

Structural chemistry of borosilicates, part II: Searlesite, $\text{NaBSi}_2\text{O}_5(\text{OH})$: Absolute configuration, hydrogen locations, and refinement of the structure

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Abstract

Searlesite, $\text{NaBSi}_2\text{O}_5(\text{OH})_2$ is monoclinic, space group $P2_1$, with cell dimensions: $a = 7.9814(12)$, $b = 6.0657(8)$, $c = 4.9054(4)\text{\AA}$, and $\beta = 93.95(1)^\circ$. The absolute configuration and hydrogen positions have been determined from a refinement of the structure using 811 reflections measured by $\text{CuK}\alpha$ radiation, and the atomic coordinates determined by Kravchenko (1964). The structure has been refined using anisotropic temperature factors for all atoms except hydrogen to an R factor of 0.035 for 1694 reflections measured by $\text{MoK}\alpha$ radiation. The crystal structure of searlesite consists of highly kinked pyroxene-type silicate chains parallel to the c axis, connected through corner-sharing $\text{BO}_2(\text{OH})_2$ tetrahedra to form borosilicate sheets parallel to the (100) plane; these sheets are held together by spiral columns of edge-sharing Na-O octahedra running parallel to the b axis (as found by Kravchenko, 1964) and by one of the two types of hydrogen bonds. Within the tetrahedral $\text{BO}_2(\text{OH})_2$ group, the O-H distances are 0.87 and 0.88 \AA and the B-O-H angles are 114° and 113° . Both hydrogen atoms are involved in hydrogen bonds, the $\text{H}\cdots\text{O}$ distances being 2.32 and 2.04 \AA , and the $\text{O-H}\cdots\text{O}$ angles 147° and 170° . The bridging B-O distances (av. 1.490 \AA) are much longer than the non-bridging B-O distances (av. 1.455 \AA). Within each of the two crystallographically distinct SiO_4 tetrahedra, the Si-O bond involving oxygen belonging to the Si-O-B bridge is significantly shorter (av. 1.591 \AA) than those involving oxygens belonging to the Si-O-Si bridges (av. Si-O 1.617 \AA). The average B-O , Si(1)-O and Si(2)-O distances are 1.472, 1.614, and 1.608 \AA respectively. The $\text{NaO}_2(\text{OH})_4$ octahedron is highly distorted; the average Na-O distance is 2.485 \AA .

Introduction

In part I of this series of papers on the structural chemistry of borosilicates, we have described the structure of garrelsite, $\text{NaBa}_3\text{Si}_2\text{B}_7\text{O}_{16}(\text{OH})_4$ (Ghose, Ulbrich, and Wan, 1975). Garrelsite contains a new type of borosilicate chain, consisting of two types of four-membered rings with alternating B- and Si-tetrahedra; in addition, there is a $[\text{B}_5\text{O}_{12}]$ polyanion, consisting of three borate tetrahedra and two borate triangles.

In this paper we present the details of the structure of searlesite, $\text{NaBSi}_2\text{O}_5(\text{OH})_2$. This mineral is widespread in the Searles Lake area in California and in the Green River formation in Utah and Wyoming. The unit cell dimensions and space group of searlesite were determined by Fahey and Axelrod (1950). The crystal structure was determined by Kravchenko (1964) using an acicular crystal from Cave Springs, Nevada. Kravchenko (1964) collected intensity data

on 1524 (1258 non zero) reflections by visual estimation from Weissenberg films. The structure was refined by the least-squares method using isotropic temperature factors to an R factor of 19.5 percent for all reflections and 13.9 percent for non-zero reflections. The hydrogen positions were not determined. We have undertaken a further refinement of the searlesite structure, first, to obtain more precise bond distances and angles (Si-O-B angles in particular) and compare them with other borosilicates; second, to determine the absolute configuration; and third, to determine the hydrogen positions directly and discuss the nature of the hydrogen bonding.

