

data_P = 0.0001 GPa

_cell_length_a 7.2790
_cell_length_b 7.2790
_cell_length_c 17.6670
_cell_angle_alpha 90.000
_cell_angle_beta 90.000
_cell_angle_gamma 120.000

loop_
_refln_index_h
_refln_index_k
_refln_index_l
_refln_F_meas
_refln_F_sigma
_refln_A_calc
_refln_B_calc
0 1 0 31.4761 0.8607 -35.4935 0.0000
-1 2 0 106.4731 1.5327 -50.7144 -92.9899
0 2 0 11.0480 1.6183 10.4496 0.0000
-1 3 0 22.4749 0.7394 -6.2152 -19.1466
0 3 0 68.7552 0.9781 67.4816 0.0000
-2 4 0 642.4675 8.4888 -322.0531 560.4602
-1 4 0 46.9626 0.7886 45.4036 -13.0470
0 4 0 12.7812 2.0517 11.7102 0.0000
-2 5 0 21.7889 1.2891 -7.6268 -18.6361
-1 5 0 65.3228 1.0816 -40.2248 -55.2537
0 5 0 28.6093 2.2012 -30.2867 0.0000
-3 6 0 78.9332 2.6285 79.3154 10.8845
-2 6 0 12.5676 2.9242 -5.0128 -10.2303
-1 6 0 47.8507 1.4933 -36.4415 -30.5902
0 6 0 345.8121 8.1303 349.4019 0.0000
-3 7 0 46.2495 2.0182 36.0397 24.6265
-2 7 0 44.2268 1.5211 -22.2551 39.8030
-1 7 0 34.5484 2.5070 -8.5389 29.8393
0 7 0 13.0622 6.5097 -6.4700 0.0000
-4 8 0 290.0575 10.8920 -146.0501 -251.5210
-3 8 0 50.0775 2.2974 -17.4859 39.6354
-2 8 0 13.6761 5.0447 -7.9633 10.6834
-1 8 0 47.2233 2.6973 -13.5190 -47.3749
0 8 0 14.0758 6.4895 -1.3851 0.0000
-4 9 0 7.5195 9.2484 13.8649 -4.2789
-3 9 0 41.7330 3.6253 38.1317 -5.5907
-2 9 0 37.1349 5.4535 8.9507 -32.3935
-1 1 1 80.0014 1.5954 75.2265 0.0000
0 1 1 34.0846 1.2304 -18.4553 31.9655
-2 2 1 11.8365 1.6790 -7.4771 0.0000
-1 2 1 51.7693 0.7407 -13.4375 52.3906
0 2 1 211.5199 2.6353 106.1019 -183.7738
-3 3 1 50.3632 1.0955 55.2121 0.0000
-2 3 1 20.8055 0.9278 -2.5283 -21.4860
-1 3 1 28.3554 0.6739 -24.3421 7.4832
0 3 1 71.8688 0.9941 -36.5311 63.2737

