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Table S1. Positional and thermal parameters of Groundstate SNP at 50K

Atom	occupation	x	y	z	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)	Uiso
Fe(g)	0.500000	0.500762	0.280393	0.500000	0.002583	0.003830	0.003085	-0.000215	0.000000	0.000000	0.003166
esd	0.000000	0.000018	0.000009	0.000000	0.000046	0.000038	0.000040	0.000028	0.000000	0.000000	0.000024
N(4g)	0.500000	0.727079	0.357971	0.500000	0.004584	0.005866	0.006355	-0.000349	0.000000	0.000000	0.005602
esd	0.000000	0.000117	0.000058	0.000000	0.000237	0.000213	0.000233	0.000168	0.000000	0.000000	0.000131
O(1g)	0.500000	0.887747	0.405099	0.500000	0.006349	0.011215	0.018031	-0.004020	0.000000	0.000000	0.011865
esd	0.000000	0.000117	0.000063	0.000000	0.000248	0.000250	0.000313	0.000195	0.000000	0.000000	0.000157
C(1g)	0.500000	0.249726	0.182898	0.500000	0.005995	0.007005	0.006700	-0.001114	0.000000	0.000000	0.006567
esd	0.000000	0.000140	0.000069	0.000000	0.000282	0.000251	0.000268	0.000203	0.000000	0.000000	0.000154
C(2g)	1.000000	0.607364	0.179566	0.587970	0.005433	0.007475	0.006142	0.000349	-0.000011	0.001015	0.006350
esd	0.000000	0.000098	0.000048	0.000038	0.000190	0.000176	0.000186	0.000139	0.000162	0.000142	0.000106
C(3g)	1.000000	0.345754	0.362080	0.410862	0.005931	0.008026	0.005999	0.000494	0.000228	0.000767	0.006652
esd	0.000000	0.000097	0.000049	0.000039	0.000192	0.000179	0.000189	0.000142	0.000161	0.000142	0.000108
N(1g)	0.500000	0.099061	0.123919	0.500000	0.007722	0.009992	0.010259	-0.002922	0.000000	0.000000	0.009324
esd	0.000000	0.000135	0.000068	0.000000	0.000274	0.000262	0.000277	0.000210	0.000000	0.000000	0.000156
N(2g)	1.000000	0.667060	0.119639	0.642042	0.008521	0.010757	0.009312	0.001306	-0.000166	0.003429	0.009530
esd	0.000000	0.000094	0.000048	0.000038	0.000196	0.000184	0.000193	0.000149	0.000164	0.000152	0.000110
N(3g)	1.000000	0.250160	0.405723	0.355595	0.009502	0.013719	0.008208	0.002196	-0.000577	0.002985	0.010476
esd	0.000000	0.000097	0.000052	0.000038	0.000200	0.000207	0.000191	0.000163	0.000165	0.000159	0.000115
Na(1)	0.500000	0.500000	0.000000	0.245955	0.006446	0.008087	0.005775	-0.001345	0.000000	0.000000	0.006769
esd	0.000000	0.000000	0.000000	0.000027	0.000153	0.000135	0.000137	0.000105	0.000000	0.000000	0.000082
Na(2)	0.500000	0.000000	0.000000	0.378131	0.007216	0.008966	0.007086	0.000501	0.000000	0.000000	0.007756
esd	0.000000	0.000000	0.000000	0.000028	0.000157	0.000142	0.000144	0.000109	0.000000	0.000000	0.000085
O(2)	1.000000	0.171827	0.122505	0.268831	0.009971	0.011243	0.010923	0.000716	-0.001991	0.000823	0.010712
esd	0.000000	0.000087	0.000045	0.000036	0.000191	0.000175	0.000186	0.000141	0.000159	0.000144	0.000106
H(1)	1.000000	0.176742	0.185907	0.284453							0.039252
esd	0.000000	0.002513	0.001320	0.001069							0.004232
H(2)	1.000000	0.058829	0.122577	0.235035							0.052398
esd	0.000000	0.003359	0.001585	0.001140							0.004809

PLANE AND CONTOURS AS IN FIG. 3.