Crystal data

The cell dimensions of an acicular crystal from Cave Springs, Nevada, were determined by the least-squares refinement of 15 reflections with 2θ values between 35° and 45° measured with $\text{MoK}\alpha$ radiation

SEARLESITE, - FINAL STRUCTURE FACTORS LISTING

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DE
0	11	3	.744 *	.500	-.329	-.377	.243	
0	11	4	2.665	2.399	1.043	2.161	.266	
0	11	5	2.112	2.030	-2.024	-.157	.082	
0	11	6	2.724	2.589	-.482	-2.544	.134	
0	11	7	2.492	2.299	2.168	-.766	.193	
0	12	0	11.015	11.050	10.791	-2.379	-.035	
0	12	1	1.730	1.739	.927	1.472	-.009	
0	12	2	7.872	7.905	-7.894	.409	-.033	
0	12	3	3.974	3.781	2.646	-2.701	.193	
0	12	4	6.299	6.207	5.755	2.326	.092	
0	12	5	2.125	2.050	.612	1.956	.075	
0	12	6	3.411	3.281	2.627	-1.966	.130	
0	13	1	4.988	4.953	3.765	-3.217	.036	
0	13	2	5.903	5.891	-4.261	-4.068	.012	
0	13	3	3.965	4.043	-3.759	1.491	-.079	
0	13	4	8.423	8.309	7.657	3.226	.114	
0	13	5	2.329	2.301	-.695	-2.194	.028	
0	14	0	8.736	8.768	3.362	-8.098	-.032	
0	14	1	1.392	1.269	-.919	.874	.124	
0	14	2	5.892	5.979	-.325	5.971	-.087	
0	14	3	2.469	2.454	2.439	-.271	.015	
0	14	4	2.531	2.636	.108	-2.634	-.106	
0	15	0	.442 *	.000	.000	.000	.442	
0	15	1	1.710	1.631	1.255	-1.041	.080	
1	0	-10	4.192	3.888	3.885	.138	.304	
1	0	-9	1.036	1.109	1.109	-.008	-.073	
1	0	-8	1.892	1.878	-1.872	-.147	.014	
1	0	-7	6.790	6.725	-6.725	-.008	.066	
1	0	-6	.688	.560	.558	.054	.128	
1	0	-5	4.097	4.403	4.403	-.012	-.305	
1	0	-4	10.601	12.338	-12.338	-.014	-1.737	
1	0	-3	37.889	42.131	-42.131	-.137	-4.241	
1	0	-2	31.431	35.320	-35.319	-.208	-3.889	
1	0	-1	36.665	40.794	40.794	.123	-4.129	
1	0	0	23.018	22.118	22.117	.176	.901	
1	0	1	49.590	56.059	-56.058	-.244	-6.468	
1	0	2	12.796	14.330	-14.329	-.184	-1.534	
1	0	3	12.825	11.396	11.395	.128	1.430	
1	0	4	3.730	3.520	-3.520	.030	.210	
1	0	5	5.406	6.299	-6.298	-.053	-.893	
1	0	6	7.081	6.858	-6.858	-.018	.223	
1	0	7	7.400	7.418	-7.418	-.096	-.018	
1	0	8	2.002	1.771	1.771	-.024	.231	
1	0	9	5.764	5.543	5.542	.135	.220	
1	0	10	.558 *	.558	.557	.025	.001	
1	1	-10	4.843	4.509	.267	-4.501	.334	
1	1	-9	3.266	3.077	-3.075	-.096	.189	
1	1	-8	1.525	1.599	-.085	-1.597	-.074	
1	1	-7	3.245	3.254	3.139	-.858	-.009	
1	1	-6	15.223	15.967	3.516	15.575	-.744	
1	1	-5	4.718	4.739	-2.452	-4.055	-.020	
1	1	-4	20.201	22.129	-7.004	-20.991	-1.928	
1	1	-3	11.264	11.840	4.944	10.758	-.576	