-4	4	1	176.1012	2.7652	-177.9987	0.0000
-3	4	1	45.5812	0.7523	37.3189	-24.1059
-2	4	1	19.2901	1.1350	-16.3266	9.3268
-1	4	1	39.5673	0.8252	29.8216	-21.9792
0	4	1	11.4699	2.2427	-0.9898	1.7144
-5	5	1	34.9081	2.3664	36.9474	0.0000
-4	5	1	48.2902	1.1207	48.6435	8.8707
-3	5	1	68.8195	1.0276	-41.8125	51.0077
-2	5	1	21.4208	1.3493	0.3666	-21.2617
-1	5	1	34.2172	1.1080	3.8486	-36.0711
0	5	1	38.4602	1.7997	-20.8079	36.0404
-6	6	1	20.1191	4.0486	18.9937	0.0000
-5	6	1	18.3280	2.7743	-16.4158	6.4111
-4	6	1	13.8416	2.8770	-7.6820	10.8390
-3	6	1	25.0859	1.9760	-24.9583	-6.6691
-2	6	1	109.7735	1.7590	57.2521	93.2670
-1	6	1	42.6358	1.6496	-37.0693	-20.5441
0	6	1	11.2556	4.4755	-1.2741	2.2067
-7	7	1	36.8937	6.4862	44.6257	0.0000
-6	7	1	27.0369	2.3751	-25.4533	0.2820
-5	7	1	23.5625	2.2032	-18.7487	14.5442
-4	7	1	29.3721	2.3121	27.9290	12.7250
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-1	7	1	29.6924	2.0264	25.1364	20.2862
0	7	1	18.0266	4.6073	-7.6103	13.1814
-8	8	1	20.6883	5.2137	19.8295	0.0000
-7	8	1	28.9207	3.5436	-3.5240	34.0592
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-3	8	1	14.4244	7.1715	16.6432	11.0913
-2	8	1	15.8053	7.0216	0.7847	-10.7481
-1	8	1	21.5022	5.1852	7.0800	19.9347
0	8	1	56.9838	3.0371	30.3582	-52.5818
-7	9	1	39.9605	3.5658	-22.6183	34.7166
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-5	9	1	30.5398	8.2108	-7.2559	-34.9165
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-3	9	1	20.9527	5.3986	16.6212	13.5560
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0	1	2	118.7026	1.6599	-58.9302	-102.0701
-2	2	2	654.5281	12.0737	659.9313	0.0001
-1	2	2	57.8660	0.8060	-57.6805	-15.8638
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0	3	2	78.8289	1.0698	40.1073	69.4680
-4	4	2	13.1043	2.2278	-1.1910	0.0000
-3	4	2	101.1724	1.0903	-44.1108	-91.2860
-2	4	2	9.3634	1.6895	-5.1765	1.8550
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-4	5	2	55.8377	1.1613	9.9038	-55.4760
-3	5	2	67.8861	1.3227	19.4705	-62.0625
-2	5	2	121.0110	1.5643	119.7536	-3.3873
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0	5	2	26.8050	2.8287	-13.4889	-23.3635
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0	6	2	17.1568	3.3992	-6.0819	-10.5342
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-6	7	2	65.9397	1.8977	-36.7435	-49.0557
-5	7	2	19.7106	2.7145	6.8607	-17.0527
-4	7	2	21.2395	2.6942	-21.4794	-4.4778
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0	7	2	65.4832	3.7060	-31.6560	-54.8298
-8	8	2	239.4240	6.8130	242.4569	0.0000
-7	8	2	47.7512	2.6998	-33.8242	-30.4671
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-5	8	2	53.4322	4.6077	51.1162	10.7916
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-3	8	2	41.0076	3.5322	-32.6511	-27.5497
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-5	9	2	40.9888	3.3028	31.0179	30.2652
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-3	3	3	112.7276	1.9967	105.1921	0.0000
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-4	6	3	18.6456	2.3695	-6.7225	19.7939
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-6	8	3	7.1010	6.5864	4.2480	10.1467
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-1	3	4	17.3601	0.9157	14.7028	-6.6349
0	3	4	23.6118	1.2211	13.4117	-23.2295
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-3	4	4	65.2904	0.8924	-62.7502	-19.4698
-2	4	4	12.5271	1.6627	-1.5320	12.5563
-1	4	4	58.2521	0.7816	57.8025	9.8296
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-4	5	4	18.1394	2.3578	-12.5249	13.3272
-3	5	4	68.7225	1.3890	-30.9787	62.0041
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-6	9	4	22.0979	4.7162	-7.9948	-7.6106
-5	9	4	40.8406	2.7116	-20.0165	-31.8725
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0	1	5	99.3733	1.4972	-48.9784	-84.8332
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0	6	5	12.7924	4.3076	-7.0816	-12.2658
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-7	8	5	21.1101	3.7567	18.1022	-14.8016
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0	0	6	624.3206	15.3925	657.4933	0.0003
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0	2	6	10.6702	1.8139	3.9691	0.0000
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-3	4	6	38.3135	1.3204	38.8558	-10.7319
-2	4	6	499.8252	6.6345	-248.3504	424.8686
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0	4	6	20.2360	2.6450	17.4877	0.0000
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-4	5	6	30.2841	1.9137	-19.8921	-23.7288
-3	5	6	24.3153	2.0195	-11.1543	-23.0716
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0	5	6	57.1652	1.4807	-54.8568	0.0000
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-4	6	6	13.6587	3.3887	-12.3249	2.2822
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-7	7	6	0.0000	8.1495	-1.5410	0.0000
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-4	7	6	57.4381	2.0557	42.9407	39.8967
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0	7	6	18.5075	10.5843	-9.1347	0.0000
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-6	8	6	17.8218	4.9505	-11.3158	15.3870
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-3	8	6	44.9314	2.6550	-6.3893	42.6534
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-1	8	6	41.0218	5.9644	-7.8007	-32.7232
0	8	6	12.6848	13.9878	1.4368	0.0000
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-5	9	6	22.9975	5.2660	15.3918	-5.5895
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0	1	7	37.1898	1.0778	-18.6297	32.2674
-2	2	7	9.5423	2.1051	8.9154	0.0000
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0	2	7	122.9324	1.7562	62.9740	-109.0739
-3	3	7	22.9825	1.7112	24.9009	0.0000
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-1	3	7	40.5388	0.7799	-34.8305	19.6793
0	3	7	65.8395	1.5371	-33.2706	57.6266
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0	5	7	85.4530	2.5473	-42.0041	72.7529
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0	7	7	24.2582	8.5508	-13.1107	22.7085
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-1	2	8	72.0545	0.8641	-61.0486	-36.4796
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-2	3	8	23.3107	1.6204	11.2349	23.8327
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0	4	8	463.2506	8.8514	-232.1656	-402.1231
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0	5	8	13.5226	4.2593	-5.2913	-9.1648
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-5	7	8	16.5185	9.5768	3.6609	-13.0316
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-3	8	8	34.9850	3.3677	-20.5075	-30.5819
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-1	8	8	17.7175	10.2422	-18.9806	-23.9188
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-1	7	9	37.2301	2.8718	37.9593	5.3369
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-3	4	10	51.4162	2.3828	-53.0183	-6.6438

