10 (0.54)
F5_$1     2.7479 (0.0167)  152.23 (0.61) 104.42 (0.55)  55.24 (0.34) 118.13 (0.53)  59.82 (0.35) 138.24 (0.61)
F15_$6    2.7482 (0.0169)   44.53 (0.36)  90.72 (0.51) 111.22 (0.48)  58.04 (0.45) 118.62 (0.47)  60.92 (0.49) 159.61 (0.56)
F10_$6    2.8046 (0.0156)  123.63 (0.54) 116.27 (0.54)  65.17 (0.35)  72.51 (0.42)  58.20 (0.38) 158.70 (0.65)  63.05 (0.46)
OW3_$9    2.9479 (0.0185)   89.01 (0.48)  66.39 (0.46)  97.83 (0.45) 126.23 (0.57)  97.32 (0.47)  61.21 (0.51)  77.21 (0.48)
OW3_$6    3.0042 (0.0184)   98.23 (0.50) 130.88 (0.56)  56.48 (0.36) 133.24 (0.62) 162.66 (0.53)  68.49 (0.49) 103.32 (0.51)
              F13 -          V1            F6_$9         Sr3_$4        F2            Sr5_$9        F17_$9        F5_$1

F14 -       Distance       Angles
Sr2       2.3701 (0.0120)
Sr3_$6    2.4068 (0.0121)  120.67 (0.48)
Sr1       2.4394 (0.0119)  113.80 (0.50) 119.54 (0.48)
OW3       2.9455 (0.0194)  154.02 (0.58)  58.78 (0.39)  60.77 (0.39)
OW2_$6    2.9699 (0.0191)   63.60 (0.42)  57.08 (0.39) 154.25 (0.58) 109.33 (0.54)
OW1_$1    3.0757 (0.0190)   57.50 (0.38) 149.55 (0.56)  56.87 (0.37) 108.47 (0.54) 111.46 (0.56)
              F14 -          Sr2           Sr3_$6        Sr1           OW3           OW2_$6

F15 -       Distance       Angles
V1_$3     1.9276 (0.0131)
Sr4       2.5165 (0.0115)  108.29 (0.51)
Sr1_$1    2.5065 (0.0122)  138.72 (0.56) 111.03 (0.45)
F2_$3     2.5890 (0.0167)   52.74 (0.39)  60.05 (0.37) 147.37 (0.57)
F13_$3    2.7482 (0.0168)   46.19 (0.36)  79.47 (0.39) 154.89 (0.54)  57.73 (0.41)
F18_$3    2.7537 (0.0178)   42.34 (0.38) 118.07 (0.52) 105.59 (0.49)  62.03 (0.44)  87.72 (0.50)
F17_$8    2.7663 (0.0192)   37.43 (0.39) 137.83 (0.57) 109.75 (0.51)  89.94 (0.55)  58.83 (0.45)  58.75 (0.47)
F3_$1     2.8601 (0.0177)  162.21 (0.62)  62.11 (0.35)  56.45 (0.35) 121.89 (0.54) 116.02 (0.51) 154.66 (0.59) 140.30 (0.59)
              F15 -          V1_$3         Sr4           Sr1_$1        F2_$3         F13_$3        F18_$3        F17_$8

F16 -       Distance       Angles
V2        1.8749 (0.0123)
Sr2_$1    2.4642 (0.0120)  134.96 (0.59)
F5_$6     2.7243 (0.0183)   46.36 (0.40) 149.72 (0.57)
F4        2.7534 (0.0168)   48.10 (0.36) 152.63 (0.63)  56.69 (0.48)
F12       2.7512 (0.0169)   37.17 (0.35) 102.15 (0.48)  63.05 (0.48)  85.23 (0.49)
F7_$9     2.8030 (0.0177)   43.50 (0.40) 106.34 (0.52)  88.32 (0.50)  55.36 (0.44)  57.73 (0.47)
OW2_$17   2.8053 (0.0200)   99.52 (0.58) 125.27 (0.56)  62.84 (0.49)  65.11 (0.50) 125.89 (0.65) 120.10 (0.57)
OW2_$16   2.9871 (0.0207)  105.46 (0.59)  62.41 (0.41) 145.46 (0.61)  90.23 (0.55) 108.69 (0.61)  62.10 (0.48) 115.18 (0.52)
OW1       3.0555 (0.0179)   95.80 (0.51)  57.17 (0.35)  93.42 (0.51) 142.78 (0.57)  59.75 (0.43) 107.69 (0.51) 124.18 (0.60)
              F16 -          V2            Sr2_$1        F5_$6         F4            F12           F7_$9         OW2_$17

F17 -       Distance       Angles
V1_$10    1.7026 (0.0132)
Sr3_$6    2.5348 (0.0145)  151.51 (0.97)
F18_$10   2.7078 (0.0189)   42.67 (0.42) 136.18 (0.66)
F13_$10   2.7085 (0.0170)   46.90 (0.41) 119.42 (0.63)  89.47 (0.52)
F15_$8    2.7663 (0.0192)   43.47 (0.49) 161.69 (0.69)  60.39 (0.48)  60.25 (0.46)
F6        2.7898 (0.0191)   42.65 (0.46) 109.23 (0.68)  58.47 (0.46)  55.73 (0.43)  85.92 (0.49)
OW3       2.8871 (0.0226)   96.94 (0.71)  58.53 (0.46) 122.64 (0.70)  63.49 (0.50) 123.66 (0.61)  64.68 (0.53)
O_$10     3.1136 (0.0183)  132.26 (0.69)  57.11 (0.40)  89.73 (0.52) 172.27 (0.83) 125.51 (0.69) 117.69 (0.65) 110.78 (0.68)
              F17 -          V1_$10        Sr3_$6        F18_$10       F13_$10       F15_$8        F6            OW3

F18 -       Distance       Angles
V1        1.8577 (0.0134)
Sr1       2.4379 (0.0132)  161.06 (0.72)
F6_$9     2.6859 (0.0175)   45.70 (0.41) 116.09 (0.56)
F17_$9    2.7077 (0.0189)   38.40 (0.38) 146.97 (0.62)  62.29 (0.51)
F2        2.7564 (0.0160)   49.33 (0.38) 119.91 (0.54)  56.41 (0.46)  87.74 (0.51)
F15_$6    2.7537 (0.0178)   44.33 (0.41) 148.64 (0.62)  88.22 (0.52)  60.86 (0.50)  56.05 (0.43)
OW1_$1    2.8366 (0.0201)  100.70 (0.61)  60.65 (0.41)  60.44 (0.48) 121.60 (0.68)  70.21 (0.50) 126.26 (0.59)
OW1_$6    2.9580 (0.0195)   94.24 (0.59) 104.06 (0.53) 130.52 (0.62)  68.26 (0.55) 124.66 (0.63)  68.80 (0.49) 164.12 (0.51)
              F18 -          V1            Sr1           F6_$9         F17_$9        F2            F15_$6        OW1_$1

OW1 -       Distance       Angles
Sr1_$1    2.6852 (0.0143)
Sr2_$1    2.6915 (0.0142)   97.07 (0.46)
F6_$3     2.7827 (0.0188)  105.38 (0.54)  97.90 (0.52)
F18_$1    2.8366 (0.0200)   52.31 (0.38)  84.81 (0.50)  57.10 (0.45)
F12       2.9045 (0.0192)   55.70 (0.39)  92.99 (0.51) 159.40 (0.65) 106.95 (0.60)
F18_$3    2.9580 (0.0194)   95.84 (0.49) 161.06 (0.65)  65.22 (0.48)  92.22 (0.41) 105.74 (0.60)
F11       3.0582 (0.0194)  148.78 (0.60)  51.99 (0.35)  78.51 (0.51) 112.81 (0.59) 121.71 (0.60) 113.24 (0.60)
F16       3.0555 (0.0179)   97.17 (0.49)  50.29 (0.33) 143.44 (0.62) 124.43 (0.62)  54.91 (0.42) 141.03 (0.63)  67.61 (0.45)
F14_$1    3.0757 (0.0190)   49.54 (0.33)  47.96 (0.32) 112.86 (0.59)  63.13 (0.46)  62.97 (0.47) 144.81 (0.62)  99.92 (0.52)
O_$3      3.1605 (0.0218)  145.21 (0.62)  92.67 (0.49) 106.22 (0.57) 162.37 (0.65)  90.60 (0.56)  84.50 (0.55)  53.80 (0.44)
              OW1 -          Sr1_$1        Sr2_$1        F6_$3         F18_$1        F12           F18_$3        F11

OW2 -       Distance       Angles
Sr3       2.6160 (0.0157)
F16_$11   2.8053 (0.0199)  142.05 (0.68)
Sr2_$3    2.8596 (0.0156)   98.49 (0.48)  93.05 (0.54)
```

```
F5_$7     2.8835 (0.0193)  152.54 (0.72)  57.21 (0.47)  99.30 (0.54)
O_$1      2.9658 (0.0227)   58.57 (0.43) 158.07 (0.72)  89.36 (0.52) 100.89 (0.62)
F14_$3    2.9699 (0.0191)   50.56 (0.36) 128.86 (0.68)  47.93 (0.33) 142.73 (0.66)  66.95 (0.50)
F16_$13   2.9871 (0.0206)   96.08 (0.52)  64.82 (0.52)  49.80 (0.35) 111.37 (0.63) 130.29 (0.64)  64.40 (0.45)
F4_$11    2.9915 (0.0205)  147.76 (0.63)  56.61 (0.45)  49.41 (0.34)  52.52 (0.44) 110.92 (0.62)  97.31 (0.55)  66.72 (0.48)
F7_$14    2.9908 (0.0205)   51.13 (0.37)  92.59 (0.57)  92.32 (0.51) 147.90 (0.68) 109.11 (0.61)  63.44 (0.45)  55.93 (0.43)
              OW2 -          Sr3           F16_$11       Sr2_$3        F5_$7         O_$1          F14_$3        F16_$13

OW3 -       Distance       Angles
Sr3_$6    2.6684 (0.0152)
Sr1       2.7585 (0.0152)  100.97 (0.49)
F12       2.8832 (0.0201)  144.77 (0.61)  95.39 (0.55)
F3        2.8760 (0.0191)  153.65 (0.64)  53.93 (0.37)  56.02 (0.45)
F17       2.8871 (0.0226)   54.12 (0.39)  94.73 (0.52) 154.92 (0.71) 114.29 (0.60)
F14       2.9455 (0.0193)   50.48 (0.35)  50.51 (0.34) 135.05 (0.67) 104.10 (0.56)  67.45 (0.51)
F13_$10   2.9479 (0.0186)  107.37 (0.56)  99.48 (0.50) 100.33 (0.56)  73.30 (0.48)  55.30 (0.45) 112.22 (0.57)
F7_$3     3.0115 (0.0189)   50.51 (0.35)  94.75 (0.51)  97.48 (0.57) 130.51 (0.66) 104.49 (0.58)  63.47 (0.44) 155.98 (0.66)
F13_$3    3.0042 (0.0182)   53.71 (0.35) 152.62 (0.62) 101.49 (0.54) 152.48 (0.65)  78.89 (0.52) 103.30 (0.54)  98.52 (0.53)
F6        3.0379 (0.0186)   98.93 (0.52)  51.23 (0.35) 115.53 (0.58)  60.30 (0.43)  56.11 (0.44)  69.03 (0.45)  50.84 (0.40)
F12_$1    3.0999 (0.0219)   91.62 (0.50)  52.71 (0.36)  73.91 (0.54)  79.22 (0.53) 129.68 (0.65)  62.23 (0.45) 149.62 (0.63)
              OW3 -          Sr3_$6        Sr1           F12           F3            F17           F14           F13_$10


FMAP and GRID set by program

FMAP   2   1  31
GRID    -1.786  -2  -1     1.786   2   1

R1 =  0.0465 for   1513 unique reflections after merging for Fourier


Electron density synthesis with coefficients Fo-Fc

Highest peak    2.61  at -0.0029  0.3436  0.2492  [  0.59 A from F1 ]
Deepest hole   -1.38  at  0.0167  0.2798  0.2399  [  1.16 A from F1 ]

Mean =    0.00,   Rms deviation from mean =    0.28 e/A^3,   Highest memory used =  7803 / 33255


Fourier peaks appended to .res file

             x       y       z       sof     U      Peak   Distances to nearest atoms (including symmetry equivalents)