SEARLESITE, - FINAL STRUCTURE FACTORS LISTING

STRUCT

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DE
1	1	-2	6.730	7.280	-5.887	4.283	-.550	
1	1	-1	14.382	14.435	5.321	-13.418	-.053	
1	1	0	13.073	11.702	8.845	-7.662	1.371	
1	1	1	29.694	29.255	-27.210	10.747	.438	
1	1	2	12.301	11.741	3.488	11.211	.559	
1	1	3	22.247	22.464	16.233	15.529	-.218	
1	1	4	25.074	26.475	2.045	26.396	-1.401	
1	1	5	9.380	9.321	-7.102	-6.036	.059	
1	1	6	11.197	11.049	-3.676	-10.419	.149	
1	1	7	11.983	11.702	5.012	10.574	.281	
1	1	8	2.751	2.552	-.099	2.550	.200	
1	1	9	5.243	5.011	-1.484	-4.787	.232	
1	1	10	.768	.681	.253	.632	.087	
1	2	-10	8.934	8.574	7.898	-3.337	.360	
1	2	-9	4.822	4.600	-4.495	-.980	.222	
1	2	-8	6.842	6.797	-6.028	3.140	.045	
1	2	-7	8.983	9.307	9.231	1.191	-.324	
1	2	-6	4.642	4.865	-3.657	-3.208	-.223	
1	2	-5	16.449	17.582	-16.220	-6.785	-1.133	
1	2	-4	4.930	5.210	-3.646	3.721	-.280	
1	2	-3	15.654	16.424	-5.035	15.633	-.770	
1	2	-2	41.118	43.898	-43.494	5.948	-2.780	
1	2	-1	22.142	21.232	-12.502	-17.161	.911	
1	2	1	46.062	44.967	-43.186	12.532	1.095	
1	2	2	19.056	19.311	-15.397	11.655	-.255	
1	2	3	22.747	23.000	20.518	-10.393	-.253	
1	2	4	20.468	20.665	-20.079	-4.883	-.197	
1	2	5	6.791	6.590	-6.589	.090	.201	
1	2	6	6.772	6.597	5.086	4.201	.175	
1	2	7	9.813	9.379	-8.405	4.163	.434	
1	2	8	3.574	3.422	-2.959	-1.720	.152	
1	2	9	6.708	6.183	5.428	-2.960	.525	
1	2	10	4.298	3.903	3.604	-1.498	.395	
1	3	-10	2.757	2.621	-2.157	-1.489	.137	
1	3	-9	4.224	4.179	-2.262	3.514	.045	
1	3	-8	3.661	3.541	-2.190	-2.783	.120	
1	3	-7	8.510	8.607	4.534	-7.316	-.097	
1	3	-6	16.339	17.339	9.746	14.341	-1.001	
1	3	-5	5.492	5.741	-4.961	2.889	-.248	
1	3	-4	23.901	25.872	-12.892	-22.432	-1.971	
1	3	-3	9.897	10.292	.054	10.292	-.395	
1	3	-2	16.070	16.361	11.193	11.933	-.291	
1	3	-1	15.537	15.059	-3.672	-14.605	.477	
1	3	0	21.919	19.777	-18.158	-7.835	2.142	
1	3	1	13.325	12.511	-3.437	12.029	.814	
1	3	2	18.826	17.195	4.769	16.520	1.631	
1	3	3	14.375	14.266	13.478	4.674	.109	
1	3	4	15.808	16.198	9.039	13.441	-.390	
1	3	5	8.760	8.621	-8.583	.804	.140	
1	3	6	7.581	7.519	-6.656	-3.498	.062	
1	3	7	10.548	10.118	3.119	9.625	.430	
1	3	8	5.573	5.169	3.876	-3.420	.404	
1	3	9	5.537	5.216	-2.296	-4.683	.321	

SEARLESITE, - FINAL STRUCTURE FACTORS LISTING

STRUCT

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DE
1	3	10	6.600	5.815	-3.023	4.967	.785	
1	4	-10	3.506	3.311	.465	-3.278	.195	
1	4	-9	2.581	2.270	-1.745	-1.452	.311	
1	4	-8	3.079	2.913	2.007	2.112	.166	
1	4	-7	3.352	3.189	2.208	2.300	.163	
1	4	-6	8.251	8.539	-5.564	-6.478	-.288	
1	4	-5	12.099	12.605	-12.346	-2.540	-.506	
1	4	-4	7.586	8.043	-5.011	6.291	-.457	
1	4	-3	7.810	8.016	.851	7.971	-.206	
1	4	-2	18.167	18.211	-15.174	10.068	-.044	
1	4	-1	19.386	18.989	-15.799	-10.534	.397	
1	4	0	26.353	24.095	-9.202	-22.268	2.258	
1	4	1	12.948	11.991	-11.755	2.372	.957	
1	4	2	15.223	14.419	8.137	11.904	.804	
1	4	3	2.873	2.651	-1.344	-2.285	.221	
1	4	4	22.415	22.054	-19.050	-11.113	.361	
1	4	5	3.419	3.217	-3.080	.929	.202	
1	4	6	8.958	8.705	4.819	7.250	.252	
1	4	7	4.601	4.401	-2.907	3.304	.200	
1	4	8	2.699	2.496	-1.630	-1.891	.203	
1	4	9	4.871	4.482	.972	-4.376	.388	
1	4	10	1.061	.885	.116	-.877	.176	
1	5	-10	3.761	3.472	-.632	-3.414	.289	
1	5	-9	5.405	5.355	-.995	5.261	.051	
1	5	-8	2.750	2.632	-2.044	1.658	.118	
1	5	-7	7.701	7.852	1.776	-7.648	-.150	
1	5	-6	7.969	8.145	8.139	-.311	-.176	
1	5	-5	2.677	2.692	-2.340	1.331	-.016	
1	5	-4	9.944	10.279	-8.786	5.336	-.335	
1	5	-3	6.621	6.646	3.134	5.860	-.025	
1	5	-2	13.285	13.360	-1.926	-13.221	-.076	
1	5	-1	14.852	14.434	-4.181	-13.815	.418	
1	5	0	17.710	16.654	-2.502	16.465	1.056	
1	5	1	30.623	28.785	-8.475	27.509	1.838	
1	5	2	11.264	10.505	5.242	-9.104	.759	
1	5	3	17.389	16.738	12.525	-11.104	.651	
1	5	4	15.923	15.530	3.112	15.215	.393	
1	5	5	9.699	9.490	-5.484	7.746	.209	
1	5	6	1.507	1.222	-1.218	.093	.285	
1	5	7	3.468	3.414	3.258	1.020	.055	
1	5	8	3.645	3.610	-2.972	-2.048	.036	
1	5	9	1.960	2.088	-1.868	-.931	-.127	
1	6	-9	2.943	2.923	-2.922	-.070	.020	
1	6	-8	.795 *	.801	.713	.366	-.006	
1	6	-7	7.433	7.687	5.901	-4.926	-.254	
1	6	-6	8.122	8.176	-8.109	1.042	-.054	
1	6	-5	15.133	15.637	-14.902	4.739	-.504	
1	6	-4	6.402	6.665	6.383	1.918	-.262	
1	6	-3	7.092	7.136	6.655	-2.576	-.045	
1	6	-2	22.722	22.620	-22.332	3.602	.102	
1	6	-1	9.732	8.986	-7.279	5.269	.745	
1	6	0	14.619	13.255	4.014	-12.632	1.365	
1	6	1	24.875	23.660	-23.660	-.033	1.215	