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-3	6	10	30.1230	2.0364	-18.3103	23.9384
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-3	4	11	34.2580	2.3190	-26.4549	-20.7468
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-3	3	15	11.7671	5.5282	11.3036	-0.0003
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data_P = 2.25 GPa

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 _cell_angle_alpha 90.000
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loop_
 _refln_index_h
 _refln_index_k
 _refln_index_l
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 _refln_B_calc

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data_P = 4.23 GPa

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 _cell_angle_alpha 90.000
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loop_
 _refln_index_h
 _refln_index_k
 _refln_index_l
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 _refln_B_calc

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-4	5	2	53.3227	1.7963	10.4005	-54.1028
-3	5	2	73.4254	2.5224	15.1445	-68.6553
-2	5	2	113.8916	2.0140	115.9955	11.6756
-1	5	2	29.6372	1.4684	28.7952	1.8382

0	5	2	29.4347	2.5252	-14.4848	-25.0884
-6	6	2	5.5882	8.8332	12.0429	0.0000
-5	6	2	35.9746	2.1932	31.3874	8.0197
-4	6	2	372.8096	6.2602	-179.6634	310.8823
-3	6	2	40.3156	2.1877	35.8327	-1.8826
-2	6	2	5.7552	8.4344	9.4009	1.6572
-1	6	2	55.0275	1.3202	-30.1643	47.5810
-6	7	2	53.4790	2.4039	-15.2983	-52.5818
-5	7	2	6.1118	14.2639	-6.3512	-5.1429
-4	7	2	18.3968	4.3506	-17.9889	1.8854
-3	7	2	31.3296	4.6849	-17.7522	-27.9154
-2	7	2	43.0607	3.7243	-43.9399	4.7082
-1	7	2	47.2119	4.0103	-34.0251	32.9459
-1	2	3	75.8874	4.1455	-49.5826	-49.7485
0	2	3	3.0006	6.7346	-2.4952	0.0001
-3	3	3	97.7187	2.6302	101.5917	0.0000
-2	3	3	27.6338	0.8394	-6.6888	-27.5310
-1	3	3	10.9090	3.4101	8.5349	5.0018
-3	4	3	50.3439	0.9449	-21.8490	42.1782
-2	4	3	138.3043	1.7450	69.2047	-118.5414
-1	4	3	52.9525	1.5517	-10.3029	49.7878
0	4	3	7.6570	5.4727	-10.8538	0.0000
-4	5	3	38.4714	2.7440	-9.1566	-36.2006
-3	5	3	65.9791	1.5014	-35.8762	59.1661
-2	5	3	53.7858	1.6522	-29.7473	41.4348
-1	5	3	62.2202	3.2816	-8.6148	-65.1109
0	5	3	10.8477	8.8380	-17.0098	0.0000
-6	6	3	97.5017	7.2735	-95.6794	0.0000
-5	6	3	23.5621	3.3158	21.9628	-8.8674
-4	6	3	6.3147	10.0989	1.0061	7.0856
-3	6	3	52.5867	2.5650	48.7145	-16.8523
-2	6	3	5.1887	8.6406	-3.5602	8.3012
-1	6	3	26.5329	2.5186	24.2616	-0.8837
0	6	3	94.3823	8.0334	-88.6743	0.0000
-6	7	3	29.6681	2.4424	35.2434	-3.5171
-5	7	3	35.2555	4.4502	-27.8648	31.4861
-4	7	3	10.4406	8.9749	5.9904	-10.5613
-3	7	3	5.8091	12.2823	-8.3011	-5.4000
-2	7	3	5.8161	10.6621	-7.7706	0.9467
-1	7	3	42.3883	3.4792	42.8048	1.0079
-3	3	4	76.5507	2.5590	-74.3333	0.0000
-2	3	4	92.1720	1.6855	-53.5356	-88.6691
-1	3	4	4.5828	5.7788	4.4383	-1.8831
0	3	4	35.2421	5.5105	13.0990	-22.6882
-4	4	4	412.1054	10.8438	416.0302	0.0001
-3	4	4	66.7821	2.0188	-59.6841	-29.4772
-2	4	4	5.5705	5.6132	2.2153	-1.7646
-1	4	4	56.3477	1.3995	53.0777	9.7968
-5	5	4	5.6683	12.7057	8.2675	0.0000
-4	5	4	10.3338	4.7750	-4.2767	14.4958
-3	5	4	62.1269	1.6229	-25.4009	58.9183
-2	5	4	69.6460	1.6111	51.5338	46.1074
-1	5	4	53.5946	1.3950	49.1389	29.9404
0	5	4	62.9196	2.2469	-32.6556	56.5612