Q1    1   0.9971  0.1564  0.7492   1.00000  0.05    2.61   0.59 F1  2.17 F11  2.23 V3  2.36 F9
Q2    1   0.6686  0.1585  0.5854   1.00000  0.05    2.17   0.64 F3  1.98 V2  2.29 OW3  2.39 F5
Q3    1   0.3322  0.1553  0.9131   1.00000  0.05    1.95   1.04 F13  2.01 F15  2.08 V1  2.25 F7
Q4    1   0.9159 -0.0893  0.5765   1.00000  0.05    1.45   1.48 F4  1.64 F7  2.19 V2  2.40 SR4
Q5    1   0.5063  0.3489  0.5096   1.00000  0.05    1.39   0.81 OW3  2.51 F17  2.56 F13  2.60 F13
Q6    1   0.6808 -0.0896  0.7679   1.00000  0.05    1.36   1.79 F8  2.40 F15  2.65 F9  2.75 F14
Q7    1   0.6822  0.4145  0.7367   1.00000  0.05    1.31   1.24 F6  1.77 F2  1.96 OW1  2.16 V1
Q8    1   0.1485  0.0721  0.8122   1.00000  0.05    1.18   1.43 F2  1.82 F10  1.91 F1  1.98 SR5
Q9    1   0.0756  0.5824  0.4088   1.00000  0.05    1.16   1.46 F10  1.77 F5  2.22 SR5  2.24 F9
Q10   1  -0.0163  0.0859  0.0600   1.00000  0.05    1.15   1.54 OW2  2.04 F10  2.16 F5  2.40 O
Q11   1   0.9939  0.0373  0.7502   1.00000  0.05    1.13   0.41 F1  2.13 V3  2.26 F9  2.48 SR4
Q12   1   0.7257  0.0194  0.4736   1.00000  0.05    1.13   1.08 V2  1.20 F12  1.68 F16  1.98 F7
Q13   1   0.4931  0.1602  0.4886   1.00000  0.05    1.09   1.32 OW3  1.81 F12  2.60 F12  2.68 F15
Q14   1   0.1598  0.4134  0.9874   1.00000  0.05    1.09   1.27 F7  1.63 F16  1.63 V2  2.27 F4
Q15   1   0.8655 -0.0181  0.8440   1.00000  0.05    1.09   1.01 V3  1.29 O  1.47 F9  2.16 F8
Q16   1   0.3535 -0.1425  0.9363   1.00000  0.05    1.06   1.51 F13  1.89 OW3  2.01 F5  2.24 F3
Q17   1   0.4308  0.1598  0.4602   1.00000  0.05    1.01   1.67 OW3  2.12 F15  2.25 F12  2.25 F7
Q18   1   0.8394  0.1455  0.5885   1.00000  0.05    1.00   1.07 F4  1.43 V2  1.69 F3  1.75 F5
Q19   1   0.1591 -0.0820  0.6603   1.00000  0.05    1.00   1.39 SR2  1.42 F11  2.03 OW1  2.41 F16
Q20   1   0.4437  0.0964  0.5968   1.00000  0.05    1.00   1.05 SR1  1.85 F12  1.97 F14  2.12 OW3

Shortest distances between peaks (including symmetry equivalents)

    13  17  0.76      1  11  0.98      9  10  1.03      4  14  1.31     12  14  1.56      5  13  1.60      5  16  1.64
     2  16  1.69      8  11  1.84      5  17  1.90      2  18  1.91      1   8  1.93      3  17  1.95      4  18  2.15
    12  20  2.23     10  15  2.23      6  15  2.27      7  19  2.30      3   5  2.32      2  13  2.33      9  15  2.40
     9  18  2.42     14  18  2.43     13  20  2.44      3  16  2.48      3  13  2.50      5   5  2.50     12  18  2.50
    13  16  2.52      3   8  2.53      2   5  2.54      8   9  2.63      2  20  2.65      4  12  2.66     13  13  2.66
     7   8  2.70     11  15  2.71     16  18  2.71     17  20  2.74      2  12  2.74      4  19  2.76     13  17  2.85
     2  17  2.88     10  18  2.89     12  17  2.89     10  10  2.89      5  20  2.92     13  20  2.92     17  20  2.94
    12  13  2.95


Time profile in seconds
-----------------------

     5.84: Read and process instructions
     0.00: Fit rigid groups
     0.00: Interpret restraints etc.
     0.02: Generate connectivity array
     0.24: Analyse DFIX/DANG restraints
     0.00: Analyse SAME/SADI restraints
     0.00: Generate CHIV restraints
     0.00: Check if bonds in residues restrained
     0.00: Generate DELU restraints
     0.00: Generate SIMU restraints
     0.00: Generate ISOR restraints
     0.00: Generate NCSY restraints
     0.00: Analyse other restraints etc.
     0.60: Read intensity data, sort/merge etc.
```

```
      0.00: Set up constraints
      0.00: OSF, H-atoms from difference map
      0.08: Set up l.s. refinement
      0.01: Generate idealized H-atoms
      2.81: Structure factors and derivatives
      6.99: Sum l.s. matrices
      0.00: Generate and apply antibumping restraints
      0.04: Apply other restraints
      0.44: Solve l.s. equations
      0.00: Generate HTAB table
      0.27: Other dependent quantities, CIF, tables
      0.44: Analysis of variance
      0.04: Merge reflections for Fourier and .fcf
      0.29: Fourier summations
      0.24: Peaksearch
      0.02: Analyse peaklist

 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 +  sv108b            finished at 19:06:31   Total CPU time:      18.4 secs  +
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

Solving the structure

From the simulated powder data, several tests have shown that solving the structure was relatively easy by either direct methods with SHELXS or by using the ESPOIR pseudo-direct space program in "scratch" mode (atoms moving independently). The "|Fobs|" were extracted by the Le Bail method with the FULLPROF program. From a total of > 7700 reflections, only the first low diffracting angle 2000 reflections were used (for solving, a limitation to a 1 Å resolution is recommended...). Several tests were performed with SHELXS by using either these 2000 hkl or reduced sets (produced by applying the OVERLAP program) eliminating reflections having a neighbouring one at less than 0.005 and 0.01°(2θ).

SHELXS tests

2000 hkl dataset :

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+  SHELXS-97 - CRYSTAL STRUCTURE SOLUTION - MSDOS 32-BIT VERSION  +
+  Copyright(C) George M. Sheldrick 1986-97         Release 97-1  +
+  i0                          started at 12:56:13 on 24-Aug-2002  +
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

TITL Sr5V3X22   P21/c
CELL 0.79764  11.243328   8.195712  19.949343  90.0 106.728287  90.0
LATT 1
SYMM  X,.5-Y,.5+Z
SFAC SR V F
UNIT 20 12 88

V =     1760.48     At vol =    14.7     F(000) =    1828.0     mu =  16.75 mm-1

Max single Patterson vector =  34.1    cell wt =   4035.68    rho =  3.807

TREF 200
HKLF 4


   2000  Reflections read, of which     0  rejected

   Maximum h, k, l and 2-Theta =   11.    8.   20.   48.30

   2000  Unique reflections, of which   1996  observed

   R(int) = 0.0000     R(sigma) = 0.0100      Friedel opposites merged


NUMBER OF UNIQUE DATA AS A FUNCTION OF RESOLUTION IN ANGSTROMS

Resolution  Inf    5.00    3.50    2.50    2.00    1.70    1.50    1.40    1.30    1.20    1.10    1.00    0.90

N(observed)      14.     27.     76.    108.    149.    173.    119.    172.    228.    319.    453.    158.

N(measured)      14.     27.     77.    108.    149.    175.    119.    172.    228.    320.    453.    158.

N(theory)        14.     27.     77.    108.    149.    175.    119.    172.    228.    320.    453.    684.
```

Two-theta 0.0 9.2 13.1 18.4 23.0 27.1 30.8 33.1 35.7 38.8 42.5 47.0 52.6

Highest memory for sort/merge = 4468 / 10000

Observed E .GT. 1.200 1.300 1.400 1.500 1.600 1.700 1.800 1.900 2.000 2.100

Number	519	412	328	245	195	152	122	95	69	47

	Centric	Acentric	0kl	h0l	hk0	Rest
Mean Abs(E*E-1)	0.968	0.736	0.850	0.798	0.781	0.758

0.3 seconds elapsed time

SUMMARY OF PARAMETERS FOR Sr5V3X22 P21/c

```
ESEL  Emin  1.200    Emax  5.000    DelU 0.005    renorm 0.700    axis 0
OMIT  s  4.00    2theta(lim)  180.0
INIT  nn   12    nf   16    s+  0.800    s-  0.200    wr  0.200
PHAN  steps   10   cool 0.900   Boltz 0.400   ns  170   mtpr   40   mnqr  10
TREF  np      200.    nE   280    kapscal  0.900    ntan   2    wn -0.950
FMAP  code  8
PLAN  npeaks   -35    del1 0.500    del2 1.500
MORE  verbosity  1
TIME  t    9999999.
```

170 Reflections and 1418. unique TPR for phase annealing

280 Phases refined using 4885. unique TPR
449 Reflections and 9779. unique TPR for R(alpha)

0.8 seconds elapsed time

1501 Unique negative quartets found, 1501 used for phase refinement

0.9 seconds elapsed time

Highest memory used to derive phase relations = 3500 / 28347

ONE-PHASE SEMINVARIANTS

h	k	l	E	P+	Phi
0	0	6	3.035	0.47	
-4	0	8	2.899	0.99	
2	6	2	2.704	0.41	
4	0	4	2.550	1.00	
-2	6	10	2.662	0.40	
-2	6	4	2.128	0.42	
-4	0	2	2.034	0.61	
2	2	2	2.040	0.43	
-2	2	4	1.975	0.44	
-6	0	10	2.043	0.59	
-4	4	8	2.454	0.74	
0	4	0	1.792	0.00	
0	6	8	2.461	0.41	
0	4	6	2.131	0.44	
-2	0	18	2.476	0.28	
-8	0	4	1.957	0.97	
2	6	8	1.840	0.45	
4	0	6	1.863	0.27	
-2	0	4	1.587	0.79	
2	0	2	1.609	0.29	
4	4	4	1.981	0.72	
0	6	0	1.975	0.00	
0	0	14	1.672	0.20	
-6	2	18	1.942	0.71	
-6	6	6	1.484	0.48	
0	0	12	1.429	0.99	
6	0	4	1.331	0.21	
-2	2	10	1.269	0.55	
-6	0	2	1.360	0.21	
-4	2	2	1.432	0.46	
-6	0	4	1.277	0.67	
-4	4	2	1.477	0.45	
-4	0	16	1.297	0.33	
-4	6	2	1.302	0.46	
4	4	6	1.746	0.60	
2	6	6	1.475	0.45	

```
 -6   4  10   1.432   0.45
 -2   0  16   1.416   0.63
  2   2  14   1.458   0.45

Expected value of Sigma-1 = 0.883


Following phases held constant with unit weights for the initial 4 weighted
tangent cycles (before phase annealing):

  h   k   l     E     Phase/Comment

 -4   0   8   2.899     0    sigma-1 = 0.994
  4   0   4   2.550     0    sigma-1 = 0.998
  2   2   1   2.306   random phase
 -1   2   3   2.600   random phase
 -2   2   3   2.395   random phase
  1   2   3   2.350   random phase
  0   2   7   2.716   random phase
  0   4   0   1.792   180    sigma-1 = 0.000
 -8   0   4   1.957     0    sigma-1 = 0.965
  3   3   2   2.010   random phase
  4   0   6   1.863   random phase
  2   0   2   1.609   random phase
 -3   1   8   1.744   random phase
  0   6   0   1.975   180    sigma-1 = 0.000
  2   3   4   1.496   random phase
  1   3   6   1.592   random phase
 -2   2   7   1.629   random phase

All other phases random with initial weights of 0.200 replaced by 0.2*alpha
(or 1 if less) during first 4 cycles - unit weights for all phases thereafter


    185 Unique NQR employed in phase annealing


    100 Parallel refinements,  highest memory =    5280 /   64833

      0.1 seconds elapsed time

STRUCTURE SOLUTION for  Sr5V3X22   P21/c


Phase annealing cycle:     1   Beta =  0.07968
Ralpha 0.134 0.073 0.235 0.148 0.043 0.217 0.102 0.148 0.531 0.439 0.045 0.047 0.433 0.166 0.589 0.045 0.313 0.068 0.044 0.220
Nqual -0.087 0.048 0.044-0.288-0.809-0.405 0.478-0.594-0.013-0.029-0.781-0.919-0.205 0.055 0.192-0.919 0.395-0.923-0.808-0.260
Mabs   0.894 1.028 0.788 0.843 1.064 0.787 0.953 0.856 0.615 0.652 1.091 1.132 0.649 0.842 0.598 1.093 0.720 1.074 1.080 0.768