SEARLESITE, - FINAL STRUCTURE FACTORS LISTING

STRUC

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	D
1	6	2	2.008	1.821	1.808	-.218	.187	
1	6	3	18.649	17.938	15.565	-8.916	.711	
1	6	4	20.956	20.596	-10.159	7.558	.360	
1	6	5	12.424	11.891	-11.682	2.221	.533	
1	6	6	11.683	11.286	11.023	-2.424	.397	
1	6	7	4.167	3.714	3.004	2.184	.452	
1	6	8	5.895	5.478	-5.474	.206	.417	
1	6	9	2.686	2.166	-1.628	-1.428	.521	
1	7	-9	5.219	5.162	2.273	4.634	.058	
1	7	-8	.433 *	.165	-.161	.038	.267	
1	7	-7	6.585	8.636	-2.912	-8.131	-.051	
1	7	-6	4.116	4.094	3.558	2.025	.022	
1	7	-5	2.344	2.454	.974	2.253	-.110	
1	7	-4	4.780	4.741	-1.772	-4.397	.039	
1	7	-3	11.492	11.516	4.773	10.480	-.024	
1	7	-2	10.382	10.668	-9.327	-5.177	-.286	
1	7	-1	18.362	18.142	-11.963	-13.646	.219	
1	7	0	18.136	17.342	7.708	15.535	.794	
1	7	1	18.020	17.066	7.216	15.465	.954	
1	7	2	8.185	8.018	-4.437	-6.679	.167	
1	7	3	9.174	8.755	-1.905	-8.545	.419	
1	7	4	12.565	12.292	7.333	9.865	.274	
1	7	5	5.688	5.391	1.414	5.202	.297	
1	7	6	3.064	3.097	-2.325	-2.046	-.033	
1	7	7	6.314	5.841	1.720	5.582	.472	
1	7	8	4.038	3.868	-3.000	-2.441	.170	
1	7	9	3.981	3.590	-2.716	-2.348	.391	
1	8	-9	3.380	3.143	-2.910	-1.189	.237	
1	8	-8	3.446	3.572	-.891	-3.459	-.126	
1	8	-7	3.949	3.920	3.472	-1.821	.029	
1	8	-6	3.747	3.861	-3.692	1.129	-.114	
1	8	-5	10.566	10.777	-7.623	7.618	-.211	
1	8	-4	1.016	.502	-.499	-.052	.514	
1	8	-3	10.339	10.503	4.820	-9.332	-.164	
1	8	-2	5.607	6.483	-4.211	4.930	-.876	
1	8	-1	12.479	12.576	-11.258	5.605	-.097	
1	8	0	6.442	6.305	-5.731	-2.628	.138	
1	8	1	5.817	5.637	-5.167	-2.254	.180	
1	8	2	7.292	7.172	3.456	-6.285	.120	
1	8	3	4.770	4.741	-.605	-4.702	.029	
1	8	4	13.704	13.299	-12.043	5.643	.405	
1	8	5	8.072	7.661	2.153	7.352	.411	
1	8	6	6.957	6.728	5.670	-3.622	.229	
1	8	7	5.890	5.464	-2.932	-4.610	.426	
1	8	8	3.183	2.887	-1.634	2.380	.296	
1	9	-8	1.017	.923	.126	-.914	.094	
1	9	-7	4.366	4.283	-2.513	-3.468	.083	
1	9	-6	2.251	2.352	-.328	2.329	-.101	
1	9	-5	.802 *	1.218	-1.199	-.214	-.417	
1	9	-4	7.676	8.025	5.998	-5.331	-.149	
1	9	-3	3.513	3.606	3.543	.671	-.093	
1	9	-2	15.092	15.488	-13.344	7.862	-.396	
1	9	-1	9.624	9.531	-9.531	.018	.093	