-5	6	4	51.9293	5.6665	-24.2218	-39.2763
-4	6	4	5.0527	6.6115	0.4753	9.9705
-3	6	4	38.5500	2.7076	-22.5488	28.0102
-2	6	4	325.3373	7.9934	-155.2553	-278.2390
-1	6	4	27.4734	3.1986	-7.9838	27.2234
0	6	4	11.6965	13.3339	-8.8108	15.2609
-6	7	4	53.6313	3.5091	-3.3024	-53.0460
-5	7	4	59.3156	6.4998	12.8188	-49.7573
-4	7	4	53.9845	4.3153	53.2830	-0.2149
-2	7	4	11.6267	8.4613	1.8232	-11.6700
-1	7	4	27.5300	3.5529	27.1982	-5.3363
-3	4	5	68.1044	2.1985	-49.1316	-31.5425
-1	4	5	35.6573	4.0167	-24.3661	-19.0586
0	4	5	91.1165	6.4578	47.7847	82.7656
-5	5	5	18.8529	11.3418	18.1762	-0.0001
-4	5	5	18.7104	4.3761	-9.3273	19.4350
-3	5	5	23.8633	3.6289	-20.4628	13.9387
-2	5	5	27.9301	2.1986	27.2365	11.1731
-1	5	5	53.2197	1.8792	-25.8710	-41.4757
0	5	5	37.7542	3.0860	-23.4980	-40.6998
-5	6	5	47.2909	4.2623	-8.6537	33.6868
-4	6	5	90.9681	2.7307	51.4841	-77.0670
-3	6	5	22.7139	3.4637	-11.8167	19.5197
-2	6	5	4.7894	6.2762	5.8800	-1.8270
-1	6	5	47.0635	2.6726	0.2028	40.1851
-6	7	5	23.6772	6.5900	3.7300	-26.6911
-5	7	5	68.5265	6.9540	-32.6228	49.8271
-4	7	5	49.7451	5.2225	-24.6208	37.0054
-3	7	5	21.2967	5.4862	1.2621	-24.8390
-2	7	5	5.3838	10.1147	13.7603	2.3362
-1	7	5	14.1249	8.3151	15.2390	11.8031
-1	5	6	96.2337	4.1423	-31.8129	-68.9208
0	5	6	45.9156	4.0095	-56.3187	0.0000
-4	6	6	15.7766	9.7352	-11.6715	-7.5170
-3	6	6	31.3018	5.5150	35.6320	-4.0235
-2	6	6	6.1048	13.3999	4.8090	-11.8471
-1	6	6	37.3337	5.5430	-28.4118	-33.3314
0	6	6	285.5517	19.4327	291.6429	0.0001
-4	7	6	76.8823	3.4258	49.4127	33.0621
-2	7	6	50.3283	14.4304	-18.5100	38.5105
-1	7	6	17.6329	9.0704	-10.2325	21.0424

data_P = 5.41 GPa

_cell_length_a 7.2040
 _cell_length_b 7.2040
 _cell_length_c 17.4500
 _cell_angle_alpha 90.000
 _cell_angle_beta 90.000
 _cell_angle_gamma 120.000

loop_
 _refln_index_h

			_refln_index_k	_refln_index_l	_refln_F_meas	_refln_F_sigma	_refln_A_calc	_refln_B_calc
0	1	0	31.7163	0.4097	-36.0666	0.0000		
-1	2	0	108.8995	0.9254	-69.0045	-80.2813		
0	2	0	11.0240	1.0902	11.4192	0.0000		
-1	3	0	24.6656	0.5262	-13.9038	-19.4234		
-1	4	0	46.7186	0.9242	48.5129	-7.6235		
0	4	0	12.6291	2.7280	14.8118	0.0000		
-1	5	0	59.8677	14.2363	-8.0761	-58.8101		
0	5	0	20.9054	10.3955	-17.4350	0.0000		
-1	6	0	55.9653	1.9936	-29.7757	-44.0889		
0	7	0	8.7691	11.1742	10.9508	0.0000		
-4	8	0	265.2388	3.7381	-124.9784	-226.2283		
-3	8	0	45.3690	1.9047	-28.0194	33.7688		
-2	8	0	15.2321	5.3808	-5.5603	12.6823		
-1	8	0	40.0283	2.1666	-39.4603	-10.8529		
-4	9	0	20.3733	4.9326	10.1262	-15.1647		
-3	9	0	27.1379	2.7269	22.2552	18.1857		
-2	9	0	27.8854	4.0616	4.9959	-25.4000		
0	1	1	34.8066	1.9713	-21.1040	36.5531		
-2	2	1	3.2888	4.1184	-1.7242	0.0000		
-1	2	1	51.0926	0.5531	-19.1453	50.3680		
0	2	1	207.2059	1.3263	105.7953	-183.2430		
-2	3	1	28.5960	0.6791	-6.4874	-27.3337		
-1	3	1	30.9814	0.6514	-21.3416	20.4176		
-4	4	1	164.1143	1.6766	-166.6013	0.0000		
-3	4	1	46.6390	1.0703	40.1920	-17.9075		
-1	4	1	34.0719	0.7552	27.1523	-19.0733		
0	4	1	9.0831	2.9020	4.2802	-7.4135		
-5	5	1	52.8304	8.8895	40.7407	0.0000		
-4	5	1	44.5233	2.4566	46.3187	-0.3283		
-1	5	1	19.8598	15.8519	2.9125	-25.9944		
-5	6	1	11.7068	7.3446	-13.0191	9.6343		
-1	6	1	38.6859	6.1068	-25.5587	-27.7844		
-7	7	1	30.4169	3.3792	29.4449	0.0000		
0	7	1	6.5286	14.6081	-5.1215	8.8706		
-8	8	1	12.2913	11.3487	15.1106	0.0000		
-7	8	1	27.0937	3.7029	-10.9324	28.2017		
-6	8	1	93.6526	2.1165	43.1018	-77.3857		
-5	8	1	30.9140	2.6780	-1.6475	30.2771		
-4	8	1	7.3014	10.9992	6.2506	-4.2602		
-3	8	1	20.1169	4.2976	17.7842	4.1304		
-1	8	1	11.6169	10.4706	1.8975	11.3937		
0	8	1	48.9172	2.6709	26.7760	-46.3775		
-7	9	1	29.9865	4.5641	-15.4519	28.6394		
-6	9	1	32.7511	2.4282	-18.3863	29.5824		
-5	9	1	25.5944	3.8880	-2.3006	-21.5265		
-4	9	1	8.5946	10.2285	5.2285	13.3346		
-3	9	1	11.5261	7.1521	11.7035	7.7011		
-2	9	1	7.0972	9.8063	-4.3682	-13.5358		

