

```

data_Conf1.cif
_audit_creation_method      'generated by CrystalMaker 6.3.7'
_cell_length_a              9.6007
_cell_length_b              10.2930
_cell_length_c              12.0497
_cell_angle_alpha           90.0000
_cell_angle_beta            90.0000
_cell_angle_gamma           90.0000

```

```

_symmetry_space_group_name_H-M  'P 1'
_symmetry_Int_Tables_number     1
_symmetry_cell_setting          triclinic
loop_
_symmetry_equiv_pos_as_xyz
' +x      +y      +z  '

```

```

loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
H      112    0.3017  0.0275  0.1250
H      113    0.2150  0.1527  0.2058
H      114    0.2150  0.1527  0.0442
H      115    0.0398  0.8412  0.1250
Mg      1     0.0044  0.0106 -0.0002
Mg      2     0.2492  0.4983 -0.0007
Mg      3     0.0044  0.0106  0.2502
Mg      4     0.2492  0.4983  0.2507
Mg      5     0.4930  0.2768  0.1250
Mg      6     0.7458  0.2249  0.3748
Mg      7    -0.4960 -0.2756  0.3752
Mg      8    -0.2481  0.7775  0.1250
Mg     28     0.5020  0.0012 -0.0009
Mg     29     0.7501  0.4999  0.0000
Mg     30     0.5020  0.0013  0.2509
Mg     31     0.7501  0.4999  0.2500
Mg     32     0.0014  0.2732  0.1250
Mg     33     0.2445  0.2271  0.3829
Mg     34     0.0031 -0.2751  0.3745
Mg     35     0.2597  0.7708  0.1250
Mg     56    -0.0011  0.0007  0.4998
Mg     57     0.2495  0.5037  0.5002
Mg     58    -0.0011  0.0007  0.7502
Mg     59     0.2495  0.5037  0.7498
Mg     60     0.4963  0.2779  0.6250
Mg     61     0.7458  0.2249  0.8752
Mg     62    -0.4960 -0.2756  0.8748
Mg     63    -0.2462  0.7783  0.6250
Mg     84     0.4997  0.0009  0.4998
Mg     85     0.7498  0.5015  0.5000
Mg     86     0.4997  0.0009  0.7502

```

Mg	87	0.7498	0.5015	0.7500
Mg	88	0.9954	0.2783	0.6250
Mg	89	0.2445	0.2271	0.8671
Mg	90	0.0031	-0.2751	0.8755
Mg	91	0.2537	0.7783	0.6250
O	12	0.3842	0.0840	0.1250
O	13	0.6339	0.4092	0.3752
O	14	-0.3846	-0.0907	0.3748
O	15	-0.1344	0.5909	0.1250
O	16	0.1129	0.4434	0.1250
O	17	0.3605	0.0561	0.3754
O	18	-0.1123	-0.4443	0.3754
O	19	0.1051	0.9150	0.1250
O	20	0.1280	0.1713	0.0037
O	21	0.3869	0.3369	-0.0165
O	22	-0.1388	-0.1632	0.2657
O	23	0.1111	0.6601	0.2342
O	24	-0.1388	-0.1632	-0.0157
O	25	0.1111	0.6601	0.0158
O	26	0.1280	0.1713	0.2463
O	27	0.3869	0.3369	0.2665
O	40	0.8840	0.0971	0.1250
O	41	0.1340	0.4121	0.3773
O	42	0.1151	-0.0902	0.3751
O	43	0.3653	0.5904	0.1250
O	44	0.6106	0.4453	0.1250
O	45	0.8605	0.0557	0.3743
O	46	0.3886	-0.4448	0.3746
O	47	0.6413	0.9476	0.1250
O	48	0.6360	0.1649	0.0161
O	49	0.8881	0.3389	-0.0161
O	50	0.3603	-0.1602	0.2643
O	51	0.6109	0.6632	0.2340
O	52	0.3603	-0.1602	-0.0143
O	53	0.6109	0.6632	0.0160
O	54	0.6360	0.1649	0.2339
O	55	0.8881	0.3389	0.2661
O	68	0.3836	0.0925	0.6250
O	69	0.6339	0.4092	0.8748
O	70	-0.3846	-0.0907	0.8752
O	71	-0.1350	0.5937	0.6250
O	72	0.1109	0.4483	0.6250
O	73	0.3605	0.0561	0.8746
O	74	-0.1123	-0.4443	0.8746
O	75	0.1381	0.9461	0.6250
O	76	0.1364	0.1638	0.5171
O	77	0.3876	0.3389	0.4848
O	78	-0.1387	-0.1611	0.7659
O	79	0.1114	0.6657	0.7341
O	80	-0.1387	-0.1611	0.4841
O	81	0.1114	0.6657	0.5159
O	82	0.1364	0.1638	0.7329
O	83	0.3876	0.3389	0.7652
O	96	0.8838	0.0924	0.6250

O	97	0.1340	0.4121	0.8727
O	98	0.1151	-0.0902	0.8749
O	99	0.3654	0.5939	0.6250
O	100	0.6109	0.4472	0.6250
O	101	0.8605	0.0557	0.8757
O	102	0.3886	-0.4448	0.8755
O	103	0.6377	0.9469	0.6250
O	104	0.6375	0.1641	0.5158
O	105	0.8876	0.3383	0.4845
O	106	0.3618	-0.1622	0.7669
O	107	0.6115	0.6642	0.7343
O	108	0.3618	-0.1622	0.4831
O	109	0.6115	0.6642	0.5158
O	110	0.6375	0.1641	0.7342
O	111	0.8876	0.3383	0.7655
Si	9	0.4634	0.4075	0.3750
Si	10	-0.2135	-0.0923	0.3741
Si	11	0.0364	0.5896	0.1250
Si	36	0.7137	0.0963	0.1250
Si	37	0.9633	0.4081	0.3753
Si	38	0.2856	-0.0915	0.3745
Si	39	0.5362	0.5927	0.1250
Si	64	0.2129	0.0934	0.6250
Si	65	0.4634	0.4075	0.8750
Si	66	-0.2135	-0.0923	0.8759
Si	67	0.0358	0.5960	0.6250
Si	92	0.7132	0.0944	0.6250
Si	93	0.9633	0.4081	0.8747
Si	94	0.2856	-0.0915	0.8755
Si	95	0.5362	0.5948	0.6250