SEARLESITE, - FINAL STRUCTURE FACTORS LISTING

STRUCT

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DE
1	9	0	12.059	11.568	11.128	-3.158	.491	
1	9	1	10.092	10.555	9.195	5.182	.437	
1	9	2	8.523	8.273	-8.217	.958	.251	
1	9	3	3.367	3.310	-3.306	-.155	.058	
1	9	4	5.457	5.300	4.697	2.456	.157	
1	9	5	2.448	2.262	2.158	-.677	.186	
1	9	6	2.788	2.764	2.385	1.396	.024	
1	9	7	3.426	3.276	-1.128	3.076	.150	
1	9	8	4.985	4.718	-4.702	.399	.267	
1	10	-7	4.469	4.704	.204	-4.695	-.235	
1	10	-6	1.537	1.566	.620	1.438	-.029	
1	10	-5	7.604	7.724	-3.093	7.077	-.119	
1	10	-4	2.672	2.736	2.625	-.772	-.064	
1	10	-3	7.946	8.249	-1.383	-8.133	-.303	
1	10	-2	11.917	12.120	-11.775	2.873	-.203	
1	10	-1	8.552	8.325	4.571	6.958	.227	
1	10	0	6.765	6.608	4.935	-4.395	.157	
1	10	1	13.242	13.149	-13.143	-.382	.093	
1	10	2	7.343	7.182	-6.669	-2.666	.160	
1	10	3	6.759	6.954	4.208	-5.536	-.195	
1	10	4	6.056	6.898	.571	6.875	-.842	
1	10	5	3.664	3.395	-1.835	2.857	.269	
1	10	6	5.431	5.185	1.805	-4.861	.246	
1	10	7	1.504	1.504	-1.336	-.692	-.000	
1	11	-7	2.310	3.209	-3.167	-.519	-.899	
1	11	-6	4.676	4.685	3.648	2.939	-.009	
1	11	-5	3.228	3.226	.085	-3.225	.002	
1	11	-4	8.135	8.249	-4.956	-6.565	-.114	
1	11	-3	4.841	7.622	5.267	5.510	-2.782	
1	11	-2	5.432	5.812	-2.140	5.404	-.380	
1	11	-1	7.737	7.595	-7.167	-2.512	.142	
1	11	0	5.197	5.119	4.750	1.907	.078	
1	11	1	3.394	3.135	2.660	1.658	.259	
1	11	2	4.817	4.633	-2.124	-4.117	.184	
1	11	3	1.911	2.053	-1.027	1.778	-.143	
1	11	4	7.521	7.281	2.652	6.781	.240	
1	11	5	3.053	3.160	.072	-3.159	-.107	
1	11	6	4.702	4.411	-.448	-4.388	.291	
1	11	7	6.331	6.095	2.846	5.390	.236	
1	12	-6	1.606	1.911	-.271	-1.892	-.305	
1	12	-5	4.697	4.753	3.159	3.551	-.056	
1	12	-4	1.128	1.197	.598	1.037	-.068	
1	12	-3	7.825	8.206	-6.720	-4.709	-.381	
1	12	-2	3.807	3.884	-3.253	2.122	-.078	
1	12	-1	5.112	5.419	4.268	3.339	-.307	
1	12	0	5.218	5.278	2.876	-4.426	-.060	
1	12	1	9.288	9.398	-9.398	.112	-.110	
1	12	2	6.033	6.151	-5.776	2.114	-.118	
1	12	3	4.428	4.376	3.569	-2.532	.052	
1	12	4	.446	.288	.173	.231	.157	
1	12	5	1.990	1.923	1.616	1.043	.067	
1	12	6	1.801	1.612	-.395	-1.563	.189	
1	13	-5	3.704	4.016	-4.015	.071	-.312	