-1	1	2	42.3189	1.4587	-46.1942	0.0000
0	1	2	108.2939	1.7974	-56.5464	-97.9412
-2	2	2	649.6945	3.3423	637.5391	0.0000
-1	2	2	57.7544	0.6870	-56.9536	-14.8743
0	2	2	13.4935	1.3527	-6.8552	-11.8734
-2	3	2	42.3818	0.8577	32.2945	30.8692
-1	3	2	38.4622	1.0380	-33.7616	11.6637
0	3	2	96.9996	16.8442	44.9046	77.7770
-4	4	2	9.5589	3.8302	-9.4241	0.0000
-3	4	2	94.9513	0.8989	-64.2404	-62.0697
-1	4	2	58.3961	0.8695	-20.9056	53.7666
0	4	2	472.5550	3.6422	-236.6740	-409.9315
-4	5	2	54.8482	2.2056	7.7566	-57.6975
-1	5	2	27.9640	1.5475	25.9573	1.8307
-7	7	2	48.9067	4.4527	-47.9038	0.0000
0	7	2	55.9380	3.0162	-26.5943	-46.0628
-8	8	2	219.4666	7.0057	207.8146	0.0000
-7	8	2	44.5505	3.2051	-24.5886	-34.8362
-6	8	2	6.6694	9.2245	-0.3146	-3.1189
-5	8	2	43.6928	3.0653	31.4267	-22.9471
-4	8	2	7.1577	8.8384	-9.2256	-2.5623
-3	8	2	40.6043	2.3456	-22.0823	-31.7739
-2	8	2	238.9231	3.2422	237.5706	0.2696
-1	8	2	16.7638	5.3759	-0.3871	-22.5141
0	8	2	6.6101	10.0672	-2.3633	-4.0933
-7	9	2	17.7965	6.9569	-11.2981	6.0837
-6	9	2	42.8815	2.7684	37.2611	16.6736
-5	9	2	37.9172	4.2652	37.3465	20.5249
-4	9	2	30.1971	3.3204	-26.9526	21.1734
-3	9	2	8.7664	9.5382	2.9917	11.1581
-2	9	2	16.8445	8.8516	14.0288	1.8887
-1	2	3	75.1364	3.1223	-41.2558	-55.4949
0	2	3	4.1168	4.4067	-6.4046	0.0000
-2	3	3	20.2303	1.5770	-8.8759	-19.0677
-1	3	3	4.1470	6.1656	4.1298	-5.3265
-4	4	3	1.6940	2.2761	3.0505	0.0000
-3	4	3	51.8656	1.1314	-16.0293	42.5644
-2	4	3	137.0582	0.9057	67.2827	-119.7963
-1	4	3	53.5196	1.2219	-6.4590	52.1367
0	4	3	8.1909	6.7159	-7.9858	0.0000
-4	5	3	35.8620	1.7459	-7.0099	-34.5641
-1	5	3	55.8229	1.3355	-21.3258	-55.4757
-4	6	3	5.9400	10.6148	-1.4586	6.2386
-2	6	3	3.8409	10.7020	-5.1801	2.6565
-7	7	3	52.5829	4.2731	51.9218	0.0000
-5	7	3	28.0430	12.0631	-21.8036	29.0777
0	7	3	46.4152	2.7057	41.4555	0.0000
-7	8	3	18.2822	6.2508	-18.8458	-12.1568
-6	8	3	6.4645	10.9308	4.5572	1.9297
-5	8	3	27.9600	3.0605	-18.5307	-22.4517
-4	8	3	81.0106	2.3824	40.4256	68.0509
-3	8	3	30.9167	2.7996	-19.5226	-25.9270
-1	8	3	16.2963	6.8818	-15.5952	-12.3777
-6	9	3	10.7965	10.7928	7.7735	9.6829