Phase annealing cycle:     2   Beta =  0.08853
Ralpha 0.092 0.074 0.098 0.111 0.052 0.094 0.094 0.118 0.539 0.312 0.053 0.052 0.383 0.126 0.534 0.051 0.239 0.052 0.051 0.099
Nqual -0.238 0.149-0.523-0.686-0.951-0.729 0.077-0.649-0.558 0.087-0.954-0.951-0.274-0.512-0.401-0.953 0.324-0.950-0.950-0.362
Mabs   0.994 1.100 0.975 0.936 1.152 0.955 1.013 0.921 0.614 0.719 1.151 1.152 0.682 0.930 0.616 1.152 0.793 1.134 1.148 0.953

Phase annealing cycle:     3   Beta =  0.09837
Ralpha 0.090 0.073 0.087 0.114 0.052 0.090 0.090 0.117 0.458 0.255 0.052 0.053 0.353 0.110 0.484 0.052 0.222 0.052 0.051 0.101
Nqual -0.331 0.089-0.215-0.654-0.951-0.758 0.292-0.641-0.567-0.039-0.953-0.954-0.313-0.506-0.397-0.954 0.207-0.953-0.951-0.426
Mabs   1.002 1.093 1.007 0.931 1.152 0.989 1.026 0.932 0.648 0.761 1.149 1.151 0.691 0.942 0.632 1.148 0.800 1.149 1.155 0.955

Phase annealing cycle:     4   Beta =  0.10930
Ralpha 0.088 0.075 0.088 0.119 0.052 0.085 0.081 0.124 0.465 0.197 0.052 0.051 0.356 0.112 0.431 0.051 0.215 0.052 0.051 0.101
Nqual -0.237-0.119-0.164-0.637-0.950-0.755 0.126-0.630-0.565-0.261-0.950-0.952-0.298-0.451-0.126-0.953 0.267-0.950-0.949-0.648
Mabs   1.007 1.089 1.010 0.945 1.150 0.996 1.039 0.915 0.647 0.814 1.150 1.145 0.692 0.946 0.653 1.152 0.809 1.150 1.146 0.964

Phase annealing cycle:     5   Beta =  0.12144
Ralpha 0.088 0.070 0.089 0.096 0.052 0.086 0.064 0.117 0.438 0.172 0.052 0.050 0.344 0.111 0.471 0.052 0.222 0.052 0.050 0.092
Nqual -0.165-0.015-0.257-0.417-0.951-0.762 0.388-0.687-0.529-0.176-0.951-0.950-0.451-0.393-0.385-0.951 0.291-0.951-0.950-0.633
Mabs   1.010 1.098 1.006 0.997 1.152 0.996 1.106 0.926 0.662 0.830 1.152 1.151 0.698 0.947 0.640 1.152 0.807 1.152 1.151 0.974

Phase annealing cycle:     6   Beta =  0.13494
Ralpha 0.089 0.071 0.088 0.083 0.053 0.085 0.065 0.118 0.449 0.122 0.051 0.051 0.336 0.115 0.449 0.052 0.218 0.052 0.051 0.097
Nqual -0.238 0.052-0.224-0.361-0.950-0.729 0.601-0.649-0.648-0.234-0.950-0.951-0.463-0.584-0.539-0.951 0.243-0.950-0.951-0.554
Mabs   1.007 1.093 1.008 1.037 1.150 0.996 1.147 0.927 0.654 0.902 1.148 1.155 0.710 0.943 0.644 1.152 0.812 1.150 1.155 0.980

Phase annealing cycle:     7   Beta =  0.14993
Ralpha 0.089 0.073 0.089 0.070 0.052 0.086 0.065 0.126 0.427 0.115 0.051 0.051 0.263 0.109 0.435 0.051 0.213 0.051 0.052 0.094
Nqual -0.244-0.017-0.262-0.095-0.950-0.769 0.754-0.683-0.656-0.398-0.951-0.950-0.472-0.540-0.542-0.950 0.251-0.950-0.950-0.662
Mabs   1.006 1.103 1.005 1.094 1.150 0.995 1.146 0.920 0.666 0.950 1.155 1.148 0.747 0.947 0.651 1.148 0.810 1.148 1.150 0.977

Phase annealing cycle:     8   Beta =  0.16659
Ralpha 0.089 0.073 0.089 0.071 0.051 0.086 0.064 0.124 0.192 0.105 0.052 0.051 0.260 0.110 0.425 0.051 0.211 0.050 0.051 0.096
Nqual -0.256 0.137-0.263 0.044-0.950-0.769 0.581-0.612-0.311-0.321-0.950-0.951-0.406-0.532-0.550-0.951 0.113-0.950-0.950-0.643
Mabs   1.006 1.100 1.006 1.105 1.148 0.995 1.146 0.928 0.814 0.965 1.150 1.155 0.753 0.945 0.654 1.155 0.807 1.151 1.148 0.978

Phase annealing cycle:     9   Beta =  0.18510
Ralpha 0.089 0.072 0.089 0.072 0.050 0.088 0.066 0.119 0.077 0.105 0.052 0.051 0.202 0.108 0.392 0.051 0.214 0.051 0.051 0.087
Nqual -0.239 0.022-0.238 0.099-0.950-0.768 0.724-0.650 0.019-0.327-0.951-0.950-0.255-0.492-0.324-0.950 0.130-0.951-0.951-0.577
Mabs   1.006 1.097 1.007 1.107 1.151 0.992 1.147 0.928 1.085 0.967 1.152 1.148 0.806 0.948 0.670 1.148 0.805 1.155 1.155 0.984

Phase annealing cycle:    10   Beta =  0.20566
Ralpha 0.088 0.071 0.089 0.070 0.051 0.087 0.064 0.124 0.081 0.102 0.052 0.051 0.160 0.110 0.401 0.051 0.221 0.052 0.052 0.097
Nqual -0.224 0.044-0.245 0.100-0.951-0.792 0.714-0.704 0.054-0.236-0.950-0.951-0.044-0.491-0.408-0.951 0.111-0.951-0.951-0.607
Mabs   1.008 1.096 1.006 1.104 1.155 0.994 1.151 0.918 1.090 0.976 1.150 1.155 0.851 0.947 0.664 1.155 0.801 1.152 1.152 0.982
```

Phase refinement cycle: 1

Ralpha 0.450 0.317 0.447 0.290 0.236 0.503 0.257 0.699 0.307 0.422 0.236 0.238 0.541 0.616 2.115 0.236 0.991 0.236 0.236 0.533

Nqual -0.205 0.002-0.201 0.168-0.945-0.726 0.702-0.525 0.205 0.148-0.945-0.945 0.094-0.412-0.311-0.945 0.291-0.945-0.945-0.476

Mabs 0.628 0.683 0.629 0.699 0.710 0.605 0.713 0.554 0.689 0.637 0.710 0.710 0.597 0.577 0.389 0.710 0.503 0.710 0.710 0.596

Try	Ralpha	Nqual	Sigma-1	M(abs)	CFOM	Seminvariants
1740051.	0.140	-0.292	0.797	0.959	0.573	-+-+- +-+-+ ---++ ++---+ ---+- ++++- -+-++ +--+
311647.	0.117	0.089	0.805	1.081	1.197	+++++ ++--+ --+-+ +++-- -----+ +---+ +-+-+ ----
1558235.	0.140	-0.292	0.797	0.959	0.573	-+-+- +-+-+ ---++ ++---+ ---+- ++++- -+-++ +--+
1499719.	0.115	0.316	0.826	1.105	1.718	+++++ ++--+ --+-+ ++--- -----+ +---+ +-+-+ ----
1207139.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
1841391.	0.160	-0.801	0.812	0.882	0.182	-+-+- +-+-- --++- ++---+ ---+- +++-+ +++-+ -+++
818347.	0.110	0.720	0.810	1.079	2.900	-++++ ---+- ---+- +--+- -----+ ++-+- +++++ +++-
1994583.	0.185	-0.515	0.837	0.852	0.375	+++++ ++--+ --+-+ ++--- -----+ +---+ +---+ +---
1584307.	0.120	0.502	0.787	1.072	2.229	-+-+- +-+-+ ---++ ++---+ ---+- +++-- -++++ ---+
1630079.	0.116	0.354	0.787	1.027	1.817	-+-+- +-+-+ ---++ ++---+ ---+- +++-- -++++ ---+
1858939.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
906087.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
336131.	0.140	-0.009	0.797	0.949	1.026	-+-+- +-+-+ ---++ ++---+ ---+- +++-- -+-++ +--+
1680655.	0.179	-0.538	0.752	0.862	0.349	-++++ ---++ --+++ +-++- --+-+ ++--+ -+-+- +---
14667.	0.677	-0.493	0.823	0.565	0.886	-+++- +-+-- --++- ++--- ---+- +-+++ +++-+ -+++
73335.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
366675.	0.238	0.528	0.690	0.814	2.421	-+-++ +-+-- ---+- ++--+ ----- -+--- +++++ +++-
1833375.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
778267.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
1794183.	0.164	-0.518	0.812	0.879	0.351	-+-+- +-+-- --++- ++--+ ---+- +++-+ +++-+ -+++
1258951.	0.116	0.262	0.826	1.098	1.584	+++++ ++--+ --+-+ ++--- -----+ +---+ +-+-+ ----
1020547.	0.116	0.148	0.826	1.098	1.323	+++++ ++--+ --+-+ ++--- -----+ +---+ +-+-+ ----
82475.	0.116	0.314	0.787	1.050	1.715	-+-+- +-+-+ ---++ ++---+ ---+- +++-- -++++ ---+
1720771.	0.140	-0.292	0.797	0.959	0.573	-+-+- +-+-+ ---++ ++---+ ---+- +++-- -+-++ +--+
1400219.	0.126	0.779	0.836	0.992	3.117	-++++ ---+- ---+- +--+- -----+ ++--- +++++ +++-
1920767.	0.214	-0.395	0.872	0.795	0.522	++-+- -++++ ----+ +--++ ---+- +-+-- +-+++ +--+
932211.	0.124	0.355	0.883	1.019	1.827	++-+- -++++ --+-- +--++ ----- +-+-+ +---- +-++
347851.	0.115	0.316	0.826	1.105	1.718	+++++ ++--+ --+-+ ++--- -----+ +---+ +-+-+ ----
1468343.	0.157	-0.073	0.793	0.899	0.927	-++++ ---++ --+++ +--+- -----+ ++--- -+++- ----
1119043.	0.116	0.148	0.826	1.098	1.323	+++++ ++--+ --+-+ ++--- -----+ +---+ +-+-+ ----
1215227.	0.112	0.865	0.810	1.098	3.405	-++++ ---+- ---+- +--+- -----+ ++-+- +++++ +++-
1881831.	0.116	0.148	0.826	1.098	1.323	+++++ ++--+ --+-+ ++--- -----+ +---+ +-+-+ ----
624491.	0.116	0.148	0.826	1.098	1.323	+++++ ++--+ --+-+ ++--- -----+ +---+ +-+-+ ----
1090651.	0.198	-0.355	0.769	0.846	0.552	+++++ ++--+ --+-+ -+--- -----+ +---+ +---+ +---
1538335.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
1025303.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
229299.	0.115	0.316	0.826	1.105	1.718	+++++ ++--+ --+-+ ++--- -----+ +---+ +-+-+ ----
1099691.	0.115	0.316	0.826	1.105	1.718	+++++ ++--+ --+-+ ++--- -----+ +---+ +-+-+ ----
1578763.	0.223	-0.488	0.868	0.785	0.437	++-+- -++++ ----+ +--++ ---+- +-+-+ +-+++ +--+
426927.	0.197	-0.035	0.897	0.840	1.035	++-+- -++++ ----+ +--++ ---+- +-+-+ +---+ +-++
1058799.	0.116	0.148	0.826	1.098	1.323	+++++ ++--+ --+-+ ++--- -----+ +---+ +-+-+ ----
1990807.	0.121	0.430	0.857	1.004	2.025	++-+- -+++- --+-- +--++ ---+- +-+++ ----+ ++++
1538171.	0.116	0.262	0.826	1.098	1.584	+++++ ++--+ --+-+ ++--- -----+ +---+ +-+-+ ----
1554891.	0.214	-0.309	0.766	0.806	0.625	-++++ ----++ --+++ +--+- --+-+ ++---+ -++++ +---
1304151.	0.126	0.779	0.836	0.992	3.117	-++++ ---+- ---+- +--+- -----+ ++--- +++++ +++-
1423391.	0.157	-0.073	0.793	0.899	0.927	-++++ ---++ --+++ +--+- -----+ ++--- -+++- ----
1565427.	0.132	-0.042	0.787	1.011	0.955	-+-+- +-+-+ ---++ ++---+ ---+- +++-- -++++ ---+
187415.	0.222	-0.457	0.837	0.803	0.465	+++++ ++--+ --+-+ ++--- -----+ +---+ +---+ +---
1815259.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
471459.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
883319.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
1009099.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
1364423.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
76071.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
851191.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
1560375.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
1781795.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
1172603.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
1480847.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
58695.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
1369591.	0.091	-0.976	0.852	1.049	0.091*	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
1545471.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
1435899.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
245891.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
1986123.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
1566619.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
1201403.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
344671.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
2095191.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-
1313191.	0.091	-0.976	0.852	1.049	0.091	+++++ ++--- ----- ++--- -----+ +---- ---++ -++-

CFOM Range	Frequency
0.000 - 0.020	0
0.020 - 0.040	0
0.040 - 0.060	0
0.060 - 0.080	0
0.080 - 0.100	87
0.100 - 0.120	0
0.120 - 0.140	0
0.140 - 0.160	0
0.160 - 0.180	1

