

```

data_Conf4.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

```

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_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    0.2175  0.1459  0.2081
H      113    0.1921  0.1681  0.0583
H      114    0.2095  0.9873  0.1280
H      115    0.3455  0.1053  0.0442
Mg      1     0.0051  0.0023  0.0024
Mg      2     0.2495  0.4969 -0.0003
Mg      3     0.0056  0.0032  0.2485
Mg      4     0.2494  0.4968  0.2504
Mg      5     0.4972  0.2763  0.1265
Mg      6     0.7464  0.2230  0.3748
Mg      7    -0.4956 -0.2764  0.3747
Mg      8    -0.2423  0.7748  0.1258
Mg     28     0.5127 -0.0122 -0.0008
Mg     29     0.7500  0.4992 -0.0003
Mg     30     0.4984 -0.0010  0.2479
Mg     31     0.7501  0.4993  0.2501
Mg     32     0.9957  0.2731  0.1257
Mg     33     0.2440  0.2265  0.3821
Mg     34     0.0038 -0.2764  0.3741
Mg     35     0.2534  0.7680  0.1256
Mg     56    -0.0008 -0.0004  0.4994
Mg     57     0.2498  0.5024  0.5001
Mg     58     0.0011 -0.0012  0.7503
Mg     59     0.2501  0.5016  0.7498
Mg     60     0.4967  0.2760  0.6248
Mg     61     0.7481  0.2220  0.8753
Mg     62    -0.4948 -0.2795  0.8743
Mg     63    -0.2453  0.7764  0.6246
Mg     84     0.5006 -0.0001  0.4990
Mg     85     0.7500  0.4999  0.4999
Mg     86     0.5009 -0.0004  0.7508

```

Mg	87	0.7500	0.4992	0.7498
Mg	88	0.9955	0.2767	0.6249
Mg	89	0.2427	0.2263	0.8672
Mg	90	0.0057	-0.2778	0.8758
Mg	91	0.2541	0.7772	0.6251
O	12	0.3842	0.0943	0.1197
O	13	0.6342	0.4077	0.3753
O	14	-0.3844	-0.0916	0.3739
O	15	-0.1340	0.5901	0.1251
O	16	0.1118	0.4422	0.1250
O	17	0.3607	0.0555	0.3731
O	18	-0.1121	-0.4454	0.3753
O	19	0.1282	0.9285	0.1250
O	20	0.1202	0.1726	0.0007
O	21	0.3869	0.3336	-0.0163
O	22	-0.1370	-0.1641	0.2660
O	23	0.1123	0.6584	0.2347
O	24	-0.1361	-0.1651	-0.0157
O	25	0.1127	0.6583	0.0155
O	26	0.1287	0.1697	0.2448
O	27	0.3877	0.3360	0.2669
O	40	0.8849	0.0918	0.1262
O	41	0.1341	0.4106	0.3771
O	42	0.1157	-0.0920	0.3755
O	43	0.3658	0.5886	0.1251
O	44	0.6114	0.4447	0.1248
O	45	0.8613	0.0543	0.3741
O	46	0.3889	-0.4458	0.3749
O	47	0.6417	0.9435	0.1267
O	48	0.6404	0.1592	0.0147
O	49	0.8863	0.3390	-0.0158
O	50	0.3610	-0.1622	0.2645
O	51	0.6117	0.6619	0.2341
O	52	0.3641	-0.1657	-0.0140
O	53	0.6120	0.6620	0.0159
O	54	0.6365	0.1622	0.2335
O	55	0.8873	0.3376	0.2663
O	68	0.3844	0.0910	0.6256
O	69	0.6339	0.4065	0.8748
O	70	-0.3809	-0.0954	0.8733
O	71	-0.1345	0.5914	0.6250
O	72	0.1115	0.4462	0.6250
O	73	0.3624	0.0545	0.8821
O	74	-0.1122	-0.4452	0.8742
O	75	0.1388	0.9449	0.6247
O	76	0.1373	0.1627	0.5171
O	77	0.3877	0.3377	0.4851
O	78	-0.1354	-0.1642	0.7650
O	79	0.1126	0.6635	0.7339
O	80	-0.1388	-0.1624	0.4840
O	81	0.1116	0.6638	0.5160
O	82	0.1375	0.1615	0.7334
O	83	0.3873	0.3358	0.7652
O	96	0.8845	0.0911	0.6251

O	97	0.1340	0.4111	0.8728
O	98	0.1174	-0.0928	0.8758
O	99	0.3657	0.5927	0.6253
O	100	0.6110	0.4453	0.6249
O	101	0.8632	0.0525	0.8752
O	102	0.3893	-0.4480	0.8754
O	103	0.6385	0.9451	0.6249
O	104	0.6380	0.1626	0.5161
O	105	0.8880	0.3371	0.4844
O	106	0.3631	-0.1609	0.7673
O	107	0.6121	0.6621	0.7340
O	108	0.3623	-0.1619	0.4834
O	109	0.6117	0.6625	0.5156
O	110	0.6383	0.1618	0.7346
O	111	0.8884	0.3366	0.7659
Si	9	0.4636	0.4066	0.3754
Si	10	-0.2133	-0.0933	0.3739
Si	11	0.0368	0.5898	0.1251
Si	36	0.7148	0.0925	0.1254
Si	37	0.9634	0.4072	0.3753
Si	38	0.2860	-0.0926	0.3743
Si	39	0.5365	0.5923	0.1250
Si	64	0.2136	0.0920	0.6248
Si	65	0.4635	0.4040	0.8750
Si	66	-0.2096	-0.0956	0.8749
Si	67	0.0362	0.5937	0.6250
Si	92	0.7138	0.0925	0.6251
Si	93	0.9633	0.4073	0.8750
Si	94	0.2876	-0.0943	0.8780
Si	95	0.5365	0.5930	0.6248