-5	9	3	38.2867	6.9922	-26.3300	-32.9709
-4	9	3	31.1404	4.0897	-20.4518	-29.1405
-3	9	3	8.7976	9.7271	9.6690	8.0729
-4	4	4	402.3295	6.0089	414.5871	0.0000
-3	4	4	63.7012	1.2797	-56.4124	-33.6906
-2	4	4	4.5311	5.8151	-1.4195	-6.1203
-1	4	4	54.9717	1.1779	51.3458	-22.7122
0	4	4	5.2917	8.2801	-3.1159	5.3970
-4	5	4	7.6287	7.2415	-7.3634	13.2208
-3	5	4	65.6901	6.3003	-39.0954	49.9909
-2	5	4	84.9392	4.0365	60.1166	52.6457
-1	5	4	58.6695	1.7836	48.1507	31.2946
-4	6	4	6.9051	8.2765	3.1533	3.5468
-3	6	4	26.9411	7.4297	-19.2176	27.1061
-2	6	4	324.4455	2.5602	-164.4445	-280.4954
-7	7	4	28.2013	4.6626	33.3089	0.0001
-5	7	4	52.2001	3.5559	15.4801	-51.6695
-2	7	4	11.6411	9.0937	0.5677	-9.1562
0	7	4	53.2880	3.4753	29.0457	-50.3085
-7	8	4	17.9710	8.1045	13.7789	11.9033
-6	8	4	248.0865	4.6332	-117.9103	209.5662
-5	8	4	43.0221	2.3975	42.1210	-11.9669
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-3	8	4	22.3014	3.5586	13.3945	19.5510
-1	8	4	42.8517	4.4645	41.8623	0.4272
0	8	4	191.8434	4.2876	-96.6298	167.3676
-6	9	4	6.5630	11.6460	-11.6103	4.9182
-5	9	4	33.9752	5.6884	-2.1326	-26.7452
-4	9	4	51.7359	4.8372	-44.1092	23.1961
-3	9	4	49.7564	4.8376	-34.5233	28.6273
-2	9	4	22.8319	8.5478	-5.0539	-23.9185
-3	4	5	57.0487	1.7835	-36.2470	-39.7407
-2	4	5	12.2161	4.9934	12.8138	3.8047
-1	4	5	28.2385	2.1087	-24.0786	-16.2759
-4	5	5	29.5353	2.7896	-14.7537	21.3783
-3	5	5	24.2975	3.7330	-19.6056	11.2806
-2	5	5	29.3097	3.1751	27.8961	3.3713
-1	5	5	56.0272	3.9476	-26.4037	-46.2903
-4	6	5	79.8517	4.8800	43.7001	-74.9625
-3	6	5	24.3555	5.6525	-8.9562	26.1783
-2	6	5	10.3812	12.6013	7.9548	0.1349
0	7	5	6.5584	11.6320	-6.5827	-11.4017
-5	8	5	32.5013	3.9168	22.7816	-13.6742
-4	8	5	8.7838	10.2151	-7.3646	-1.1184
-3	8	5	28.1345	4.8786	22.7211	-15.6289
-2	8	5	81.9359	4.2263	-81.5717	1.0425
-1	8	5	29.0071	7.3943	34.5861	-4.7263
-3	5	6	23.8632	13.4714	-9.2128	-23.1835
0	6	6	303.3370	6.1305	301.4092	0.0001
-4	7	6	48.8294	9.0804	48.5435	24.0719
-7	8	6	37.2546	7.5394	-29.5005	4.5762
-5	8	6	47.9046	8.5567	-27.6463	26.5468
-4	8	6	249.2783	5.7577	-116.7912	-209.2365
-3	8	6	52.1763	6.1983	-18.8850	37.4972

data_P = 6.38 GPa

_cell_length_a 7.1820
_cell_length_b 7.1820
_cell_length_c 17.4650
_cell_angle_alpha 90.000
_cell_angle_beta 90.000
_cell_angle_gamma 120.000

loop_

_refln_index_h
_refln_index_k
_refln_index_l
_refln_F_meas
_refln_F_sigma
_refln_A_calc
_refln_B_calc

