

data\_veat

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\_chemical\_name\_systematic  
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\_chemical\_name\_common ?  
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\_chemical\_formula\_weight 629.44

loop\_  
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'B' 'B' 0.0013 0.0007  
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
'H' 'H' 0.0000 0.0000  
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
'O' 'O' 0.0106 0.0060  
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
'Sr' 'Sr' -1.5307 3.2498  
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
'Ca' 'Ca' 0.2262 0.3064  
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

\_symmetry\_cell\_setting ?  
\_symmetry\_space\_group\_name\_H-M ?

loop\_  
\_symmetry\_equiv\_pos\_as\_xyz  
'x, y, z'  
'x, -y, z+1/2'  
'x+1/2, y+1/2, z'  
'x+1/2, -y+1/2, z+1/2'

\_cell\_length\_a 6.6070(10)  
\_cell\_length\_b 11.712(2)  
\_cell\_length\_c 20.685(4)  
\_cell\_angle\_alpha 90.00  
\_cell\_angle\_beta 92.00(3)  
\_cell\_angle\_gamma 90.00  
\_cell\_volume 1599.7(5)  
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_exptl_special_details
;
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;

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_computing_cell_refinement      ?
_computing_data_reduction       ?
_computing_structure_solution   'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'

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\_computing\_molecular\_graphics ?  
\_computing\_publication\_material ?

\_refine\_special\_details

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Refinement of  $F^2$  against ALL reflections. The weighted R-factor wR and goodness of fit S are based on  $F^2$ , conventional R-factors R are based on F, with F set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\sigma(F^2)$  is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on  $F^2$  are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

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\_atom\_sites\_solution\_hydrogens geom  
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'Flack H D (1983), Acta Cryst. A39, 876-881'  
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loop\_

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\_atom\_site\_refinement\_flags  
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 Sr2 Sr 0.90046(3) -0.03728(2) 0.599674(12) 0.01406(5) Uani 0.4787(5) 1 d P . .  
 Ca2 Ca 0.90046(3) -0.03728(2) 0.599674(12) 0.01406(5) Uani 0.52 1 d P . .  
 B1 B 0.6298(3) 0.10495(17) 0.71821(10) 0.0112(4) Uani 1 1 d . . .  
 B2 B 0.9210(3) 0.29187(19) 0.86676(11) 0.0172(5) Uani 1 1 d . . .  
 B3 B 1.2054(3) 0.16975(17) 0.58534(10) 0.0117(4) Uani 1 1 d . . .  
 B4 B 0.7733(3) 0.56177(17) 0.72396(10) 0.0123(4) Uani 1 1 d . . .  
 B5 B 0.5625(3) 0.21317(17) 0.58033(10) 0.0115(4) Uani 1 1 d . . .  
 B6 B 0.9170(3) 0.40588(18) 0.46028(10) 0.0165(5) Uani 1 1 d . . .  
 B7 B 1.4131(3) 0.37624(19) 0.84453(10) 0.0161(5) Uani 1 1 d . . .  
 B8 B 0.9242(3) -0.02903(16) 0.74006(10) 0.0104(4) Uani 1 1 d . . .  
 B9 B 0.9102(3) 0.30440(18) 0.56329(10) 0.0108(4) Uani 1 1 d . . .  
 B10 B 1.3919(3) 0.26032(17) 0.74332(10) 0.0105(4) Uani 1 1 d . . .  
 B11 B 0.9427(3) 0.48615(17) 1.06241(10) 0.0106(4) Uani 1 1 d . . .  
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 OH5 O 0.9265(3) 0.39053(13) 0.83304(7) 0.0307(5) Uani 1 1 d . . .  
 OH6 O 0.9195(3) 0.28373(14) 0.93207(7) 0.0347(5) Uani 1 1 d . . .  
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 O8 O 1.24678(19) 0.05615(11) 0.58803(7) 0.0133(3) Uani 1 1 d . . .  
 O9 O 1.00892(19) 0.20200(11) 0.59045(6) 0.0124(3) Uani 1 1 d . . .  
 O10 O 1.23158(19) 0.17507(10) 0.72737(6) 0.0126(3) Uani 1 1 d . . .  
 O11 O 0.63717(18) 0.47511(11) 0.71920(6) 0.0131(3) Uani 1 1 d . . .  
 O12 O 0.60609(19) 0.09991(11) 0.57796(6) 0.0124(3) Uani 1 1 d . . .  
 O13 O 0.69558(18) 0.30054(11) 0.58479(6) 0.0132(3) Uani 1 1 d . . .  
 O14 O 0.9146(2) 0.30444(12) 0.49212(6) 0.0154(3) Uani 1 1 d . . .  
 OH15 O 0.4136(3) 0.08760(13) 0.89391(7) 0.0328(4) Uani 1 1 d . . .  
 O16 O 0.9181(2) 0.49160(12) 0.99184(6) 0.0156(3) Uani 1 1 d . . .  
 O17 O 1.4115(2) 0.27265(11) 0.81443(6) 0.0145(3) Uani 1 1 d . . .  
 O18 O 0.9141(2) -0.02357(11) 0.81022(6) 0.0145(3) Uani 1 1 d . . .  
 OH19 O 0.9194(3) 0.11520(12) 0.41017(7) 0.0290(4) Uani 1 1 d . . .  
 O20 O 1.00514(18) 0.40661(11) 0.59166(6) 0.0105(3) Uani 1 1 d . . .  
 O21 O 1.33308(18) 0.36744(10) 0.71303(6) 0.0111(3) Uani 1 1 d . . .  
 OW22 O 0.8907(3) -0.06724(14) 0.48725(8) 0.0329(5) Uani 1 1 d . . .  
 H4 H 0.922(4) 0.139(2) 0.8336(11) 0.016(6) Uiso 1 1 d . . .  
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 H6 H 0.875(5) 0.333(3) 0.9477(14) 0.045(9) Uiso 1 1 d . . .  
 H15 H 0.410(4) 0.145(2) 0.8739(13) 0.030(7) Uiso 1 1 d . . .  
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loop\_