```
0.180 - 0.200      2
0.200 - 0.220      6
0.220 - 0.240      0
0.240 - 0.260      1
0.260 - 0.280      0
0.280 - 0.300      0
0.300 - 0.320      0
0.320 - 0.340      0
0.340 - 0.360      2
0.360 - 0.380      1
0.380 - 0.400      0
0.400 - 0.420      0
0.420 - 0.440      1
0.440 - 0.460      3
0.460 - 0.480      2
0.480 - 0.500      1
0.500 - 0.520      0
0.520 - 0.540      2
0.540 - 0.560      1
0.560 - 0.580      4
0.580 - 0.600      0
0.600 - 9.999     86

     200. Phase sets refined - best is code    50527.  with CFOM =  0.0901


      3.3 seconds elapsed time


Tangent expanded to  519  out of  519  E greater than  1.200
Highest memory used =  2197 /  2953

      0.2 seconds elapsed time


FMAP and GRID set by program

FMAP   8   2  10
GRID    -3.571  -2  -2     3.571   2   2


E-Fourier for  Sr5V3X22   P21/c

Maximum =  314.32,  minimum =  -72.81       highest memory used =  8837 /  5860

      0.1 seconds elapsed time


Heavy-atom assignments:

         x       y       z    s.o.f.   Height

SR1   0.0062  0.0886  0.1443  1.0000   314.3
SR2   0.6485  0.0841  0.1422  1.0000   268.7
SR3   0.7626  0.0872  0.5170  1.0000   263.2
SR4   0.3376  0.1730  0.6752  1.0000   236.2
SR5   0.6582  0.1566  0.8309  1.0000   228.8
V6    0.3956  0.0792  0.3255  1.0000   175.1
V7    0.9165  0.0931  0.3406  1.0000   165.9
V8    0.2603  0.0804  0.0235  1.0000   128.8


Peak list optimization
RE = 0.496 for  22 surviving atoms and  519 E-values    Highest memory used =  1652 /  4671

      0.1 seconds elapsed time


E-Fourier for  Sr5V3X22   P21/c

Maximum =  283.29,  minimum =  -92.00       highest memory used =  8901 /  5860

      0.1 seconds elapsed time


Peak list optimization
RE = 0.482 for  26 surviving atoms and  519 E-values    Highest memory used =  1716 /  4671

      0.2 seconds elapsed time


E-Fourier for  Sr5V3X22   P21/c

Maximum =  254.31,  minimum =  -79.74       highest memory used =  8901 /  5860

      0.1 seconds elapsed time

Molecule  1     scale 0.407 inches = 1.035 cm per Angstrom


Atom Peak     x       y       z     SOF  Height  Distances and Angles

SR1    0.  0.0062  0.0886  0.1443  1.000  3.44   0 SR2  4.010
```

```
                                        0 SR3  4.124  60.9
                                        0 SR4  4.093 150.8 101.5
                                        0 SR5  4.177 150.0 143.1  57.3
                                        0 2    4.468 119.8  75.7  72.4  69.3
                                        0 3    4.717 144.2  83.4  32.3  62.7  41.4
                                        0 4    4.562  34.5  85.1 129.1 131.8 154.3 153.3
                                        0 5    3.319  94.9  36.3  76.8 106.8  42.6  50.1 121.3
                                        0 8    4.047  61.1  36.5 119.8 123.6  59.1  89.6  95.3  43.5
                                        0 9    3.767  90.8 147.3  96.5  69.4 136.2 123.8  62.5 173.2 143.2
                                        0 10   2.396 105.3  59.5  81.0  85.9  16.7  48.7 139.2  29.1  44.2 151.4
                                        0 13   3.905 102.8 163.6  92.7  52.6 116.9 112.9  79.6 158.8 139.2  19.5 132.0
                                        0 14   2.560  92.3 148.4  95.0  68.1 135.4 122.3  63.8 171.8 144.6   1.5 150.8
                                        0 15   2.520  69.9 130.4 119.9  85.3 139.3 145.8  48.4 163.2 120.0  23.5 146.5
                                        0 16   4.088  79.4 115.1 129.7  73.0  84.1 117.9  88.8 113.9  80.4  70.8  88.9
                                        0 17   3.302  95.6  36.1  65.8 112.5  61.3  49.8 111.0  23.3  60.7 152.2  50.9
                                        0 20   3.062  84.0 107.3 124.8  71.9  70.7 106.7  99.7 100.7  71.1  83.6  75.0
                                        0 21   4.692  61.5 119.3 120.3  97.5 153.9 151.5  34.7 155.5 118.9  29.4 156.6
                                        0 22   4.404 109.0  50.0  64.7  93.4  34.5  36.2 134.3  14.2  55.1 159.9  26.2
                                        0 23   3.636  38.1  58.5 153.2 127.0  84.6 121.8  70.7  77.0  33.6 109.8  73.4
                                        0 24   3.731  43.5  89.8 165.6 108.4 102.3 143.6  60.1 108.8  65.4  77.9  97.5
                                        0 26   4.293 102.9 131.8  70.5  73.4 137.4 102.5  68.4 140.4 162.7  33.9 150.7
                                        0 30   2.332 130.0  90.3  68.3  55.0  14.5  41.5 162.5  56.4  71.4 121.9  31.1

SR2    0. -0.3515  0.0841  0.1422  1.000  2.82   0 SR1  4.010
                                        0 SR3  4.122  60.9
                                        0 1    4.648 120.5  69.6
                                        0 4    2.596  84.5 120.5  94.3
                                        0 6    2.642 114.9 165.3 120.7  71.2
                                        0 7    4.157 116.4  55.5  31.8 126.1 126.9
                                        0 8    4.098  59.9  36.3  97.1 143.4 129.0  70.3
                                        0 11   2.914 112.4  77.2  21.3  73.6 116.2  52.6 110.8
                                        0 12   3.093 101.4  41.4  47.3 138.7 136.3  18.1  52.2  66.3
                                        0 15   3.936  37.0  97.7 141.2  59.7  80.3 152.7  91.2 122.1 138.3
                                        0 18   4.154  83.6  37.6  37.4  97.1 156.0  43.8  72.8  39.8  44.3 112.5
                                        0 19   2.882  93.9 131.1 145.1  95.1  34.5 129.0  95.2 149.7 124.8  70.8 167.3
                                        0 20   4.786  39.5  81.3 150.8 102.2  87.6 126.0  55.9 151.4 108.0  43.0 115.8
                                        0 21   4.489  66.7 124.2 128.5  34.3  59.4 160.0 122.6 107.5 164.2  31.6 121.4
                                        0 23   2.521  62.9  65.0 121.9 139.6 100.4  91.2  29.0 138.9  74.6  80.1 101.8
                                        0 24   2.877  63.1 103.6 165.1 100.5  63.8 133.4  71.8 173.3 118.7  51.2 140.2
                                        0 25   4.518 111.2  51.9  46.8 141.1 125.7  15.0  58.1  67.5  10.7 147.6  52.4
                                        0 27   4.014  78.0  36.1  81.1 156.1 131.1  51.9  19.5  98.2  34.2 110.6  65.2
                                        0 28   4.203  96.7  36.2  47.0 135.3 142.2  20.9  50.8  64.7   5.9 133.7  39.4
                                        0 29   4.658  92.7  45.3  72.7 163.0 124.7  41.4  33.8  92.2  25.9 124.8  65.9

SR3    0. -0.2374  0.4128  0.0170  1.000  3.59   0 SR1  4.124
                                        0 SR2  4.122  58.2
                                        0 5    2.443  53.6 108.5
                                        0 7    3.853 120.9  62.7 161.8
                                        0 8    2.563  70.1  71.3  68.4  93.5
                                        0 10   3.566  35.4  84.5  24.7 140.2  52.7
                                        0 11   4.491  84.3  39.3 137.1  46.2 107.8 118.2
                                        0 12   2.726 105.8  48.6 143.9  18.9  76.9 121.3  46.7
                                        0 17   2.428  53.2 109.5  31.8 163.1  98.1  46.4 117.9 158.2
                                        0 18   2.665 104.6  71.9 142.3  53.1 138.9 139.1  32.8  65.2 111.0
                                        0 22   3.610  69.0 124.7  16.2 163.1  76.8  40.6 149.8 153.3  33.7 141.2
                                        0 23   3.817  54.3  36.8  84.7  79.5  34.9  60.8  75.1  60.6 103.2 107.8  98.8
                                        0 25   3.798 125.4  69.4 146.6  17.9  80.0 131.6  62.5  20.9 178.0  70.4 145.5
                                        0 27   2.522  95.8  69.6  97.9  64.4  31.4  84.1  93.6  51.1 129.0 116.2 102.6
                                        0 28   2.584 131.0  73.6 152.7  15.0  87.6 139.5  61.2  25.3 174.1  64.9 148.3
                                        0 29   3.414 112.7  75.7 112.7  50.9  49.1 101.7  88.9  42.4 144.6 104.0 113.8
                                        0 30   4.747  29.4  81.2  27.3 140.0  56.9   6.4 113.1 121.3  44.1 132.8  43.6

SR4    0.  0.3376  0.3270  0.1752  1.000  4.73   0 SR1  4.093
                                        0 SR5  3.966  62.4
                                        0 V6   3.523  77.9  56.6
                                        0 V7   3.535  66.7 129.1 112.3
                                        0 V8   3.534  67.0  53.4 109.8 106.5
                                        0 3    2.522  87.6  88.7 145.2  89.8  35.9
                                        0 5    4.643  44.1  88.7 122.0  53.1  53.6  51.0
                                        0 10   4.408  32.5  67.5 105.9  70.3  41.3  55.1  21.3
                                        0 17   4.071  47.7 101.8 122.5  37.2  69.4  61.2  16.0  35.2
                                        0 22   4.553  61.0  94.1 137.9  60.7  47.6  34.2  17.9  32.2  27.2
                                        0 30   3.891  33.8  51.6  95.6  85.5  33.2  58.4  37.1  16.1  51.2  44.8

SR5    0.  0.3418 -0.1566  0.1691  1.000  3.40   0 SR1  4.177
                                        0 SR4  3.966  60.3
                                        0 V6   3.570  76.3  55.4
                                        0 V8   3.394  67.1  56.7 112.0
                                        0 3    4.652  64.3  32.8  88.3  24.4
                                        0 9    4.533  51.0  87.0  54.3 118.1 109.4
                                        0 10   4.665  30.8  60.8 100.2  38.6  45.7  81.1
                                        0 13   3.590  59.8  99.9  62.9 126.4 121.2  12.9  88.0
                                        0 14   4.005  36.4  78.0  58.0 103.4  96.2  14.7  66.7  25.1
                                        0 15   4.698  32.3  83.2  69.2  98.6  96.0  22.0  60.4  27.8  11.3
                                        0 20   4.345  42.1  99.8 110.8  75.7  89.2  62.1  43.7  60.6  53.7  42.5
                                        0 30   3.422  33.9  63.1 103.6  36.7  45.9  83.8   3.5  90.2  69.5  62.7  43.2

V6     0.  0.3956  0.0792  0.3255  1.000  4.53   0 SR4  3.523
                                        0 SR5  3.570  68.0
                                        0 9    3.794 106.5  75.9
                                        0 13   3.733 105.8  58.8  20.0
                                        0 14   3.690  88.0  66.9  18.5  26.4
                                        0 26   2.541 104.8 110.8  38.5  58.4  43.8
```

```
V7     0.  0.0835  0.5931  0.1594  1.000  4.99   0 SR4  3.535
                                                 0 5    3.789  78.6
                                                 0 17   2.478  83.3   4.7