0	1	0	28.7994	0.4918	-31.2213	0.0000
-1	2	0	108.4453	0.5857	-72.8603	-84.3014
0	2	0	11.0131	1.0236	11.4583	0.0000
-1	3	0	25.0516	0.5553	-10.6909	-23.6011
0	3	0	85.8175	2.1623	72.5502	0.0000
-2	4	0	660.7145	1.9242	-321.9837	563.4987
-1	4	0	51.1958	0.9861	49.8059	-11.1864
0	4	0	5.2971	6.5294	6.3601	0.0000
-2	5	0	20.2537	3.3100	-11.1053	-14.9655
-1	5	0	69.2938	1.3114	-17.7646	-72.3445
0	5	0	31.3234	4.5102	-32.2283	0.0000
-3	6	0	89.5196	1.8382	80.4278	-28.9890
-2	6	0	13.7467	12.8735	-2.9988	-9.1557
-1	6	0	58.7438	1.9611	-41.1820	-43.3391
0	6	0	365.6747	3.4588	359.1821	0.0000
-3	7	0	61.8208	2.0482	47.9183	24.3019
-2	7	0	53.7362	2.7464	-31.4536	39.2348
-1	7	0	37.2712	3.1191	-9.3293	35.5310
-4	8	0	300.3727	2.8366	-153.3078	-258.7926
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loop_
 _refln_index_h
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-2	8	1	6.9565	11.8555	7.4717	5.3159
-1	8	1	15.1146	4.7558	4.2863	16.4667
0	8	1	62.0772	6.3990	31.5472	-54.6413
-7	9	1	40.5645	3.5386	-20.6538	32.7275
-6	9	1	35.9250	2.3276	-22.6704	27.7274
-5	9	1	28.3879	3.5217	-16.9880	-21.5599
-4	9	1	10.3741	9.3017	6.6923	10.9917
-3	9	1	15.1756	8.4211	13.1633	8.8956
-2	9	1	22.7613	6.6895	-11.4700	-15.2514
-1	1	2	44.2594	2.2891	-47.7993	0.0000
0	1	2	115.2776	1.9071	-60.0016	-103.9258
-2	2	2	649.5694	4.2514	648.4468	0.0001
-1	2	2	58.7831	1.0737	-61.2119	-1.3745
0	2	2	11.6706	1.6196	-5.7784	-10.0084
-3	3	2	48.5072	9.9579	-48.4719	0.0000
-2	3	2	42.6075	1.1110	29.2071	30.8031
-1	3	2	39.5042	0.8597	-27.4610	28.7109
0	3	2	46.3850	11.4982	33.1386	57.3977
-4	4	2	4.9599	8.4257	-0.2059	0.0000
-3	4	2	95.7856	0.6170	-63.3388	-67.7332
-2	4	2	9.0124	6.5191	-4.2852	-1.3666
-1	4	2	58.7692	0.9259	-16.1596	54.0853
0	4	2	473.1767	2.6822	-236.4690	-409.5765
-4	5	2	53.8584	0.9970	11.7476	-50.9243
-1	5	2	32.9750	1.4846	28.4074	13.1808
-7	7	2	52.4533	3.1783	-47.7525	0.0000
0	7	2	59.6126	3.5496	-26.2276	-45.4275
-8	8	2	202.7084	13.8343	201.7787	0.0000
-7	8	2	48.2685	2.0704	-31.3363	-30.4967
-5	8	2	53.1314	2.6871	40.6655	-14.5868
-4	8	2	6.8520	9.1263	-10.6068	7.1540
-3	8	2	34.6372	2.3378	-24.2878	-25.4794
-2	8	2	232.9581	1.9745	225.5989	-0.9451
-1	8	2	22.4448	3.7786	-11.9808	-21.0419
-7	9	2	17.7223	8.8300	-12.7551	14.0150
-6	9	2	45.2647	2.2089	34.3824	19.4631
-5	9	2	39.7597	2.8375	32.8156	25.3337
-4	9	2	35.9804	3.2807	-24.6271	26.3846
-3	9	2	8.9494	9.5618	-4.4946	13.8868
-2	9	2	6.7626	14.7087	6.7864	2.3304
-1	2	3	75.0014	1.3292	-34.0826	-62.1884
0	2	3	6.9308	5.4498	-10.6102	0.0000
-2	3	3	25.2454	2.9362	-7.6840	-29.8402
-1	3	3	4.0766	9.2005	-11.3433	6.5446
-4	4	3	10.6997	5.5602	4.4034	0.0000
-3	4	3	53.2509	1.1017	-7.9074	50.9098
-2	4	3	142.2374	1.1547	70.2732	-117.8531