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\_atom\_site\_aniso\_U\_22

\_atom\_site\_aniso\_U\_33

\_atom\_site\_aniso\_U\_23

\_atom\_site\_aniso\_U\_13

\_atom\_site\_aniso\_U\_12

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Ca1 0.00968(6) 0.00849(6) 0.01550(7) -0.00014(7) 0.00143(5) -0.00026(7)  
 Sr2 0.01432(10) 0.01208(10) 0.01587(10) -0.00099(9) 0.00185(8) 0.00055(9)  
 Ca2 0.01432(10) 0.01208(10) 0.01587(10) -0.00099(9) 0.00185(8) 0.00055(9)  
 B1 0.0121(8) 0.0073(8) 0.0142(8) 0.0002(7) -0.0016(7) -0.0013(7)  
 B2 0.0211(10) 0.0134(9) 0.0173(9) 0.0004(8) 0.0035(8) 0.0032(8)  
 B3 0.0092(8) 0.0128(9) 0.0131(8) 0.0007(7) 0.0011(7) 0.0017(7)  
 B4 0.0100(8) 0.0101(8) 0.0167(9) 0.0015(7) -0.0010(7) 0.0015(7)  
 B5 0.0105(8) 0.0124(9) 0.0117(8) -0.0025(7) 0.0018(7) 0.0025(7)  
 B6 0.0240(10) 0.0100(9) 0.0155(9) -0.0015(8) 0.0004(8) -0.0005(8)  
 B7 0.0172(9) 0.0177(9) 0.0138(9) -0.0015(8) 0.0033(7) -0.0001(8)  
 B8 0.0102(8) 0.0038(7) 0.0173(9) -0.0011(7) 0.0015(7) -0.0012(6)  
 B9 0.0098(8) 0.0110(8) 0.0120(8) 0.0012(7) 0.0042(7) 0.0011(7)  
 B10 0.0116(8) 0.0082(8) 0.0121(8) -0.0014(7) 0.0038(7) 0.0001(7)  
 B11 0.0099(8) 0.0058(8) 0.0160(8) 0.0001(7) -0.0006(7) 0.0004(7)  
 O1 0.0114(5) 0.0067(5) 0.0216(6) -0.0028(5) 0.0021(5) 0.0020(5)  
 O2 0.0097(6) 0.0084(5) 0.0215(6) 0.0011(5) 0.0030(5) 0.0030(4)  
 O3 0.0109(5) 0.0064(5) 0.0169(6) 0.0033(5) 0.0026(5) 0.0024(4)  
 OH4 0.0436(9) 0.0112(6) 0.0207(7) -0.0021(6) 0.0017(7) 0.0008(6)  
 OH5 0.0635(11) 0.0122(7) 0.0166(7) -0.0012(6) 0.0025(7) -0.0022(8)  
 OH6 0.0751(13) 0.0140(7) 0.0152(7) -0.0014(6) 0.0058(8) 0.0013(8)  
 O7 0.0128(6) 0.0053(5) 0.0208(6) -0.0008(5) 0.0010(5) -0.0017(5)  
 O8 0.0093(5) 0.0092(6) 0.0215(6) 0.0007(5) 0.0019(5) 0.0005(5)  
 O9 0.0096(5) 0.0092(6) 0.0186(6) 0.0034(5) 0.0018(5) 0.0020(5)  
 O10 0.0113(5) 0.0059(5) 0.0205(6) 0.0003(5) 0.0004(5) -0.0020(5)  
 O11 0.0088(5) 0.0084(5) 0.0224(6) -0.0012(5) 0.0025(5) -0.0007(4)  
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 O13 0.0098(5) 0.0081(5) 0.0220(6) -0.0006(5) 0.0035(5) 0.0016(5)  
 O14 0.0240(7) 0.0111(6) 0.0112(6) -0.0014(5) 0.0012(5) -0.0039(5)  
 OH15 0.0700(11) 0.0132(7) 0.0153(7) 0.0023(6) 0.0029(7) 0.0035(8)  
 O16 0.0243(7) 0.0094(6) 0.0129(6) 0.0010(5) -0.0005(5) -0.0018(5)  
 O17 0.0231(6) 0.0079(6) 0.0127(6) 0.0010(5) 0.0023(5) -0.0001(5)  
 O18 0.0222(6) 0.0071(6) 0.0142(6) -0.0017(5) -0.0003(5) 0.0015(5)  
 OH19 0.0645(11) 0.0091(6) 0.0135(7) -0.0005(6) 0.0020(7) 0.0007(7)  
 O20 0.0104(5) 0.0092(6) 0.0119(6) -0.0002(5) -0.0006(4) -0.0008(5)  
 O21 0.0124(6) 0.0050(5) 0.0157(6) 0.0006(5) 0.0004(5) 0.0005(5)  
 OW22 0.0606(12) 0.0129(7) 0.0253(8) 0.0030(6) 0.0052(8) 0.0002(7)