V8     0.  0.2603  0.0804  0.0235  1.000  3.54   0 SR4  3.534
                                                 0 SR5  3.394  69.8
                                                 0 2    2.014 129.9 129.0
                                                 0 3    2.100  44.8 113.6 104.6
                                                 0 5    3.819  78.2 113.6  51.9  68.7
                                                 0 10   2.919  85.6  95.0  51.1  90.7  24.7
                                                 0 22   3.395  82.1 133.9  50.7  56.7  22.0  45.7
                                                 0 30   2.149  82.6  72.3  66.5 104.0  46.5  23.2  68.2

1    127. -0.5731  0.5686  0.1253  1.000  3.73   0 SR2  4.648
                                                 0 7    2.459  63.0
                                                 0 11   2.204  28.7  90.8
                                                 0 12   3.417  41.7  24.3  67.7
                                                 0 18   2.858  61.9  70.9  62.2  54.3
                                                 0 25   3.644  64.7   1.7  92.5  25.7  71.2
                                                 0 28   3.552  59.9  20.4  83.4  19.2  50.8  20.6

2    122.  0.1041  0.0746 -0.0574  1.000  3.05   0 SR1  4.468
                                                 0 V8   2.014  70.3
                                                 0 3    3.255  73.4  38.6
                                                 0 5    3.023  48.0  96.5  70.5
                                                 0 8    4.216  55.5 125.3 111.4  41.8
                                                 0 10   2.278  17.5  85.4  79.5  33.6  39.8
                                                 0 17   4.084  45.1  83.8  57.6  13.3  54.0  35.2
                                                 0 20   4.503  39.9  86.2 108.0  78.9  57.6  46.5  81.6
                                                 0 22   2.630  71.4  93.0  56.7  28.4  65.1  60.4  26.3 106.7
                                                 0 30   2.286  14.8  59.6  71.9  62.1  68.1  32.2  57.5  36.4  83.2

3    113.  0.2956  0.3298  0.0440  1.000  4.33   0 SR1  4.717
                                                 0 SR4  2.522  60.1
                                                 0 SR5  4.652  52.9  58.5
                                                 0 V8   2.100  63.9  99.3  42.0
                                                 0 2    3.255  65.2 122.1  74.6  36.8
                                                 0 5    3.629  44.5  96.4  92.8  78.7  51.8
                                                 0 10   3.616  29.9  90.0  67.3  53.8  38.3  27.0
                                                 0 17   3.612  44.3  81.1  97.2  95.7  72.8  21.3  41.9
                                                 0 22   2.847  65.9 115.9 110.5  85.2  50.5  21.6  43.3  35.2
                                                 0 30   3.348  27.5  81.7  47.3  38.5  40.5  47.3  20.5  59.2  63.2

4    111. -0.2626  0.0981  0.2774  1.000  3.35   0 SR1  4.562
                                                 0 SR2  2.596  61.0
                                                 0 6    3.049  93.9  55.1
                                                 0 9    4.374  49.8 102.2  96.8
                                                 0 11   3.311  93.2  57.6  95.8 141.6
                                                 0 14   4.128  33.8  89.1  96.8  16.0 126.1
                                                 0 15   3.451  33.1  79.8  83.9  22.4 125.6  13.2
                                                 0 19   4.046  72.3  45.2  21.7  81.4  98.5  77.8  64.7
                                                 0 21   2.762  75.2 113.8  83.6  27.9 168.3  42.8  42.8  76.7
                                                 0 24   4.213  50.1  42.2  43.9  66.6  99.7  59.1  46.4  22.2  71.8

5    110. -0.0405  0.3181  0.0020  1.000  3.63   0 SR1  3.319
                                                 0 SR3  2.443  90.1
                                                 0 SR4  4.643  59.1 124.9
                                                 0 V7   3.789  72.5  80.8  48.3
                                                 0 V8   3.819  72.4 162.3  48.2  96.2
                                                 0 2    3.023  89.4 150.0  79.7 127.3  31.6
                                                 0 3    3.629  85.4 152.0  32.7  71.5  32.6  57.7
                                                 0 8    2.815  82.1  57.8 140.3 131.2 115.1  92.4 147.7
                                                 0 10   1.690  43.5 118.1  71.5 109.3  46.3  48.2  76.1  74.4
                                                 0 17   1.336  77.7  73.4  56.9   8.8 104.7 135.4  78.6 126.8 116.7
                                                 0 22   1.437 131.4 135.4  77.5  95.4  62.2  60.4  46.9 131.7 105.2  97.3
                                                 0 23   4.337  54.8  61.2 113.7 111.6 104.7  94.7 133.2  27.6  58.5 110.8 151.6
                                                 0 27   3.745  91.0  41.8 149.5 120.9 133.0 108.1 165.4  18.0  91.6 114.5 132.4
                                                 0 30   2.810  43.8 129.2  56.7  98.7  33.7  46.0  61.1  90.0  15.6 106.9  95.5

6    108. -0.4218 -0.1793  0.1970  1.000  2.12   0 SR2  2.642
                                                 0 4    3.049  53.7
                                                 0 11   4.721  33.6  44.3
                                                 0 15   4.355  63.0  52.0  82.9
                                                 0 19   1.656  80.7 115.4 113.6  68.2
                                                 0 21   3.880  84.7  45.0  88.7  32.6  94.7
                                                 0 23   3.967  38.7  85.3  71.2  61.9  42.5  94.2
                                                 0 24   2.922  62.0  89.7  95.4  45.3  25.7  76.0  30.7

7    104. -0.5808  0.4286  0.0151  1.000  3.05   0 SR2  4.157
                                                 0 SR3  3.853  61.8
                                                 0 1    2.459  85.2 103.3
                                                 0 8    4.755  54.3  32.6 128.1
                                                 0 11   3.326  44.1  77.0  41.5  90.2
                                                 0 12   1.551  38.3  34.8 115.0  16.1  75.1
                                                 0 18   3.101  68.0  43.4  60.5  73.7  49.0  68.2
                                                 0 25   1.189 100.0  78.5 174.7  55.6 143.5  69.3 120.3
                                                 0 27   3.580  62.0  39.5 138.0  10.0  99.9  24.9  82.1  45.6
                                                 0 28   1.514  81.3  26.3 125.0  32.0 103.3  44.8  65.0  55.3  31.4
                                                 0 29   3.149  77.9  57.3 158.7  30.7 119.3  44.4 100.7  25.1  20.7  39.9