-1	4	3	55.2567	1.2738	5.6763	53.4749
-4	5	3	46.1187	1.5579	-34.3850	-25.2029
-1	5	3	64.3629	1.0714	-34.8757	-55.2564
-4	6	3	6.0552	9.9731	-3.8845	6.5437
-2	6	3	6.2493	8.5239	1.6057	-2.9560
-7	7	3	56.3751	3.2741	52.4409	0.0000
-5	7	3	23.8605	9.1964	-15.1503	31.2354
0	7	3	51.7081	4.8738	48.8560	0.0000
-7	8	3	34.9954	2.6336	1.1638	-34.1936
-6	8	3	11.8514	8.8595	-5.7593	7.7121
-5	8	3	29.7697	2.8883	-25.8581	-17.3478
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-3	8	3	22.8976	4.0241	-21.7183	-18.7042
-2	8	3	6.4111	8.6015	1.1083	6.4596
-1	8	3	25.4161	3.0805	-5.8346	-29.9535
-6	9	3	22.2124	5.0227	16.3988	-11.0760
-5	9	3	44.3821	3.9019	-20.1280	-37.9310
-4	9	3	38.3785	3.7968	-17.8778	-35.1024
-3	9	3	19.1118	5.5823	17.0443	-6.3520
0	2	4	478.6554	4.3020	-230.3913	399.0493
-4	4	4	414.3544	4.5111	416.1025	0.0002
-3	4	4	64.9163	1.3922	-61.9498	-25.5670
-2	4	4	5.1804	5.9749	1.4472	9.8266
-1	4	4	59.0892	1.4484	59.5926	-1.3199
0	4	4	12.8883	7.4415	-5.9747	10.3485
-4	5	4	22.6921	2.6393	-13.3621	14.8070
-3	5	4	61.4268	3.8531	-33.1737	58.4676
-2	5	4	73.0747	3.0440	50.1890	54.3620
-1	5	4	55.4322	2.4020	43.5587	35.5789
-4	6	4	9.1436	8.3712	9.2442	-0.3131
-3	6	4	25.1226	5.2925	-9.6732	30.8062
-2	6	4	325.5447	4.0178	-158.8806	-284.2101
-7	7	4	37.9175	3.7113	37.8580	0.0000
-5	7	4	56.3309	3.0322	15.2880	-46.2560
-2	7	4	6.4692	12.1490	4.5919	-4.9784
0	7	4	54.7352	3.5458	25.9596	-44.9634
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-6	8	4	237.5285	1.1365	-118.0864	198.1597
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-4	8	4	8.3702	14.9897	-1.3087	-7.0935
-3	8	4	22.3403	4.3778	-8.5534	24.7824
-2	8	4	9.9386	8.7637	-6.5138	-9.8378
-1	8	4	40.2785	3.1580	38.5135	-12.7074
-6	9	4	6.6573	12.4871	-10.0766	-3.8804
-5	9	4	32.1032	4.6224	-11.5257	-28.1990
-4	9	4	48.3710	5.6336	-42.7691	14.4077
-3	9	4	40.3995	6.3895	-34.6448	21.2652
-3	4	5	68.6517	2.4094	-29.0122	-58.0905
-2	4	5	16.3767	6.1791	13.7558	10.3542
-1	4	5	52.4686	2.9681	-36.7690	-29.4185
-4	5	5	16.0826	5.3005	-14.3018	10.5699
-3	5	5	21.9953	3.5790	-17.7857	12.8091
-2	5	5	43.8702	2.8540	37.6050	0.1425
-1	5	5	54.1460	4.2424	-13.5741	-47.1135

-3	6	5	26.2268	3.4311	-0.1019	22.9460
0	7	5	22.1230	9.9678	-10.6731	-18.4863
-7	8	5	12.0833	9.4467	16.6919	-10.3968
-6	8	5	8.2703	8.9240	2.8960	-13.5016
-5	8	5	35.3217	3.1907	37.5044	11.2515
-4	8	5	8.2396	10.9723	-9.8380	-5.7496
-3	8	5	29.3085	4.5098	27.7682	-19.1857
-2	8	5	84.9599	2.2845	-89.0269	-4.0887
-1	8	5	24.3688	6.3491	28.4202	-10.9443
-6	9	5	6.7890	12.7778	-0.0187	-14.1676
-5	9	5	12.0411	10.8510	4.2898	-11.3658
-4	9	5	18.0541	13.6757	-7.9051	17.6464
-3	9	5	30.9982	9.2847	36.8509	8.6139
-1	4	6	39.2690	5.5424	46.2133	-7.9415
-5	5	6	11.5607	9.4900	-19.8634	-0.0001
-3	5	6	21.8436	7.0851	-5.0610	-16.1067
-2	5	6	14.0478	9.8240	-0.4609	-17.6497
0	5	6	51.3679	8.0380	-58.2336	0.0000
-6	6	6	247.7610	43.7269	276.0499	0.0001
-7	8	6	22.7768	5.5822	-22.5225	-17.0766
-6	8	6	6.2899	12.2359	-6.5752	5.0499
-5	8	6	33.3784	5.1821	-19.6928	28.4389
-4	8	6	239.1144	1.5589	-113.5396	-205.9320
-3	8	6	34.4333	7.9586	-11.9275	35.9564
-2	8	6	8.2661	10.8018	2.1472	9.7928
-1	8	6	26.3637	7.8717	-27.0485	-15.5456
-1	7	7	30.1262	10.6662	18.1151	-11.2498
-3	8	7	28.8945	13.9348	-18.1382	7.8093