\_geom\_special\_details

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All esds (except the esd in the dihedral angle between two l.s. planes)  
 are estimated using the full covariance matrix. The cell esds are taken  
 into account individually in the estimation of esds in distances, angles  
 and torsion angles; correlations between esds in cell parameters are only  
 used when they are defined by crystal symmetry. An approximate (isotropic)  
 treatment of cell esds is used for estimating esds involving l.s. planes.

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loop\_

\_geom\_bond\_atom\_site\_label\_1

\_geom\_bond\_atom\_site\_label\_2

\_geom\_bond\_distance

\_geom\_bond\_site\_symmetry\_2

\_geom\_bond\_publ\_flag

Sr1 O1 2.5295(13) . ?

Sr1 O10 2.5432(13) . ?  
 Sr1 O2 2.5598(13) . ?  
 Sr1 OH5 2.6678(16) . ?  
 Sr1 OH4 2.6941(16) . ?  
 Sr1 O21 2.7301(13) . ?  
 Sr1 O11 2.7514(13) . ?  
 Sr1 O20 2.7975(13) . ?  
 Sr1 O3 2.8798(14) . ?  
 Sr1 O9 2.8840(14) . ?  
 Sr1 O13 3.0236(16) . ?  
 Sr1 B9 3.084(2) . ?  
 Sr2 OW22 2.3505(17) . ?  
 Sr2 O12 2.5505(13) . ?  
 Sr2 O7 2.5545(14) . ?  
 Sr2 O8 2.5552(13) . ?  
 Sr2 O21 2.6485(14) 3\_445 ?  
 Sr2 O3 2.6679(14) . ?  
 Sr2 O20 2.6928(13) 3\_445 ?  
 Sr2 O13 2.7471(13) 3\_545 ?  
 Sr2 O11 2.8826(15) 3\_545 ?  
 Sr2 O9 2.9005(14) . ?  
 Sr2 B8 2.904(2) . ?  
 Sr2 B5 3.143(2) 3\_545 ?  
 B1 O3 1.358(2) . ?  
 B1 O1 1.358(2) . ?  
 B1 O2 1.378(2) 3\_445 ?  
 B2 OH5 1.351(3) . ?  
 B2 OH6 1.355(3) . ?  
 B2 OH4 1.355(3) . ?  
 B3 O8 1.359(2) . ?  
 B3 O9 1.360(2) . ?  
 B3 O7 1.383(2) 3 ?  
 B4 O11 1.357(2) . ?  
 B4 O10 1.358(2) 3\_455 ?  
 B4 O2 1.399(2) . ?  
 B5 O13 1.350(2) . ?  
 B5 O12 1.359(2) . ?  
 B5 O7 1.405(2) 3\_455 ?  
 B5 Sr2 3.143(2) 3\_455 ?  
 B5 Ca2 3.143(2) 3\_455 ?  
 B6 O14 1.359(3) . ?  
 B6 O16 1.367(2) 2\_564 ?  
 B6 OH15 1.375(3) 4\_554 ?  
 B7 OH19 1.361(3) 4 ?  
 B7 O17 1.364(3) . ?  
 B7 O18 1.372(3) 3 ?  
 B8 O21 1.457(2) 3\_445 ?  
 B8 O18 1.456(2) . ?  
 B8 O11 1.487(2) 3\_545 ?  
 B8 O3 1.490(2) . ?  
 B9 O20 1.464(2) . ?  
 B9 O9 1.468(2) . ?  
 B9 O14 1.473(2) . ?  
 B9 O13 1.502(2) . ?

