

TITL gib08 in P2(1)/c  
 CELL 0.71073 10.2919 22.9186 26.2672 90.000 94.839 90.000  
 ZERR 4.00 0.0002 0.0005 0.0004 0.000 0.001 0.000  
 LATT 1  
 SYMM -X, 0.5+Y, 0.5-Z  
 SFAC C H N F P O  
 UNIT 224 312 8 48 8 48  
 L.S. 4  
 BOND  
 FMAP 2  
 PLAN 20  
 FREE f3 f3''  
 OMIT -2 0 4  
 OMIT -7 1 11  
 OMIT 0 1 1  
 OMIT -1 2 2  
 OMIT 1 1 0  
 OMIT -3 0 6  
 OMIT 0 1 2  
 OMIT 0 0 2  
 OMIT -1 3 2  
 OMIT 0 2 3  
 OMIT -2 1 2  
 OMIT 1 2 0  
 OMIT 2 3 0  
 OMIT -7 1 12  
 WGHT 0.116100 16.400799  
 FVAR 0.22661 0.36285 0.36756 0.54230  
 HKLF 4  
 WGHT 0.0845 16.7393  
 O1 6 1.24197 0.06501 0.15858 11.00000 0.03910 0.04060 =  
     0.02909 0.00209 0.00451 -0.00227  
 O2 6 1.12190 0.11380 0.07276 11.00000 0.03207 0.05294 =  
     0.04114 0.01345 0.00898 -0.00030  
 O3 6 0.91651 0.19874 0.06077 11.00000 0.03732 0.03201 =  
     0.03643 0.00212 0.00306 -0.00627  
 O4 6 0.66459 0.19823 0.10071 11.00000 0.03953 0.03913 =  
     0.03298 0.01298 0.00566 0.00122  
 O5 6 0.55831 0.09770 0.14387 11.00000 0.03694 0.03597 =  
     0.03001 0.00544 0.00566 0.00161  
 O6 6 0.51500 0.06103 0.31973 11.00000 0.04104 0.04279 =  
     0.02704 0.01008 0.00514 0.00799  
 O7 6 0.62710 0.10639 0.40804 11.00000 0.03195 0.04430 =  
     0.03776 -0.00199 0.01287 0.00250  
 O8 6 0.82788 0.18584 0.43438 11.00000 0.04174 0.03760 =  
     0.03979 -0.00529 0.00198 0.00854  
 O9 6 1.07738 0.17414 0.39369 11.00000 0.03626 0.06662 =  
     0.03586 -0.01371 0.00164 0.01237  
 O10 6 1.19521 0.08527 0.33658 11.00000 0.04034 0.06063 =  
     0.03061 0.00831 0.01184 0.00692  
 O12 6 0.51541 0.24673 0.25427 11.00000 0.18273 0.17200 =  
     0.20129 -0.06654 0.01538 -0.01610  
 N1 3 0.89629 0.07867 0.38526 11.00000 0.06644 0.04990 =  
     0.02458 0.00344 0.00977 0.02949  
 AFIX 3  
 H1A 2 0.82741 0.10372 0.38805 11.00000 8.80000  
 H1D 2 0.97074 0.10092 0.38551 11.00000 8.80000

AFIX	0							
N2	3	0.82103	0.09116	0.10439	11.00000	0.02954	0.03125	=
		0.02098	0.00106	0.00170	-0.00026			
AFIX	3							
H2A	2	0.85171	0.12698	0.09509	11.00000	8.80000		
H2D	2	0.73769	0.09619	0.11383	11.00000	8.80000		
AFIX	0							
C1	1	1.23032	0.03172	0.11271	11.00000	0.03759	0.04355	=
		0.03861	-0.00736	0.00488	0.00387			
AFIX	3							
H1B	2	1.14848	0.00881	0.11027	11.00000	8.80000		
H1C	2	1.30473	0.00448	0.11176	11.00000	8.80000		
AFIX	0							
C2	1	1.22962	0.07477	0.06952	11.00000	0.03718	0.06225	=
		0.03057	-0.00438	0.00933	-0.00006			
AFIX	3							
H2B	2	1.31240	0.09699	0.07185	11.00000	8.80000		
H2C	2	1.22106	0.05394	0.03638	11.00000	8.80000		
AFIX	0							
C3	1	1.13343	0.16765	0.04667	11.00000	0.04352	0.06177	=
		0.04090	0.01760	0.00769	-0.00918			
AFIX	3							
H3A	2	1.10522	0.16245	0.00998	11.00000	8.80000		
H3B	2	1.22575	0.18027	0.04957	11.00000	8.80000		