SEARLESITE, - FINAL STRUCTURE FACTORS LISTING

STRUCT DE

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DE
1	13	-4	5.261	5.316	-1.981	-4.934	-.055	
1	13	-3	2.545	2.661	2.639	-.340	-.116	
1	13	-2	6.032	6.279	.138	6.277	-.247	
1	13	-1	2.941	3.073	-1.321	2.774	-.131	
1	13	0	2.729	3.393	1.280	-3.143	-.664	
1	13	1	2.319	2.461	-.688	-2.363	-.142	
1	13	2	4.483	4.341	-3.800	2.098	.142	
1	13	3	5.135	5.145	4.322	2.792	-.010	
1	13	4	3.341	3.276	3.241	.482	.065	
1	13	5	5.135	5.259	-4.583	-2.580	-.124	
1	14	-4	1.163	1.217	.830	-.890	-.054	
1	14	-3	1.611	1.536	.878	1.261	.074	
1	14	-2	5.789	6.063	-3.730	4.780	-.274	
1	14	-1	4.160	4.318	.356	-4.303	-.158	
1	14	0	5.923	6.176	.112	-6.175	-.253	
1	14	1	6.604	6.812	-3.002	6.114	-.208	
1	14	2	4.909	4.991	-1.276	4.825	-.082	
1	14	3	5.016	5.133	-.553	-5.103	-.117	
1	14	4	2.525	2.622	-.030	-2.621	-.097	
1	15	-1	3.065	3.029	-2.683	-1.405	.036	
1	15	0	2.342	2.445	2.440	.149	-.103	
1	15	1	3.068	3.276	-1.073	3.095	-.208	
2	0	-10	7.129	6.703	6.702	.128	.426	
2	0	-9	4.309	4.359	-4.358	-.104	-.051	
2	0	-8	3.421	3.278	-3.277	-.095	.143	
2	0	-7	12.174	12.643	12.642	.152	-.469	
2	0	-6	7.877	8.091	8.091	.098	-.214	
2	0	-5	5.511	5.319	5.319	-.015	.192	
2	0	-4	1.537	1.524	-1.524	.017	.012	
2	0	-3	16.214	16.403	-16.403	-.063	-.190	
2	0	-2	14.355	14.966	14.966	-.008	-.612	
2	0	-1	47.926	52.457	52.456	.263	-4.531	
2	0	0	22.084	20.697	20.697	.089	1.386	
2	0	1	39.548	41.435	-41.434	-.261	-1.887	
2	0	2	23.960	23.622	23.622	.032	.338	
2	0	3	44.448	49.120	49.119	.268	-4.672	
2	0	4	11.658	12.028	-12.028	-.029	-.370	
2	0	5	9.851	10.074	-10.073	-.085	-.222	
2	0	6	3.165	3.075	3.075	.008	.090	
2	0	7	7.376	7.426	-7.426	-.065	-.050	
2	0	8	1.856	1.519	1.519	.031	.337	
2	0	9	4.049	3.896	3.894	.113	.154	
2	0	10	1.066	.600	-.597	-.060	.466	
2	1	-10	4.594	4.285	-3.312	-2.719	.309	
2	1	-9	1.234	1.109	.979	.522	.124	
2	1	-8	2.489	2.544	1.321	-2.174	-.055	
2	1	-7	3.037	3.176	-.894	3.048	-.140	
2	1	-6	13.505	14.500	4.937	13.634	-.995	
2	1	-5	12.853	13.465	-2.550	-13.221	-.612	
2	1	-4	13.857	15.409	-7.410	-13.510	-1.552	
2	1	-3	26.893	29.125	4.609	28.758	-2.232	
2	1	-2	26.693	26.843	18.419	-19.527	-.151	
2	1	-1	43.608	44.975	-8.742	-44.117	-1.367	