B10 O21 1.449(2) . ?  
 B10 O17 1.479(2) . ?  
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 B11 O20 1.448(2) 2\_565 ?  
 B11 O16 1.464(2) . ?  
 B11 O8 1.500(2) 4\_455 ?  
 B11 O12 1.504(2) 4 ?  
 B11 Sr2 3.152(2) 4 ?  
 B11 Ca2 3.152(2) 4 ?  
 O1 B10 1.484(2) 1\_455 ?  
 O2 B1 1.378(2) 3 ?  
 O7 B3 1.383(2) 3\_445 ?  
 O7 B5 1.405(2) 3\_545 ?  
 O8 B11 1.500(2) 4\_554 ?  
 O10 B4 1.358(2) 3\_545 ?  
 O11 B8 1.487(2) 3\_455 ?  
 O11 Sr2 2.8826(15) 3\_455 ?  
 O11 Ca2 2.8826(15) 3\_455 ?  
 O12 B11 1.504(2) 4\_454 ?  
 O13 Ca2 2.7471(13) 3\_455 ?  
 O13 Sr2 2.7471(13) 3\_455 ?  
 OH15 B6 1.375(3) 4\_455 ?  
 O16 B6 1.367(2) 2\_565 ?  
 O18 B7 1.372(3) 3\_445 ?  
 OH19 B7 1.361(3) 4\_454 ?  
 O20 B11 1.448(2) 2\_564 ?  
 O20 Ca2 2.6928(13) 3 ?  
 O20 Sr2 2.6928(13) 3 ?  
 O21 B8 1.457(2) 3 ?  
 O21 Ca2 2.6485(14) 3 ?  
 O21 Sr2 2.6485(14) 3 ?

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 O1 Sr1 O10 115.24(4) . . ?  
 O1 Sr1 O2 120.94(4) . . ?  
 O10 Sr1 O2 121.44(4) . . ?  
 O1 Sr1 OH5 93.16(6) . . ?  
 O10 Sr1 OH5 98.19(5) . . ?  
 O2 Sr1 OH5 64.63(4) . . ?  
 O1 Sr1 OH4 71.70(5) . . ?  
 O10 Sr1 OH4 69.47(5) . . ?  
 O2 Sr1 OH4 113.61(4) . . ?  
 OH5 Sr1 OH4 49.17(5) . . ?  
 O1 Sr1 O21 168.44(4) . . ?  
 O10 Sr1 O21 53.33(4) . . ?  
 O2 Sr1 O21 69.62(4) . . ?

OH5 Sr1 O21 87.43(6) .. ?  
OH4 Sr1 O21 100.35(5) .. ?  
O1 Sr1 O11 69.74(4) .. ?  
O10 Sr1 O11 168.54(4) .. ?  
O2 Sr1 O11 51.53(4) .. ?  
OH5 Sr1 O11 70.82(5) .. ?  
OH4 Sr1 O11 103.97(5) .. ?  
O21 Sr1 O11 121.12(4) .. ?  
O1 Sr1 O20 113.86(5) .. ?  
O10 Sr1 O20 101.70(5) .. ?  
O2 Sr1 O20 70.12(4) .. ?  
OH5 Sr1 O20 134.56(4) .. ?  
OH4 Sr1 O20 171.16(4) .. ?  
O21 Sr1 O20 73.06(4) .. ?  
O11 Sr1 O20 84.65(4) .. ?  
O1 Sr1 O3 50.59(4) .. ?  
O10 Sr1 O3 65.88(4) .. ?  
O2 Sr1 O3 171.00(4) .. ?  
OH5 Sr1 O3 110.52(4) .. ?  
OH4 Sr1 O3 62.63(4) .. ?  
O21 Sr1 O3 118.56(4) .. ?  
O11 Sr1 O3 120.29(4) .. ?  
O20 Sr1 O3 114.88(4) .. ?  
O1 Sr1 O9 92.72(5) .. ?  
O10 Sr1 O9 70.93(4) .. ?  
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OH5 Sr1 O9 169.05(5) .. ?  
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