Sample 2

1. Preliminary work

1.1 Did you obtained additional informations from the
chemical formula ? If yes, how and what information ?
(for instance from CSD or ICSD or ICDD databases)

No

1.2 Did you obtained additional informations from the
powder pattern ? If yes, how and what information ?
(for instance using the JCPDS-ICDD database)

No

1.3 Did you extract the structure factors ? Yes [ ] No [X]

1.3.1 If yes, which program(s) did you use ?
1.3.2 Give the angular range:
1.3.3 Give the number of extracted structure factors:
1.3.4 Give the Rp and Rwp (conventional Rietveld, background subtracted):
1.3.5 Give the Rp and Rwp (background not subtracted):

1.3.6 If not, did you use the whole pattern ? Yes
1.3.7 Or a partial pattern (if yes, give the angular range):

2- Structure solution

2.1 Did you use direct methods ? Yes [ ] No [x]

2.1.1 If yes, was it on the whole dataset ?
2.1.2 Or on a partial dataset ?
2.1.3 Give the number of reflections:
2.1.4 Which program(s) did you use ?
2.1.5 Did you modified intensities of closely neighbouring
reflections ? If yes, explain how.

2.2 Did you use Patterson methods ? Yes [ ] No [x]

2.2.1 If yes, was it on the whole dataset ?
2.2.2 Or on a partial dataset ?
2.2.3 Give the number of reflections:
2.2.4 Which program(s) did you use ?
2.2.5 Did you modified intensities of closely neighbouring reflections ? If yes, explain how.

2.3 Did you use another method ? Yes [x] No [ ]

2.3.1 If yes, which method(s) (give details : molecule location by direct space - genetic algorithm, Monte Carlo, Simulated anneling, scratch, other) ?

Molecule location in direct space, Simulated annealing, structure determination using step intensity data

2.3.2 Which program(s) did you use ? TOPAS

2.3.3 If you used molecule location methods, how many independent molecules did you use (give details on these molecules)? How many degrees of freedom (total) ? How many torsion angles ?

30 independent atoms (no constraints/restraints) put into the cell at random positions.

2.4 Did you first locate the whole structure ? Yes [x] No [ ]

2.4.1 If not, how many atoms did you locate ?
2.4.2 Give their name and initial atomic coordinates

Atom	x	y	z
.....			
.....			
.....			

2.4.3 Were the initial atomic coordinates taken from a known structure ? Yes [ ] No [x]

If yes, which one (give reference) ?

3- Structure completion

3.1 Did you performed Fourier difference syntheses before refining the structure by the Rietveld method ? Yes [ ] No [x]
3.2 If yes, with what program ?
3.3 If yes, how many additional atoms did you obtained from Fourier difference syntheses ?
3.4 Give their name and atomic coordinates as they were obtained

Atom	x	y	z
.....			
.....			
.....			

Not applicable. Structure determined using step intensity data.

3.5 Did you made first Rietveld refinements without preliminary Fourier difference syntheses ? Yes [ ] No [x]
3.5.1 If yes, with what program ? TOPAS
3.5.2 What were the Rp and Rwp (background subtracted AND not subtracted) and RB and RF that you obtained at the first Rietveld application ?
3.5.3 Did you get the structure factors from this result and performed a Fourier difference synthesis ?
3.5.4 Did you locate additional atoms at this stage ?
3.5.5 And which one ?

Atom	x	y	z
.....			
.....			
.....			

Not applicable. Structure determined using step intensity data. Final refinement to bring profile shapes in.

3.5.6 If you repeated Rietveld refinements and Fourier synthese several times before to complete the model, give the number

of times and which atoms you locate and the Rp, Rwp
RB, RF at each times.

Atom	x	y	z
.....			
.....			
.....			

Not applicable. Structure determined using step intensity data. Final refinement to bring profile shapes in.

4- Final refinement

- Give the final atomic coordinates, thermal parameters, standard deviations, Reliability factors.....

SG: P21/c
a 11.24341
b 8.19572
c 19.94952
be 106.72849
R_exp 5.501
R_exp(background subtracted) 8.896
R_wp 6.235
R_wp(background subtracted) 10.084
R_p 4.831
R_p(background subtracted) 8.934
Weighted_Durbin_Watson 1.581
gof 1.134
Rbragg 3.06

Atom	x	y	z	B
Sr1	0.65665	0.84461	0.32505	0.5239
Sr2	0.00777	0.91642	0.64657	0.5198
Sr3	0.24055	0.41190	0.48228	0.6170
Sr4	0.66483	0.16574	0.82879	0.4529
Sr5	0.64984	0.58438	0.14694	0.5302
V1	0.59982	0.08191	0.17318	1.1054
V2	0.26552	0.92250	0.52372	1.1640
V3	0.07628	0.08487	0.15942	1.0759

O1	0.82793	0.96699	0.90809	0.1308
O2	0.58419	0.31359	0.18844	0.1308
O3	0.11025	0.18296	0.64934	0.1308
O4	0.87558	0.06916	0.53365	0.1308
O5	0.44756	0.28583	0.47252	0.1308
O6	0.10723	0.64497	0.68430	0.1308
O7	0.79596	0.39432	0.89463	0.1308
O8	0.42313	0.57497	0.10674	0.1308
O9	0.01655	0.21920	0.96883	0.1308
O10	0.74035	0.08468	0.25444	0.1308
O11	0.80852	0.77480	0.61454	0.1308
O12	0.66387	0.42889	0.61198	0.1308
O13	0.36494	0.56245	0.96444	0.1308
O14	0.02407	0.12420	0.23971	0.1308
O15	0.29755	0.81277	0.03204	0.1308
O16	0.27335	0.15152	0.54594	0.1308
O17	0.84161	0.12495	0.67026	0.1308
O18	0.06790	0.92661	0.90269	0.1308
O19	0.73803	0.59418	0.27549	0.1308
O20	0.48796	0.91495	0.74566	0.1308
O21	0.42799	0.41589	0.61897	0.1308
O22	0.42457	0.14597	0.81339	0.1308

- Give details about constraints, restraints

No constraints / restraints