SEARLESITE, - FINAL STRUCTURE FACTORS LISTING

STRUCT

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DE
2	1	0	36.433	34.264	-34.264	-.134	2.168	
2	1	1	32.909	32.346	12.094	-30.001	.563	
2	1	2	20.863	21.153	13.106	-16.603	-.290	
2	1	3	14.835	15.493	-2.614	15.271	-.659	
2	1	4	2.010	2.334	1.430	1.845	-.324	
2	1	5	20.872	21.384	-4.769	-20.845	-.512	
2	1	6	3.111	2.975	-.631	-2.907	.136	
2	1	7	12.703	12.919	4.314	12.177	-.216	
2	1	8	6.531	6.458	.829	-6.405	.073	
2	1	9	9.078	8.693	-2.964	-8.172	.385	
2	1	10	3.172	2.900	-1.985	2.114	.272	
2	2	-10	3.911	3.629	3.066	-2.294	.082	
2	2	-9	3.011	2.995	-2.206	2.026	.016	
2	2	-8	3.570	4.239	3.070	2.924	-.669	
2	2	-7	5.807	6.022	5.678	-2.004	-.215	
2	2	-6	9.869	10.044	5.490	-8.410	-.174	
2	2	-5	4.620	4.837	4.712	-1.092	-.217	
2	2	-4	12.376	13.597	-2.698	13.327	-1.221	
2	2	-3	9.649	9.963	7.913	6.053	-.314	
2	2	-2	8.933	8.433	7.358	-4.122	.500	
2	2	-1	9.911	10.183	1.793	-10.023	-.272	
2	2	0	31.426	29.434	29.238	-3.392	1.991	
2	2	1	20.789	19.003	13.476	13.399	1.786	
2	2	2	10.442	9.498	9.211	-2.319	.944	
2	2	3	14.633	14.631	9.857	-10.813	.002	
2	2	4	4.704	4.828	2.269	-4.262	-.124	
2	2	5	5.276	5.386	2.886	4.547	-.109	
2	2	6	9.499	9.398	-6.629	6.662	.101	
2	2	7	5.250	5.177	-5.095	.918	.073	
2	2	8	3.897	3.718	3.164	-1.952	.179	
2	2	9	2.599	2.625	1.829	-1.883	-.026	
2	2	10	1.404	1.188	-1.117	.406	.216	
2	3	-10	1.972	1.889	-1.672	-.880	.082	
2	3	-9	4.512	4.933	-4.379	2.271	-.421	
2	3	-8	4.801	4.845	1.555	-4.589	-.045	
2	3	-7	7.125	8.638	8.563	-1.129	-1.512	
2	3	-6	14.958	16.154	.715	16.139	-1.196	
2	3	-5	12.746	13.155	-8.159	-10.318	-.408	
2	3	-4	12.563	13.214	.329	-13.210	-.651	
2	3	-3	25.458	27.145	13.109	23.769	-1.686	
2	3	-2	11.315	11.559	-2.270	-11.333	-.244	
2	3	-1	39.622	39.045	-5.239	-38.692	.577	
2	3	0	13.659	12.412	-7.039	-10.223	1.246	
2	3	1	22.876	21.106	-21.053	1.493	1.771	
2	3	2	19.569	19.122	13.903	-13.128	.447	
2	3	3	21.227	21.501	19.949	-8.019	-.273	
2	3	4	9.727	9.650	-8.780	4.004	.077	
2	3	5	11.642	11.771	-8.827	-7.787	-.129	
2	3	6	3.284	4.138	4.006	-1.039	-.855	
2	3	7	6.522	6.702	6.041	2.901	-.179	
2	3	8	7.866	7.740	-2.217	-7.416	.125	
2	3	9	4.612	4.380	-3.836	-2.115	.232	
2	3	10	2.963	2.655	-.220	2.646	.307	