AFIX	0							
C4	1	1.05160	0.21324	0.06881	11.00000	0.03978	0.04545	=
		0.04779	0.00596	0.00143	-0.01296			
AFIX	3							
H4A	2	1.07659	0.21682	0.10590	11.00000	8.80000		
H4B	2	1.06726	0.25135	0.05267	11.00000	8.80000		
AFIX	0							
C5	1	0.83555	0.24875	0.06525	11.00000	0.05284	0.02956	=
		0.03791	0.00273	0.01215	-0.00290			
AFIX	3							
H5A	2	0.85526	0.27820	0.03942	11.00000	8.80000		
H5B	2	0.85363	0.26637	0.09953	11.00000	8.80000		
AFIX	0							
C6	1	0.69530	0.23175	0.05749	11.00000	0.04748	0.03721	=
		0.03067	0.01326	0.01024	0.00726			
AFIX	3							
H6A	2	0.63971	0.26702	0.05418	11.00000	8.80000		
H6B	2	0.67957	0.20836	0.02588	11.00000	8.80000		
AFIX	0							
C7	1	0.52894	0.18964	0.10267	11.00000	0.03680	0.04307	=
		0.03502	0.00779	0.00609	0.00449			
AFIX	3							
H7A	2	0.49286	0.16761	0.07228	11.00000	8.80000		
H7B	2	0.48361	0.22770	0.10329	11.00000	8.80000		
AFIX	0							
C8	1	0.51004	0.15581	0.15062	11.00000	0.03255	0.03601	=
		0.03544	0.00687	0.00909	0.00960			
AFIX	3							
H8A	2	0.55842	0.17462	0.18040	11.00000	8.80000		
H8B	2	0.41643	0.15460	0.15667	11.00000	8.80000		
AFIX	0							
C9	1	0.55657	0.05983	0.18536	11.00000	0.02178	0.03868	=
		0.03455	0.00539	0.00210	-0.00143			

C10	1	0.53530	0.07866	0.23413	11.00000	0.02536	0.03383 =
		0.03417	0.00264	0.00526	0.00106		
AFIX	3						
H10A	2	0.51868	0.11864	0.24062	11.00000	8.80000	
AFIX	0						
C11	1	0.53883	0.03765	0.27344	11.00000	0.02579	0.03921 =
		0.03140	0.00574	0.00333	-0.00109		
C12	1	0.56411	-0.02085	0.26463	11.00000	0.03349	0.03389 =
		0.04273	0.01007	0.00547	0.00214		
AFIX	3						
H12A	2	0.56643	-0.04850	0.29164	11.00000	8.80000	
AFIX	0						
C13	1	0.58604	-0.03803	0.21503	11.00000	0.04208	0.03460 =
		0.04752	0.00038	0.00623	0.00241		
AFIX	3						
H13A	2	0.60355	-0.07790	0.20845	11.00000	8.80000	
AFIX	0						
C14	1	0.58286	0.00148	0.17549	11.00000	0.03477	0.03802 =
		0.03627	-0.00309	0.00435	-0.00073		
AFIX	3						
H14A	2	0.59835	-0.01084	0.14200	11.00000	8.80000	
AFIX	0						
C15	1	0.53008	0.02427	0.36409	11.00000	0.02622	0.04196 =
		0.03634	0.01295	0.00254	-0.00127		
AFIX	3						
H15A	2	0.61411	0.00307	0.36542	11.00000	8.80000	
H15B	2	0.45839	-0.00458	0.36355	11.00000	8.80000	
AFIX	0						
C16	1	0.52655	0.06405	0.40914	11.00000	0.02910	0.05347 =
		0.03239	0.01161	0.00884	0.00543		
AFIX	3						
H16A	2	0.44074	0.08372	0.40817	11.00000	8.80000	
H16B	2	0.53883	0.04115	0.44113	11.00000	8.80000	
AFIX	0						
C17	1	0.61036	0.15513	0.44091	11.00000	0.04767	0.05842 =
		0.03240	-0.00818	0.01188	0.01075		
AFIX	3						
H17A	2	0.63439	0.14401	0.47689	11.00000	8.80000	
H17B	2	0.51804	0.16776	0.43779	11.00000	8.80000	
AFIX	0						
C18	1	0.69566	0.20371	0.42573	11.00000	0.03875	0.04563 =
		0.04004	-0.00702	0.00106	0.01374		
AFIX	3						