8    102. -0.2593  0.1312 -0.0413  1.000  2.63   0 SR1  4.047
                                                 0 SR2  4.098  59.0
```

							0	SR3	2.563	73.4	72.3														
							0	2	4.216	65.4	123.9	99.5													
							0	5	2.815	54.3	101.6	53.8	45.8												
							0	7	4.755	103.8	55.4	54.0	153.4	107.8											
							0	10	2.866	35.6	94.6	81.9	30.6	34.6	131.0										
							0	12	3.292	97.2	48.0	53.8	152.5	107.0	7.5	126.4									
							0	17	3.770	49.8	87.3	39.6	61.2	16.5	92.9	43.2	91.3								
							0	20	4.208	43.5	70.4	116.5	64.6	86.5	125.5	52.8	118.2	89.4							
							0	22	3.920	67.1	117.5	63.7	37.5	15.9	116.3	39.3	117.3	31.3	91.6						
							0	23	2.256	63.1	32.9	104.6	112.4	117.2	80.2	93.1	73.8	108.5	48.0	130.1					
							0	24	4.209	53.7	40.5	107.7	98.9	107.9	92.4	80.6	85.6	102.2	34.7	118.9					
							0	25	4.199	117.3	66.0	63.0	157.9	115.9	13.5	143.3	20.2	102.6	133.8	121.2					
							0	27	1.376	130.4	76.8	72.7	155.4	122.9	26.7	154.6	33.2	111.8	139.9	124.4					
							0	28	3.563	107.4	66.1	46.4	143.1	99.3	13.0	127.7	19.1	86.0	136.4	105.6					
							0	29	2.601	141.2	85.0	82.8	150.5	129.9	38.1	164.0	44.2	120.9	140.3	127.8					
							0	30	3.976	33.8	91.6	90.4	32.2	45.0	135.5	10.4	129.8	52.7	42.7	49.0					
9	99.	0.0958	-0.1471	0.3136	1.000	3.37	0	SR1	3.767																
							0	SR5	4.533	59.6															
							0	V6	3.794	79.0	49.8														
							0	4	4.374	67.7	127.2	123.1													
							0	13	1.306	86.2	37.7	77.4	140.2												
							0	14	1.210	3.2	57.0	75.9	70.4	84.9											
							0	15	1.768	34.6	84.3	113.6	48.0	93.7	37.7										
							0	16	4.556	57.9	65.5	114.3	85.5	54.9	59.3	42.7									
							0	20	4.580	41.6	56.9	102.1	82.5	58.7	42.8	35.0	16.8								
							0	21	2.325	97.9	152.0	148.5	33.8	134.0	101.0	68.7	88.9	95.4							
							0	24	4.714	50.7	87.9	127.7	55.1	85.2	53.5	19.0	30.4	31.3	64.2						
							0	26	2.400	85.2	88.2	41.2	89.7	118.5	83.3	110.9	141.7	124.9	107.5	129.8					
10	91.	0.0032	0.1237	0.0246	1.000	3.22	0	SR1	2.396																
							0	SR3	3.566	85.1															
							0	SR4	4.408	66.5	105.4														
							0	SR5	4.665	63.3	145.9	51.7													
							0	V8	2.919	105.3	145.2	53.1	46.5												
							0	2	2.278	145.8	127.9	93.0	82.5	43.5											
							0	3	3.616	101.4	110.4	34.9	67.0	35.5	62.3										
							0	5	1.690	107.4	37.2	87.2	138.8	109.0	98.2	76.9									
							0	8	2.866	100.2	45.4	150.3	147.5	153.0	109.5	145.5	71.0								
							0	14	4.796	15.1	99.8	65.9	50.1	94.8	131.9	99.3	121.7	108.2							
							0	15	4.708	17.2	93.4	78.6	60.2	106.2	138.4	112.5	121.7	95.5	13.2						
							0	16	4.698	60.5	113.3	108.8	63.4	100.4	105.3	130.0	150.5	84.2	50.8	43.3					
							0	17	2.583	83.0	42.9	65.3	115.8	104.4	114.2	69.0	27.5	87.4	96.1	99.3					
							0	20	3.366	61.5	114.3	109.1	63.1	99.6	104.2	129.6	151.3	84.5	51.7	44.4					
							0	22	2.489	128.7	70.7	77.1	118.4	77.3	66.8	51.7	33.9	93.8	137.9	145.9					
							0	23	3.741	68.7	62.9	134.5	112.2	151.9	129.9	167.9	98.9	37.0	73.0	59.8					
							0	24	4.691	52.1	83.3	117.1	86.6	129.4	130.2	150.2	120.5	62.3	51.4	38.5					
							0	27	4.150	97.3	37.2	142.2	151.5	157.4	114.4	140.6	64.4	8.2	107.1	94.9					
							0	30	1.267	71.7	155.4	58.2	9.6	41.9	74.2	67.7	143.3	145.6	57.8	66.7					
11	88.	-0.4314	0.3959	0.1846	1.000	3.64	0	SR2	2.914																
							0	SR3	4.491	63.5															
							0	1	2.204	130.0	90.6														
							0	4	3.311	48.8	96.7	169.4													
							0	6	4.721	30.1	93.5	132.2	40.0												
							0	7	3.326	83.3	56.7	47.7	131.9	97.5											
							0	12	3.289	59.5	37.1	74.0	107.6	81.2	27.1										
							0	18	2.673	96.0	32.7	71.0	118.9	126.1	61.1	57.2									
							0	25	4.339	74.1	50.9	57.0	122.9	90.3	9.4	18.1	61.1								
							0	28	3.959	73.6	34.9	63.0	120.4	96.5	21.8	15.3	45.3	17.1							
12	85.	-0.4686	0.3157	0.0183	1.000	2.94	0	SR2	3.093																
							0	SR3	2.726	90.0															
							0	1	3.417	91.0	109.2														
							0	7	1.551	123.6	126.3	40.7													
							0	8	3.292	79.8	49.3	156.0	156.4												
							0	11	3.289	54.2	96.1	38.3	77.8	124.0											
							0	18	2.906	87.6	56.4	53.0	82.1	104.2	50.7										
							0	23	3.433	45.1	75.6	136.0	157.8	39.1	98.4	112.6									
							0	25	1.586	148.1	121.2	85.2	44.5	114.2	121.8	114.3	131.1								
							0	27	2.269	95.7	59.8	167.0	138.3	19.4	143.4	116.1	51.4	94.9							
							0	28	1.169	158.4	70.6	86.9	65.9	93.6	116.9	74.0	132.7	53.1	82.8						
							0	29	2.310	118.4	84.9	147.9	107.6	51.8	172.5	134.3	74.5	63.2	32.5	70.5					
13	78.	0.1535	-0.2467	0.2823	1.000	3.12	0	SR1	3.905																
							0	SR5	3.590	67.6															
							0	V6	3.733	78.0	58.3														
							0	9	1.306	74.3	129.4	82.7													
							0	14	1.699	29.2	91.2	75.4	45.2												
							0	15	2.264	37.5	104.4	103.1	51.2	27.8											
							0	16	3.952	62.7	81.2	132.2	109.5	81.8	60.9										
							0	20	4.058	45.2	68.9	113.8	105.3	68.5	54.2	19.1									
							0	21	3.366	80.0	147.4	112.4	29.8	56.7	44.3	87.5	91.2								
							0	24	4.786	49.6	99.1	127.4	79.0	56.9	31.7	30.5	31.6	59.9							
							0	26	3.234	73.3	95.7	42.0	40.7	51.8	75.5	133.6	118.2	70.5	107.1						
14	76.	0.0732	-0.0698	0.2597	1.000	3.41	0	SR1	2.560																
							0	SR5	4.005	75.5															
							0	V6	3.690	99.0	55.1														
							0	4	4.128	82.4	157.7	133.5													
							0	9	1.210	175.3	108.3	85.6	93.6												
							0	10	4.796	14.1	63.3	96.1	94.4	167.2											
							0	13	1.699	131.9	63.7	78.2	133.7	50.0	117.9										

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                                        0 15   1.098  75.5 123.3 174.4  45.7  99.9  78.8 106.1
                                        0 16   4.074  72.0  75.0 129.6  95.3 105.9  63.3  73.8  50.0
                                        0 20   3.782  53.6  67.8 121.8  96.5 124.7  44.3  86.8  55.7  19.1
                                        0 21   2.818 121.4 155.8 129.7  41.8  54.1 130.2  93.0  54.4  93.1 106.7
                                        0 24   4.112  63.1 104.5 157.2  61.5 112.8  63.0 102.9  19.2  34.6  36.7  73.1
                                        0 26   2.559 114.0  98.5  43.4  93.3  68.7 120.8  96.8 137.8 170.1 162.6  90.1
                                        0 30   4.259  28.0  48.8  87.2 108.9 154.6  14.6 104.7  88.2  61.5  43.1 142.1

15    75. -0.0242 -0.1050  0.2361  1.000  3.09   0 SR1  2.520
                                        0 SR2  3.936  73.1
                                        0 SR5  4.698  62.4 132.5
                                        0 4    3.451  98.4  40.5 156.3
                                        0 6    4.355 107.7  36.7 151.0  44.1
                                        0 9    1.768 121.9 150.1  73.8 109.6 128.0
                                        0 10   4.708  16.3  73.1  59.5 106.1 102.9 129.1
                                        0 13   2.264 109.3 172.0  47.7 143.6 137.8  35.1 106.9
                                        0 14   1.098  79.6 141.3  45.5 121.2 163.5  42.4  88.0  46.1
                                        0 16   3.471  84.5  88.4  72.3 122.3  79.9 117.1  68.2  84.3 116.0
                                        0 19   4.043  99.2  42.3 128.7  64.8  22.4 138.6  89.4 129.9 174.0  58.0
                                        0 20   3.291  61.9  82.4  63.0 122.3  88.1 127.1  45.6  92.0 108.3  22.6  66.2
                                        0 21   2.354 148.5  87.3 140.1  52.8  62.6  66.9 158.9  93.6 103.4 120.1  80.8
                                        0 23   4.294  57.7  35.3 102.1  75.8  54.6 174.3  48.8 139.2 136.6  57.5  41.5
                                        0 24   3.097  82.6  46.4 109.1  79.9  42.1 150.3  70.5 125.7 154.0  43.1  21.0
                                        0 26   3.452  90.5 122.9  75.1  92.3 133.8  40.5 104.3  65.1  29.8 145.4 156.1
                                        0 30   4.365  24.8  88.3  44.2 121.2 115.7 115.9  15.5  91.5  77.2  64.7  99.1

16    72. -0.0777 -0.3933  0.1033  1.000  1.87   0 SR1  4.088
                                        0 9    4.556  51.3
                                        0 10   4.698  30.7  80.5
                                        0 13   3.952  58.1  15.7  83.5
                                        0 14   4.074  36.6  14.8  65.9  24.4
                                        0 15   3.471  37.8  20.2  68.5  34.8  14.0
                                        0 19   3.675  81.8  83.0  94.2  98.1  82.9  68.8
                                        0 20   1.334  33.3  82.6   3.0  85.0  68.0  71.1  96.7
                                        0 23   3.804  54.7  92.4  50.9 105.8  81.5  72.2  46.7  52.7
                                        0 24   2.437  64.0  78.4  74.8  94.0  73.5  60.2  19.5  77.3  29.9
                                        0 30   4.261  32.4  75.1  15.3  74.4  61.4  67.8 107.4  14.3  65.9  87.9

17    71. -0.0123  0.4289  0.0533  1.000  4.11   0 SR1  3.302
                                        0 SR3  2.428  90.8
                                        0 SR4  4.071  66.5 155.8
                                        0 V7   2.478  92.6 116.4  59.6
                                        0 2    4.084  73.6 105.6  76.8 136.0
                                        0 3    3.612  85.9 154.8  37.7  88.8  49.6
                                        0 5    1.336  79.1  74.7 107.1 166.5  31.3  80.1
                                        0 8    3.770  69.5  42.3 127.8 148.8  64.8 114.1  36.7
                                        0 10   2.583  46.1  90.7  79.5 132.4  30.6  69.2  35.8  49.4
                                        0 18   4.198  92.3  36.4 131.7  80.0 140.4 168.5 110.7  75.6 117.2
                                        0 22   2.082 107.6 106.1  89.4 132.5  34.0  51.9  43.2  78.3  63.4 138.9
                                        0 27   4.467  79.5  26.0 142.9 139.6  79.9 129.5  49.7  16.6  66.0  61.0  87.1
                                        0 30   3.445  40.4 106.6  61.7 115.9  34.0  56.6  51.3  66.7  17.9 126.8  67.6

18    69. -0.3327  0.5802  0.1038  1.000  4.11   0 SR2  4.154
                                        0 SR3  2.665  70.6
                                        0 1    2.858  80.7 130.9
                                        0 7    3.101  68.1  83.5  48.5
                                        0 11   2.673  44.2 114.6  46.8  69.9
                                        0 12   2.906  48.1  58.4  72.7  29.7  72.1
                                        0 17   4.198  81.3  32.7 160.1 116.0 120.8  88.9
                                        0 25   3.841  68.7  68.7  64.0  15.5  81.4  22.1 101.4
                                        0 27   4.404  55.8  30.9 100.0  53.6  93.4  27.6  62.5  40.1
                                        0 28   2.818  71.2  56.2  77.5  29.1  92.2  23.5  88.8  13.6  30.0

19    64. -0.3694 -0.2667  0.1362  1.000  1.81   0 SR2  2.882
                                        0 4    4.046  39.7
                                        0 6    1.656  64.8  42.9
                                        0 15   4.043  66.9  50.5  89.5
                                        0 16   3.675 103.5 103.4 141.0  53.2
                                        0 20   4.052  85.5  93.7 136.2  48.0  19.1
                                        0 21   4.342  73.7  38.2  63.0  32.4  78.1  78.7
                                        0 23   2.965  51.0  85.0 115.3  73.8  69.0  51.0 102.1
                                        0 24   1.600  73.7  84.8 127.6  44.0  30.6  11.8  76.2  42.4

20    61. -0.0522 -0.2503  0.0785  1.000  2.24   0 SR1  3.062
                                        0 SR2  4.786  56.4
                                        0 SR5  4.345  66.0 119.9
                                        0 2    4.503  69.4 104.3  67.5
                                        0 8    4.208  65.5  53.8 115.9  57.8
                                        0 9    4.580  54.8  72.5  61.0 114.7 115.0
                                        0 10   3.366  43.4  76.8  73.2  29.4  42.7  96.5
                                        0 13   4.058  64.8  88.4  50.4 113.0 128.8  16.0 102.1
                                        0 14   3.782  42.3  67.6  58.6 104.0 104.2  12.5  84.1  24.7
                                        0 15   3.291  46.6  54.6  74.5 114.5  99.1  17.9  90.0  33.9  16.0
                                        0 16   1.334 132.9  99.3 107.7 154.8 136.1  80.6 175.8  75.9  92.9  86.3
                                        0 19   4.052  90.4  36.9 139.7 135.9  78.3  78.8 112.3  90.6  81.8  65.9  64.2
                                        0 23   3.178  71.3  28.8 136.3  89.5  31.8 101.1  69.7 117.0  95.0  83.2 107.8
                                        0 24   2.508  83.5  29.4 137.3 129.7  72.7  77.3 105.0  90.4  78.8  62.9  71.4
                                        0 30   2.987  45.3  93.4  51.7  27.0  64.5  87.9  22.0  88.4  77.0  88.0 159.3

21    60. -0.0978 -0.1497  0.3338  1.000  3.09   0 SR1  4.692
                                        0 SR2  4.489  51.7
                                        0 4    2.762  70.1  32.0
                                        0 6    3.880  82.0  35.9  51.3
```

