

```

data_Conf6.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    0.2064  0.1240  0.2195
H      113    0.2064  0.1239  0.0305
H      114    0.2118  0.9832  0.1250
H      115    0.3233  0.1682  0.1249
Mg      1     0.0016  0.0008  0.0013
Mg      2     0.2511  0.4978 -0.0000
Mg      3     0.0017  0.0009  0.2487
Mg      4     0.2511  0.4978  0.2500
Mg      5     0.5119  0.2830  0.1250
Mg      6     0.7482  0.2240  0.3752
Mg      7    -0.4956 -0.2753  0.3748
Mg      8    -0.2444  0.7786  0.1250
Mg     28     0.4989  0.0031 -0.0008
Mg     29     0.7530  0.5017 -0.0002
Mg     30     0.4989  0.0031  0.2508
Mg     31     0.7530  0.5017  0.2502
Mg     32     0.0039  0.2699  0.1250
Mg     33     0.2437  0.2275  0.3840
Mg     34     0.0044 -0.2762  0.3743
Mg     35     0.2542  0.7686  0.1250
Mg     56    -0.0006  0.0001  0.4995
Mg     57     0.2505  0.5030  0.4999
Mg     58    -0.0006  0.0001  0.7505
Mg     59     0.2505  0.5030  0.7501
Mg     60     0.4971  0.2771  0.6250
Mg     61     0.7482  0.2240  0.8748
Mg     62    -0.4956 -0.2753  0.8752
Mg     63    -0.2459  0.7773  0.6250
Mg     84     0.4998  0.0005  0.4999
Mg     85     0.7503  0.5006  0.5000
Mg     86     0.4998  0.0005  0.7501

```

Mg	87	0.7503	0.5006	0.7500
Mg	88	0.9959	0.2771	0.6250
Mg	89	0.2437	0.2275	0.8660
Mg	90	0.0044	-0.2762	0.8757
Mg	91	0.2537	0.7774	0.6250
O	12	0.3846	0.0922	0.1250
O	13	0.6353	0.4089	0.3746
O	14	-0.3850	-0.0902	0.3747
O	15	-0.1322	0.5919	0.1250
O	16	0.1143	0.4424	0.1250
O	17	0.3590	0.0560	0.3750
O	18	-0.1109	-0.4449	0.3757
O	19	0.1270	0.9286	0.1250
O	20	0.1240	0.1673	-0.0004
O	21	0.3905	0.3363	-0.0143
O	22	-0.1386	-0.1627	0.2660
O	23	0.1136	0.6586	0.2347
O	24	-0.1386	-0.1627	-0.0160
O	25	0.1136	0.6586	0.0153
O	26	0.1240	0.1673	0.2504
O	27	0.3905	0.3363	0.2644
O	40	0.8848	0.0903	0.1250
O	41	0.1353	0.4109	0.3770
O	42	0.1152	-0.0927	0.3755
O	43	0.3682	0.5907	0.1250
O	44	0.6163	0.4498	0.1250
O	45	0.8608	0.0545	0.3751
O	46	0.3898	-0.4457	0.3742
O	47	0.6362	0.9473	0.1250
O	48	0.6404	0.1649	0.0161
O	49	0.8899	0.3384	-0.0155
O	50	0.3610	-0.1610	0.2647
O	51	0.6133	0.6654	0.2345
O	52	0.3610	-0.1610	-0.0147
O	53	0.6133	0.6654	0.0155
O	54	0.6404	0.1649	0.2339
O	55	0.8899	0.3384	0.2655
O	68	0.3839	0.0921	0.6250
O	69	0.6353	0.4089	0.8754
O	70	-0.3850	-0.0902	0.8753
O	71	-0.1344	0.5920	0.6250
O	72	0.1119	0.4466	0.6250
O	73	0.3590	0.0560	0.8750
O	74	-0.1109	-0.4449	0.8743
O	75	0.1384	0.9453	0.6250
O	76	0.1366	0.1631	0.5173
O	77	0.3885	0.3378	0.4838
O	78	-0.1390	-0.1626	0.7658
O	79	0.1119	0.6640	0.7340
O	80	-0.1390	-0.1626	0.4842
O	81	0.1119	0.6640	0.5160
O	82	0.1366	0.1631	0.7326
O	83	0.3885	0.3378	0.7662
O	96	0.8841	0.0916	0.6250

O	97	0.1353	0.4109	0.8730
O	98	0.1152	-0.0927	0.8745
O	99	0.3658	0.5929	0.6250
O	100	0.6112	0.4464	0.6250
O	101	0.8608	0.0545	0.8749
O	102	0.3898	-0.4457	0.8758
O	103	0.6379	0.9461	0.6250
O	104	0.6380	0.1635	0.5159
O	105	0.8886	0.3376	0.4842
O	106	0.3621	-0.1622	0.7664
O	107	0.6118	0.6635	0.7343
O	108	0.3621	-0.1622	0.4836
O	109	0.6118	0.6635	0.5157
O	110	0.6380	0.1635	0.7341
O	111	0.8886	0.3376	0.7658
Si	9	0.4647	0.4068	0.3743
Si	10	-0.2140	-0.0927	0.3749
Si	11	0.0384	0.5899	0.1250
Si	36	0.7147	0.0931	0.1250
Si	37	0.9644	0.4074	0.3751
Si	38	0.2857	-0.0927	0.3746
Si	39	0.5390	0.5965	0.1250
Si	64	0.2132	0.0925	0.6250
Si	65	0.4647	0.4068	0.8757
Si	66	-0.2140	-0.0927	0.8751
Si	67	0.0363	0.5940	0.6250
Si	92	0.7136	0.0935	0.6250
Si	93	0.9644	0.4074	0.8749
Si	94	0.2857	-0.0927	0.8754
Si	95	0.5365	0.5942	0.6250