H18A	2	0.67516	0.21323	0.38917	11.00000	8.80000	
H18B	2	0.68050	0.23900	0.44614	11.00000	8.80000	
AFIX	0						
C19	1	0.91717	0.23326	0.42943	11.00000	0.04992	0.03636 =
		0.03690	-0.00414	0.00675	0.00670		
AFIX	3						
H19A	2	0.90381	0.26359	0.45531	11.00000	8.80000	
H19B	2	0.90210	0.25109	0.39511	11.00000	8.80000	
AFIX	0						
C20	1	1.05319	0.20988	0.43704	11.00000	0.04592	0.05392 =
		0.02991	-0.00606	0.00229	0.01000		
AFIX	3						
H20A	2	1.11638	0.24251	0.44029	11.00000	8.80000	
H20B	2	1.06364	0.18636	0.46874	11.00000	8.80000	

AFIX	0							
C21	1	1.21179	0.17345	0.38453	11.00000	0.03627	0.07604	=
		0.04156	-0.00522	0.00622	0.00899			
AFIX	3							
H21A	2	1.26215	0.15092	0.41163	11.00000	8.80000		
H21B	2	1.24633	0.21378	0.38486	11.00000	8.80000		
AFIX	0							
C22	1	1.22528	0.14570	0.33313	11.00000	0.04505	0.05638	=
		0.04140	0.00211	0.01222	0.01387			
AFIX	3							
H22A	2	1.16489	0.16455	0.30676	11.00000	8.80000		
H22B	2	1.31544	0.15068	0.32336	11.00000	8.80000		
AFIX	0							
C23	1	1.20103	0.05170	0.29312	11.00000	0.02350	0.05124	=
		0.03352	0.00938	0.00486	0.00338			
C24	1	1.18430	-0.00771	0.29958	11.00000	0.03843	0.05715	=
		0.04382	0.01856	0.00694	-0.00465			
AFIX	3							
H24A	2	1.17303	-0.02339	0.33240	11.00000	8.80000		
AFIX	0							
C25	1	1.18431	-0.04377	0.25740	11.00000	0.05209	0.04271	=
		0.05893	0.01912	-0.00055	-0.00660			
AFIX	3							
H25A	2	1.17086	-0.08446	0.26144	11.00000	8.80000		
AFIX	0							
C26	1	1.20356	-0.02191	0.20906	11.00000	0.04184	0.04360	=
		0.04807	0.00386	-0.00120	-0.00351			
AFIX	3							
H26A	2	1.20416	-0.04720	0.18042	11.00000	8.80000		
AFIX	0							
C27	1	1.22166	0.03723	0.20389	11.00000	0.02208	0.04074	=
		0.03312	0.00709	0.00070	0.00016			
C28	1	1.22073	0.07478	0.24567	11.00000	0.02145	0.04068	=
		0.03432	0.00725	-0.00079	0.00338			
AFIX	3							
H28A	2	1.23340	0.11552	0.24163	11.00000	8.80000		
AFIX	0							
C29	1	1.14582	0.02324	0.45376	11.00000	0.04975	0.05601	=
		0.03375	0.01984	-0.01185	-0.02250			
AFIX	3							
H29A	2	1.15203	0.06233	0.46576	11.00000	8.80000		
AFIX	0							
C30	1	1.25467	-0.01105	0.45591	11.00000	0.03021	0.14457	=
		0.06703	0.06693	0.00694	0.00044			
AFIX	3							
H30A	2	1.33538	0.00435	0.47018	11.00000	8.80000		
AFIX	0							
C31	1	1.25005	-0.06602	0.43829	11.00000	0.08347	0.15405	=
		0.06328	0.07051	0.04285	0.07672			
AFIX	3							
H31A	2	1.32704	-0.08902	0.43946	11.00000	8.80000		
AFIX	0							
C32	1	1.13122	-0.08907	0.41827	11.00000	0.17079	0.03792	=
		0.04557	0.01726	0.04079	0.03849			
AFIX	3							
H32A	2	1.12695	-0.12789	0.40556	11.00000	8.80000		
AFIX	0							

C33	1	1.01812	-0.05493	0.41692	11.00000	0.06666	0.02999 =
		0.03642	0.00667	0.00369	-0.00873		
AFIX	3						
H33A	2	0.93628	-0.07056	0.40416	11.00000	8.80000	
AFIX	0						