						0	9	2.325	52.7	104.2	118.3	127.9										
						0	13	3.366	55.0	103.0	125.0	118.1	16.2									
						0	14	2.818	27.8	79.4	95.4	106.8	24.9	30.3								
						0	15	2.354	16.3	61.1	84.4	84.9	44.4	42.2	22.3							
						0	19	4.342	68.5	38.1	65.1	22.3	107.1	96.0	89.0	66.8						
						0	24	4.254	49.0	38.3	70.2	41.8	86.3	76.8	67.6	45.5	21.4					
						0	26	3.811	59.6	102.6	97.2	138.3	36.9	53.1	42.2	63.0	128.1	107.7				
22	59.	0.0433	0.3754	-0.0352	1.000	3.83	0	SR1	4.404													
						0	SR3	3.610	61.0													
						0	SR4	4.553	54.4	101.8												
						0	V8	3.395	64.3	124.2	50.2											
						0	2	2.630	74.1	114.8	85.3	36.3										
						0	3	2.847	77.9	131.7	29.9	38.1	72.8									
						0	5	1.437	34.4	28.4	84.6	95.9	91.2	111.5								
						0	8	3.920	57.8	39.5	112.2	100.3	77.4	131.9	32.4							
						0	10	2.489	25.1	68.8	70.7	57.0	52.8	85.1	40.9	46.8						
						0	17	2.082	45.6	40.3	63.4	102.6	119.7	92.9	39.5	70.4	68.1					
						0	30	3.275	31.2	87.0	56.8	37.5	43.9	65.9	58.7	66.4	20.0	76.4				
23	58.	-0.2998	-0.0392	0.0382	1.000	2.30	0	SR1	3.636													
						0	SR2	2.521	79.0													
						0	SR3	3.817	67.2	78.2												
						0	5	4.337	48.2	101.0	34.1											
						0	6	3.967	96.1	40.9	119.1	137.1										
						0	8	2.256	83.2	118.1	40.5	35.3	157.9									
						0	10	3.741	37.9	110.3	56.3	22.6	133.9	49.9								
						0	12	3.433	102.8	60.3	43.8	77.5	91.8	67.1	100.0							
						0	15	4.294	35.9	64.6	96.7	84.0	63.5	119.1	71.4	116.2						
						0	16	3.804	66.6	108.0	130.9	99.5	81.4	117.8	77.0	166.5	50.3					
						0	19	2.965	100.5	62.8	140.9	148.4	22.2	176.2	133.7	111.5	64.7	64.4				
						0	20	3.178	52.9	113.8	112.4	80.1	96.9	100.1	57.5	154.9	49.6	19.5	82.5			
						0	24	2.083	76.1	76.7	138.6	122.7	45.7	151.9	103.6	136.0	42.5	35.7	31.2			
						0	25	4.632	116.2	71.5	52.4	83.7	96.5	64.7	106.2	15.0	130.9	176.7	113.0			
						0	27	2.686	105.0	100.8	41.2	59.0	131.4	30.8	78.6	41.3	137.8	147.2	146.3			
						0	28	4.312	100.8	70.4	36.4	68.8	103.3	55.6	91.4	11.5	120.8	167.1	122.9			
						0	29	3.591	120.9	97.8	54.8	75.8	119.6	46.2	95.2	38.3	150.2	154.2	130.5			
24	58.	-0.2475	-0.2204	0.1143	1.000	2.09	0	SR1	3.731													
						0	SR2	2.877	73.4													
						0	4	4.213	69.8	37.3												
						0	6	2.922	115.9	54.2	46.4											
						0	8	4.209	60.9	67.7	98.4	117.0										
						0	9	4.714	51.4	90.4	58.4	91.7	112.3									
						0	10	4.691	30.4	82.8	94.8	136.1	37.1	79.0								
						0	13	4.786	52.8	104.9	74.1	105.0	111.8	15.8	75.3							
						0	14	4.112	37.7	85.8	59.4	99.3	98.6	13.7	65.6	20.2						
						0	15	3.097	42.0	82.3	53.7	92.6	102.5	10.7	71.1	22.6	6.7					
						0	16	2.437	80.0	153.4	129.6	142.0	101.0	71.2	75.1	55.5	71.8	76.7				
						0	19	1.600	142.5	74.1	73.0	26.7	121.1	111.0	154.6	120.4	121.7	115.0	129.9			
						0	20	2.508	54.6	125.3	120.9	163.0	72.6	71.4	43.9	58.0	64.5	71.0	31.3			
						0	21	4.254	71.6	75.3	38.1	62.2	125.8	29.5	102.0	43.2	39.3	32.8	94.8			
						0	23	2.083	71.1	58.5	93.2	103.6	14.6	121.0	50.8	123.6	107.8	110.4	114.4			
						0	27	4.768	71.7	57.1	92.1	102.0	16.1	121.2	52.0	124.4	108.2	110.7	116.0			
25	57.	-0.5888	0.3720	-0.0409	1.000	2.74	0	SR2	4.518													
						0	SR3	3.798	58.7													
						0	1	3.644	68.5	84.9												
						0	7	1.189	65.0	83.7	3.6											
						0	8	4.199	55.9	37.0	113.4	110.9										
						0	11	4.339	38.3	66.6	30.5	27.1	85.8									
						0	12	1.586	21.2	37.9	69.1	66.2	45.7	40.1								
						0	18	3.841	58.9	40.8	44.8	44.2	74.9	37.5	43.6							
						0	23	4.632	31.9	52.7	99.6	96.2	29.1	69.1	34.0	76.5						
						0	27	2.877	61.1	41.6	119.7	117.2	6.3	91.9	51.8	80.5	32.3					
						0	28	1.287	67.7	15.9	75.7	75.3	52.4	64.5	46.6	31.1	67.7	56.6				
						0	29	2.132	80.3	63.1	144.0	141.3	30.6	115.1	75.2	103.7	48.4	24.4	76.2			
26	57.	0.1994	0.0991	0.3639	1.000	4.35	0	SR1	4.293													
						0	V6	2.541	85.4													
						0	9	2.400	61.0	100.3												
						0	13	3.234	60.6	79.6	20.8											
						0	14	2.559	33.0	92.7	28.0	31.4										
						0	15	3.452	35.9	104.9	28.6	39.4	12.3									
						0	21	3.811	70.5	135.7	35.6	56.4	47.7	37.4								
27	57.	-0.3762	0.1988	-0.0570	1.000	2.58	0	SR2	4.014													
						0	SR3	2.522	74.3													
						0	5	3.745	88.5	40.3												
						0	7	3.580	66.1	76.1	116.3											
						0	8	1.376	83.7	76.0	39.1	143.3										
						0	10	4.150	78.9	58.7	24.0	128.9	17.3									
						0	12	2.269	50.1	69.1	107.1	16.8	127.4	114.7								
						0	17	4.467	79.6	25.0	15.8	100.6	51.6	34.6	91.4							
						0	18	4.404	58.9	32.9	72.3	44.2	102.8	86.2	36.3	56.5						
						0	23	2.686	38.1	94.2	83.1	102.1	57.1	62.1	87.3	84.1	93.1					
						0	24	4.768	37.0	94.2	83.8	100.9	58.2	63.0	86.1	84.6	92.4	1.2				
						0	25	2.877	80.1	89.2	129.1	17.2	160.5	145.4	33.3	114.2	59.3	112.7	111.5			
						0	28	2.419	77.2	63.0	102.7	19.0	138.0	120.9	28.7	88.0	35.7	115.2	114.1			
						0	29	1.283	112.5	124.3	151.0	60.3	156.0	168.5	75.5	145.6	100.8	125.9	125.1			
28	55.	-0.4771	0.4274	-0.0193	1.000	3.13	0	SR2	4.203													
						0	SR3	2.584	70.2													

```
                                          0 1    3.552  73.1 108.9
                                          0 7    1.514  77.9 138.7  34.5
                                          0 8    3.563  63.1  46.0 134.6 135.0
                                          0 11   3.959  41.7  83.9  33.6  54.8 101.0
                                          0 12   1.169  15.7  84.2  73.9  69.3  67.3  47.8
                                          0 18   2.818  69.4  58.9  51.8  85.9  99.6  42.4  82.5
                                          0 23   4.312  34.4  61.3 107.3 104.1  31.5  75.9  35.8  93.2
                                          0 25   1.287  95.8 156.3  83.8  49.4 110.9  98.5  80.3 135.3  96.2
                                          0 27   2.419  68.7  60.4 141.6 129.6  15.0 109.6  68.5 114.3  34.3  97.0
                                          0 29   2.213  87.4  90.4 145.0 114.0  46.6 127.4  79.7 145.9  56.3  69.4  31.8

29    54. -0.4885  0.2242 -0.0939  1.000  2.37   0 SR2  4.658
                                          0 SR3  3.414  59.0
                                          0 7    3.149  60.7  71.8
                                          0 8    2.601  61.2  48.1 111.2
                                          0 12   2.310  35.7  52.7  28.0  84.0
                                          0 23   3.591  32.4  66.0  93.2  38.7  67.1
                                          0 25   2.132  72.9  83.0  13.7 124.7  41.6 105.2
                                          0 27   1.283  52.7  37.6  98.9  12.4  72.0  37.3 112.4
                                          0 28   2.213  64.3  49.2  26.1  95.1  29.9  92.9  34.4  83.0

30    54.  0.0956  0.0352  0.0546  1.000  3.21   0 SR1  2.332
                                          0 SR3  4.747  60.3
                                          0 SR4  3.891  77.8  94.4
                                          0 SR5  3.422  91.1 148.7  65.3
                                          0 V8   2.149 141.9 123.2  64.2  70.9
                                          0 2    2.286 150.7  90.4 107.4 117.6  53.9
                                          0 3    3.348 111.0  91.9  39.9  86.8  37.5  67.6
                                          0 5    2.810  79.8  23.5  86.1 151.3  99.9  71.9  71.6
                                          0 8    3.976  74.8  32.7 127.0 156.8 131.0  79.7 115.2  45.1
                                          0 10   1.267  77.3  18.2 105.8 166.9 115.0  73.5  91.8  21.1  24.0
                                          0 14   4.259  31.0  91.2  75.8  61.7 127.4 176.3 115.7 110.4 100.0 107.6
                                          0 15   4.365  27.0  83.4  88.7  73.1 141.5 163.2 128.0 105.2  86.8  97.8  14.6
                                          0 16   4.261  69.7 100.5 130.5  78.7 134.2 119.3 165.5 122.0  79.1 102.3  57.1
                                          0 17   3.445  66.5  29.3  67.1 130.6  99.6  88.5  64.2  21.8  60.6  38.8  94.5
                                          0 20   2.987  69.0  94.9 134.8  85.1 138.3 116.6 171.9 116.0  72.8  96.1  59.9
                                          0 22   3.275 102.2  49.4  78.4 137.7  74.2  52.9  50.9  25.9  64.6  42.3 130.3
                                          0 23   4.405  55.6  49.1 129.9 126.3 159.7 105.8 141.0  69.9  30.7  51.1  72.9



     0.2 seconds elapsed time

++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+  i0            finished at 12:56:19   Total elapsed time:       6.5 secs  +
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

Well, no need at all to eliminate any overlaping data (but those at d > 1Å) : that test with 2000hkl obviously gives the structure, Sr and V atoms at the right place, as well as F/O atoms. The simulated data is of extremely good quality, just like it can be expected from third generation synchrotron sources, indeed, FWHM and shape were selected from experimental data on BM01 at ESRF. The list of heavy atoms is recalled below.

Heavy-atom assignments:

	x	y	z	s.o.f.	Height
SR1	0.0062	0.0886	0.1443	1.0000	314.3
SR2	0.6485	0.0841	0.1422	1.0000	268.7
SR3	0.7626	0.0872	0.5170	1.0000	263.2
SR4	0.3376	0.1730	0.6752	1.0000	236.2
SR5	0.6582	0.1566	0.8309	1.0000	228.8
V6	0.3956	0.0792	0.3255	1.0000	175.1
V7	0.9165	0.0931	0.3406	1.0000	165.9
V8	0.2603	0.0804	0.0235	1.0000	128.8

Applying SHELXS to a reduced dataset (elimination of reflections having a neighbouring one at less than 0.005°) of 979 reflections gives the following :

Heavy-atom assignments:

	x	y	z	s.o.f.	Height
SR1	-0.0066	0.0861	0.3551	1.0000	378.6
SR2	0.3552	0.0840	0.3568	1.0000	340.1

```
SR3    0.2386   0.0890   0.9793   1.0000    310.7
V4     0.3508   0.1502   0.6767   1.0000    250.2
V5     0.6784   0.1745   0.8359   1.0000    236.0
V6     0.5920   0.0814   0.1694   1.0000    216.4
V7     0.0876   0.0899   0.1625   1.0000    165.6
V8     0.7164   0.0983   0.4645   1.0000    140.0
```

Applying SHELXS to another reduced dataset (elimination of reflections having a neighbouring one at less than 0.01°) of 551 reflections gives the following - more difficult to interpret... :

```
Heavy-atom assignments:

          x        y        z     s.o.f.    Height

SR1    0.0794   0.0814   0.9248   1.0000    356.6
SR2    0.3364   0.0817   0.5598   1.0000    353.7
SR3    0.6985   0.0947   0.7384   1.0000    351.7
SR4    0.3151   0.0817   0.7236   1.0000    331.1
SR5    0.9774   0.1477   0.2464   1.0000    326.5
SR6    0.9830   0.0874   0.5591   1.0000    265.1
V7     0.4189   0.1060   0.1045   1.0000    223.6
V8     0.2426   0.0802   0.7545   1.0000    188.9
V9     0.6450   0.1721   0.0794   1.0000    169.3
V10    0.8629   0.0636   0.7805   1.0000    169.2
V11    0.4887   0.0832   0.6181   1.0000    163.7
V12    0.4674   0.0778   0.9363   1.0000    159.8
V13    0.4029   0.1120   0.7984   1.0000    157.5
V14    0.5938   0.0655   0.9162   1.0000    154.8
V15    0.9405   0.0829   0.6191   1.0000    151.1
V16    0.5754   0.0477   0.4277   1.0000    149.3
V17    0.3311   0.1235   0.4151   1.0000    148.8
V18    0.2225   0.1583   0.1087   1.0000    147.2
V19    0.6554   0.0727   0.8182   1.0000    143.0
V20    0.5654   0.1741   0.2652   1.0000    140.4
V21    0.3535   0.2041   0.2840   1.0000    138.7
V22    0.2501   0.0673   0.2053   1.0000    134.0
V23    0.0084   0.2181   0.8435   1.0000    127.5
V24    0.0364   0.0752   0.0001   1.0000    124.9
V25    0.8920   0.2518   0.0602   1.0000    122.0
V26    0.6594   0.2119   0.4389   1.0000    121.3
V27    0.2953   0.2290   0.7629   1.0000    115.2
V28    0.3757   0.1166   0.3824   1.0000    114.4
V29    0.6649   0.0805   0.6618   1.0000    113.4
V30    0.2268   0.2437   0.9841   1.0000    112.4
V31    0.7356   0.1123   0.9456   1.0000    111.2
V32    0.2538   0.0764   0.8991   1.0000    110.7
V33    0.3939   0.0306   0.4608   1.0000    110.5
```

So that, the SHELXS 2 first tries above obviously give the heavy atoms and more. Completing the structure by alternating Rietveld refinements and Fourier difference synthesis would be a kid game, asking for a total of a few hours of work, no more.

INDEED, even ESPOIR can solve it

Very short data (.dat file) prepared for ESPOIR in "scratch" mode (all atoms disordered at the beginning):

```
Test on Sr5V3(F/O/OH/H2O)22
11.243328   8.195712  19.949343  90.0 106.728287  90.0
```