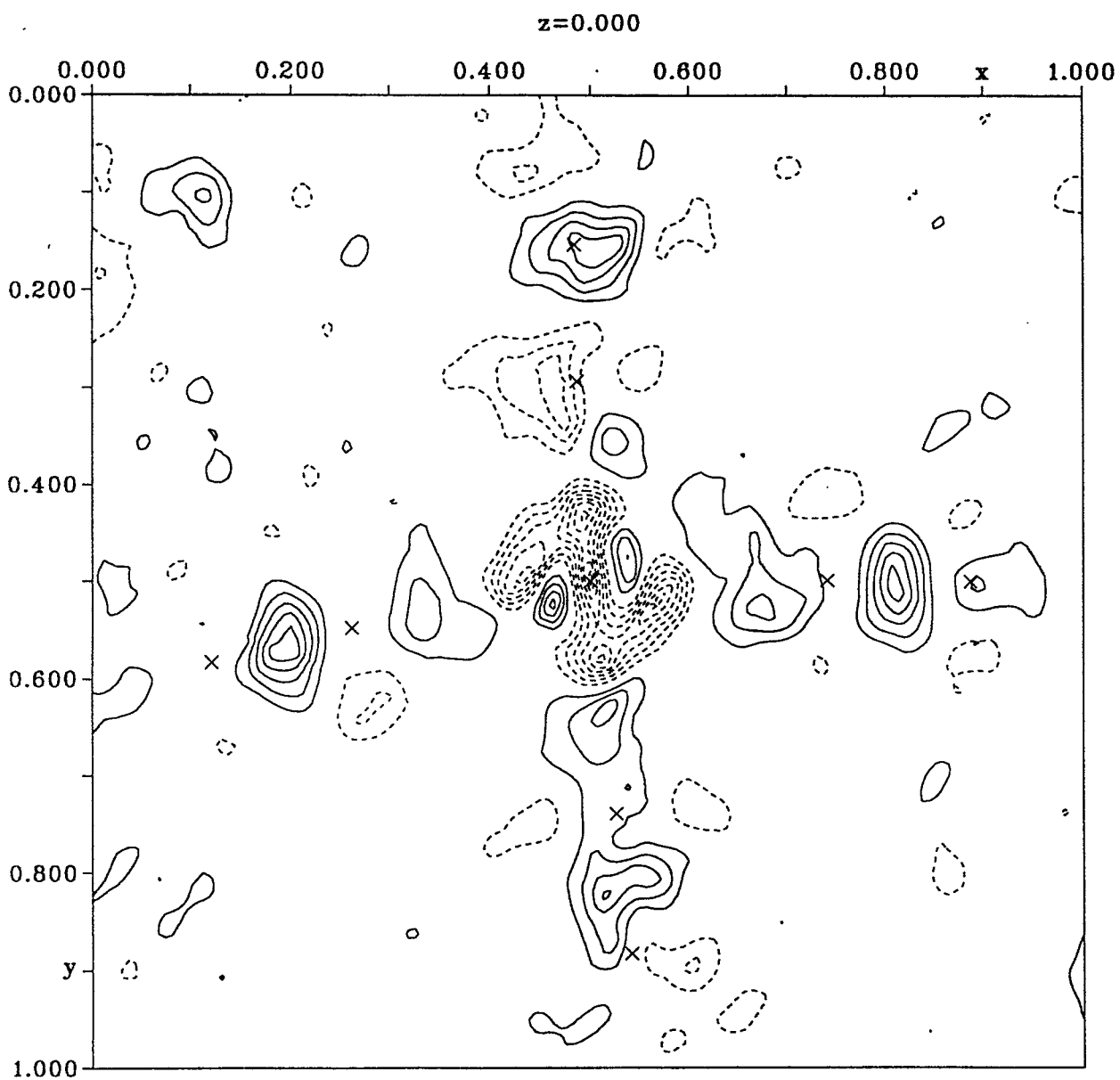


FIGURE S2. RESIDUAL MAP OF MS_2 SNP REFINEMENT
PLANE AND CONTOURS AS IN FIG. 3