C34	1	1.02755	0.00160	0.43437	11.00000	0.03342	0.03257 =
		0.01958	0.00761	0.00446	0.00182		
C35	1	0.90779	0.03924	0.43178	11.00000	0.05962	0.06415 =
		0.02449	0.01327	0.01000	0.02772		
AFIX	3						
H35A	2	0.90982	0.06356	0.46298	11.00000	8.80000	
H35B	2	0.82971	0.01392	0.43108	11.00000	8.80000	
AFIX	0						
C36	1	0.87722	0.04877	0.33613	11.00000	0.03353	0.04771 =
		0.02308	0.00668	0.00220	-0.00845		
AFIX	3						
H36A	2	0.79478	0.02637	0.33501	11.00000	8.80000	
H36B	2	0.94916	0.02051	0.33361	11.00000	8.80000	
AFIX	0						
C37	1	0.87221	0.08906	0.29025	11.00000	0.02312	0.04298 =
		0.02383	0.00819	0.00003	0.00085		
C38	1	0.88447	0.06416	0.24271	11.00000	0.02023	0.03516 =
		0.02529	0.00196	-0.00001	0.00088		
AFIX	3						
H38A	2	0.89420	0.02307	0.24015	11.00000	8.80000	
AFIX	0						
C39	1	0.88281	0.09808	0.19872	11.00000	0.02065	0.04002 =
		0.02289	0.00598	0.00121	0.00227		
C40	1	0.86985	0.15819	0.20275	11.00000	0.05027	0.03980 =
		0.02496	0.00663	-0.00251	0.00363		
AFIX	3						
H40A	2	0.87084	0.18204	0.17320	11.00000	8.80000	
AFIX	0						
C41	1	0.85551	0.18325	0.24976	11.00000	0.06751	0.03706 =
		0.03508	-0.00199	-0.00930	0.01096		
AFIX	3						
H41A	2	0.84540	0.22433	0.25227	11.00000	8.80000	
AFIX	0						
C42	1	0.85571	0.14900	0.29347	11.00000	0.04557	0.04656 =
		0.02458	-0.00436	-0.00282	0.01102		
AFIX	3						
H42A	2	0.84455	0.16664	0.32554	11.00000	8.80000	
AFIX	0						
C43	1	0.90650	0.06804	0.14913	11.00000	0.03296	0.04384 =
		0.02216	0.00630	0.00256	0.01056		
AFIX	3						
H43A	2	0.99900	0.07325	0.14242	11.00000	8.80000	
H43B	2	0.89038	0.02570	0.15262	11.00000	8.80000	
AFIX	0						
C44	1	0.81785	0.05045	0.05943	11.00000	0.04253	0.03215 =
		0.03194	-0.00572	0.00073	0.00313		
AFIX	3						
H44A	2	0.78441	0.01198	0.06944	11.00000	8.80000	
H44B	2	0.90767	0.04484	0.04948	11.00000	8.80000	
AFIX	0						
C45	1	0.73297	0.07346	0.01421	11.00000	0.04263	0.03175 =
		0.02395	-0.00599	0.00087	-0.00594		

C46	1	0.78761	0.09888	-0.02688	11.00000	0.04113	0.03960 =
		0.02960	-0.00743	0.00421	-0.00629		
AFIX	3						
H46A	2	0.87975	0.10183	-0.02655	11.00000	8.80000	
AFIX	0						
C47	1	0.70967	0.12008	-0.06845	11.00000	0.07040	0.04548 =
		0.02521	-0.00023	-0.00037	-0.00951		
AFIX	3						
H47A	2	0.74818	0.13768	-0.09627	11.00000	8.80000	
AFIX	0						
C48	1	0.57622	0.11544	-0.06916	11.00000	0.06082	0.05534 =
		0.03305	0.00054	-0.01281	0.00232		
AFIX	3						
H48A	2	0.52258	0.12951	-0.09774	11.00000	8.80000	
AFIX	0						
C49	1	0.52000	0.09050	-0.02864	11.00000	0.03935	0.07107 =
		0.04618	-0.00846	-0.00136	-0.00278		
AFIX	3						
H49A	2	0.42779	0.08800	-0.02900	11.00000	8.80000	
AFIX	0						
C50	1	0.59858	0.06900	0.01275	11.00000	0.03629	0.05523 =
		0.03202	-0.00138	0.00437	-0.00865		
AFIX	3						
H50A	2	0.55969	0.05107	0.04032	11.00000	8.80000	
END							