```
P 21/C
0.79764 4 30 3 1 1 3
0.00192   0.00092   0.00031   3
Sr  V   F
0
10. 10. 10.
1.5 1.0 0.007
50000 2000000 2000000
800000 0.350 2 100
1 10
5 3 22
1. 0 0
```

The .hkl files with 300 hkl only (recommended Natoms x 10):

```
  300
   1   0   0   53.34   52.61
   0   0   2   47.50   67.64
   1   0  -2   98.60   57.01
   0   1   1   20.50  102.46
   1   1  -1   20.64   60.59
   1   1   0   24.70   68.20
   1   0   2    8.55  157.26
   0   1   2   42.19   75.32
   1   1  -2   21.15   99.11
   1   1   1   18.34   93.48
   2   0  -2   73.75   86.61
   2   0   0   83.42   88.30
   0   1   3   35.09  102.09
   1   1  -3   12.05   67.56
   1   1   2    6.26   94.05
   1   0  -4   85.91  108.98
   0   0   4  103.42  114.57
   2   1  -1   25.33  164.53
   2   1  -2    8.92  202.31
   2   1   0   11.90  211.27
   2   0  -4  147.12  101.80
   1   1  -4   23.13   28.48
   1   1   3   50.83   32.85
   2   0   2  149.35   85.56
   2   1  -3   39.26   63.04
   2   1   1   48.18   71.28
   0   1   4   49.67   76.42
   0   2   0  105.64  115.21
   0   2   1   74.29   90.23
   1   0   4   42.80  214.63
   1   2  -1   36.93  116.38
   1   2   0   29.82   93.18
   0   2   2   29.72  115.28
   2   1  -4    8.06   84.49
   2   1   2   20.29   56.19
   3   0  -2   99.82  121.24
   1   2  -2   61.06   62.82
   1   2   1   87.40   78.20
   3   0   0  237.87  115.46
   1   1  -5   87.88   73.72
   1   1   4    7.31   31.39
   0   1   5   43.09  113.06
   0   2   3   40.30   34.69
Etc
```

Best result at test 7 ;

```
Test number :   7
 24-Aug-2002      3 hour 18 min 21 Sec

  Object number  1 at test  7.  Previous minimum R=0.189 at test  5
      0 moves acc.       0 tested; Chi**2=0.750    , R=0.750
      0 perm. acc.       0 tested
      0 events did not improve the fit, DAMP = 1.000000

  Object number  1 at test  7.  Previous minimum R=0.166 at test  7
  61427 moves acc. 1800000 tested; Chi**2=0.194    , R=0.167
    686 perm. acc.  199999 tested
  34803 events did not improve the fit, DAMP = 0.010000

 Final coordinates x,y,z and occupation numbers

Sr1      0.85973    0.58695    0.84950      1.000
Sr2      0.17651    0.86459    0.83951      1.000
Sr3      0.51901    0.06793    0.64098      1.000
Sr4      0.26771    0.07598    0.02089      1.000
Sr5      0.84348    0.65604    0.16177      1.000
V1       0.76497    0.10830    0.51388      1.000
V2       0.09174    0.60902    0.67032      1.000
V3       0.41717    0.45531    0.33294      1.000
F1       0.22187    0.41551    0.26828      1.000
F2       0.08749    0.62170    0.03707      1.000
F3       0.44283    0.87862    0.08412      1.000
F4       0.41525    0.04795    0.71152      1.000
F5       0.49100    0.36800    0.25082      1.000
F6       0.04569    0.14038    0.18089      1.000
F7       0.45884    0.27750    0.52572      1.000
F8       0.89967    0.35221    0.82657      1.000
F9       0.69051    0.38756    0.85416      1.000
F10      0.42540    0.76113    0.46065      1.000
F11      0.74186    0.68472    0.03523      1.000
F12      0.26576    0.58518    0.75495      1.000
F13      0.90937    0.61496    0.57026      1.000
F14      0.95636    0.85873    0.82417      1.000
F15      0.30847    0.41709    0.43175      1.000
F16      0.24311    0.29984    0.64032      1.000
F17      0.93832    0.37829    0.10006      1.000
F18      0.18550    0.61890    0.61767      1.000
F19      0.25077    0.94249    0.41017      1.000
F20      0.99316    0.41046    0.23051      1.000
F21      0.75894    0.76679    0.31159      1.000
F22      0.43977    0.86862    0.53995      1.000
 24-Aug-2002      4 hour  1 min 47 Sec
```

From this proposal, more moves are made on short distances (1 Å maximum) and more data (500hkl) :

Data file :

```
Test on Sr5V3(F/O/OH/H2O)22    solution a 16% relancee sur 500 hkl
11.243328   8.195712  19.949343  90.0 106.728287  90.0
P 21/C
0.79764 4 30 3 1 1 3
0.00192   0.00092   0.00031   3
Sr  V   F
0
1. 1. 1.
1.5 1.0 0.002
20000 500000 500000
200000 0.350 2 10
0 10
5 3 22
```

```
1. 0 0
     0.85973    0.58695    0.84950 1.00
     0.17651    0.86459    0.83951 1.00
     0.51901    0.06793    0.64098 1.00
     0.26771    0.07598    0.02089 1.00
     0.84348    0.65604    0.16177 1.00
     0.76497    0.10830    0.51388 1.00
     0.09174    0.60902    0.67032 1.00
     0.41717    0.45531    0.33294 1.00
     0.22187    0.41551    0.26828 1.00
     0.08749    0.62170    0.03707 1.00
     0.44283    0.87862    0.08412 1.00
     0.41525    0.04795    0.71152 1.00
     0.49100    0.36800    0.25082 1.00
     0.04569    0.14038    0.18089 1.00
     0.45884    0.27750    0.52572 1.00
     0.89967    0.35221    0.82657 1.00
     0.69051    0.38756    0.85416 1.00
     0.42540    0.76113    0.46065 1.00
     0.74186    0.68472    0.03523 1.00
     0.26576    0.58518    0.75495 1.00
     0.90937    0.61496    0.57026 1.00
     0.95636    0.85873    0.82417 1.00
     0.30847    0.41709    0.43175 1.00
     0.24311    0.29984    0.64032 1.00
     0.93832    0.37829    0.10006 1.00
     0.18550    0.61890    0.61767 1.00
     0.25077    0.94249    0.41017 1.00
     0.99316    0.41046    0.23051 1.00
     0.75894    0.76679    0.31159 1.00
     0.43977    0.86862    0.53995 1.00
```

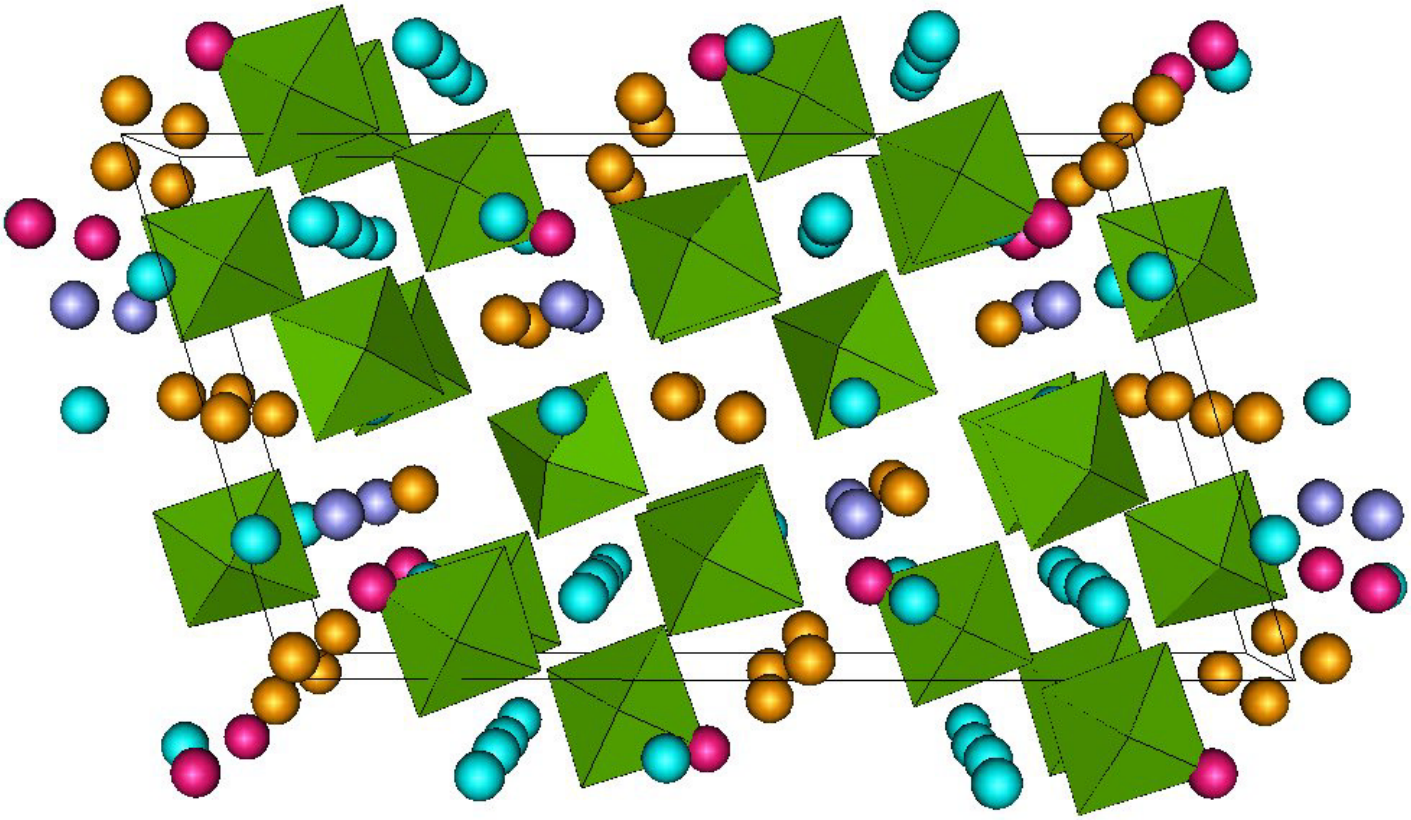
New results :

```
  Object number  1 at test  6.  Previous minimum R=0.109 at test  6
  21155 moves acc.  450000 tested; Chi**2=0.109    , R=0.109
      0 perm. acc.   49999 tested
  11640 events did not improve the fit, DAMP = 0.009999

 Final coordinates x,y,z and occupation numbers

Sr1      0.84956    0.58376    0.85312      1.000
Sr2      0.16000    0.83357    0.82698      1.000
Sr3      0.50611    0.08272    0.64595      1.000
Sr4      0.25918    0.08924    0.01584      1.000
Sr5      0.83898    0.65650    0.17379      1.000
V1       0.76663    0.07754    0.52510      1.000
V2       0.09891    0.57688    0.67177      1.000
V3       0.42489    0.41025    0.33878      1.000
F1       0.22682    0.39186    0.27895      1.000
F2       0.15241    0.54878    0.04376      1.000
F3       0.43549    0.93050    0.08585      1.000
F4       0.46401    0.14406    0.76017      1.000
F5       0.38787    0.65213    0.32801      1.000
F6       0.05137    0.10680    0.17764      1.000
F7       0.48625    0.27322    0.53523      1.000
F8       0.90058    0.32237    0.81410      1.000
F9       0.68627    0.40444    0.84016      1.000
F10      0.37727    0.90766    0.53016      1.000
F11      0.78275    0.65563    0.04490      1.000
F12      0.24781    0.57242    0.74777      1.000
F13      0.93678    0.70891    0.47065      1.000
F14      0.89546    0.83117    0.78551      1.000
F15      0.32414    0.46449    0.40122      1.000
F16      0.17257    0.59199    0.61194      1.000
```

```
F17      0.92596     0.43663     0.11097       1.000
F18      0.92086     0.60667     0.60794       1.000
F19      0.29322     0.88015     0.39621       1.000
F20      0.97569     0.41883     0.23213       1.000
F21      0.68808     0.75142     0.39495       1.000
F22      0.34068     0.70727     0.63924       1.000
 24-Aug-2002     20 hour 28 min 57 Sec

 End of this test
```

In this starting model for Rietveld refinement, most atoms are correctly located. But a little more work by alternating Fourier difference synthesis and Rietveld refinement is needed.

Poor view of the final complex structure :



Isolated VF_6 and VOF_5 octahedra in green.
Sr atoms in blue.
The O atom in the VOF_5 octahedron in red.
Water molecules in brown.
One special F atom in purple.

Projection viewed from a STRUVIR VRML plot available at the SDPDRR-2 web site.