SEARLESITE, - FINAL STRUCTURE FACTORS LISTING

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DE
2	4	-10	3.687	3.613	3.065	-1.914	.073	
2	4	-9	3.332	3.283	-2.014	2.593	.049	
2	4	-8	4.293	4.283	3.766	2.040	.010	
2	4	-7	10.262	10.847	9.106	-5.895	-.585	
2	4	-6	6.694	7.084	-6.401	-3.035	-.389	
2	4	-5	2.224	2.500	-2.486	-.258	-.275	
2	4	-4	18.616	19.636	19.356	3.304	-1.020	
2	4	-3	17.382	18.528	9.368	15.985	-1.147	
2	4	-2	12.072	12.089	-12.003	1.442	-.017	
2	4	-1	20.899	20.424	5.787	-19.586	.475	
2	4	0	30.376	28.528	27.725	-6.720	1.848	
2	4	1	21.459	20.127	.971	20.103	1.332	
2	4	2	9.328	9.082	8.945	1.567	.247	
2	4	3	25.293	25.872	14.010	-21.750	-.579	
2	4	4	13.280	13.289	-13.288	.214	-.009	
2	4	5	7.582	7.635	.992	7.570	-.053	
2	4	6	10.072	10.135	9.321	3.979	-.063	
2	4	7	7.284	7.190	-5.584	4.529	.095	
2	4	8	5.057	4.821	-3.188	-3.617	.236	
2	4	9	2.957	2.718	1.255	-2.411	.239	
2	4	10	2.291	1.981	.918	1.756	.310	
2	5	-9	4.828	4.695	-.452	4.673	.132	
2	5	-8	4.782	4.863	-.534	-4.834	-.081	
2	5	-7	5.266	5.502	1.705	-5.231	-.236	
2	5	-6	10.080	10.734	7.952	7.211	-.655	
2	5	-5	3.592	3.849	-2.971	2.446	-.256	
2	5	-4	5.619	5.945	-5.512	-2.227	-.327	
2	5	-3	12.742	13.333	12.030	5.748	-.590	
2	5	-2	26.412	27.522	4.621	-27.132	-1.111	
2	5	-1	21.864	21.382	-14.877	-15.358	.481	
2	5	0	36.051	35.324	-10.757	33.646	.727	
2	5	1	15.189	14.857	5.756	-13.697	.332	
2	5	2	36.133	36.773	3.764	-36.580	-.640	
2	5	3	2.469	2.601	-.236	2.591	-.133	
2	5	4	11.745	11.941	4.692	10.981	-.196	
2	5	5	5.740	5.606	-.756	-5.555	.134	
2	5	6	6.475	6.251	-1.849	-5.971	.224	
2	5	7	3.649	3.737	2.778	2.499	-.088	
2	5	8	5.441	5.203	-.604	-5.168	.238	
2	5	9	4.105	3.852	-3.281	-2.018	.253	
2	6	-9	2.294	2.339	2.024	1.172	-.044	
2	6	-8	3.931	4.024	3.722	-1.529	-.093	
2	6	-7	2.928	2.978	.305	-2.962	-.049	
2	6	-6	3.053	3.416	-3.372	-.545	-.363	
2	6	-5	4.735	5.106	3.422	3.790	-.372	
2	6	-4	8.182	8.504	8.478	.664	-.322	
2	6	-3	9.110	9.618	8.178	-5.063	-.508	
2	6	-2	11.945	12.478	3.150	12.073	-.533	
2	6	-1	3.232	3.357	-.998	3.205	-.124	
2	6	0	13.426	13.165	3.149	-12.783	.261	
2	6	1	8.799	8.567	8.369	1.832	.232	
2	6	2	16.028	15.529	15.374	-2.189	.499	
2	6	3	3.462	3.507	-.619	-3.452	-.045	

SEARLESITE, - FINAL STRUCTURE FACTORS LISTING

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DE
2	6	4	13.999	13.967	-13.774	2.315	.032	
2	6	5	5.447	5.385	5.000	2.001	.061	
2	6	6	9.601	9.560	9.392	1.785	.041	
2	6	7	2.985	2.785	-2.488	1.251	.200	
2	6	8	4.713	4.564	-4.071	2.063	.148	
2	6	9	1.513	1.254	-1.131	-.542	.260	
2	7	-9	5.344	5.432	.822	5.369	-.088	
2	7	-8	3.076	3.047	-1.265	-2.772	.029	
2	7	-7	6.675	6.953	-1.121	-6.862	-.277	
2	7	-6	7.859	8.412	4.346	7.202	-.552	
2	7	-5	2.950	3.215	3.189	.408	-.265	
2	7	-4	4.688	5.080	4.140	-2.945	-.392	
2	7	-3	1.597	1.553	.086	1.551	.044	
2	7	-2	15.989	15.929	-10.254	-12.191	.060	
2	7	-1	5.278	5.305	1.697	-5.027	-.027	
2	7	0	12.228	11.899	6.139	10.193	.329	
2	7	1	6.756	6.672	-6.622	-.815	.084	
2	7	2	19.031	18.783	-3.517	-18.451	.249	
2	7	3	7.435	7.397	4.075	-6.174	.038	
2	7	4	7.416	7.349	2.741	6.819	.067	
2	7	5	4.288	4.033	.720	-3.969	.255	
2	7	6	3.288	3.210	2.578	-1.913	.078	
2	7	7	1.216	.952	-.951	-.048	.264	
2	7	8	6.554	6.284	-4.543	-4.342	.270	
2	7	9	1.300	1.265	.319	1.224	.035	
2	8	-8	3.288	3.350	2.321	-2.415	-.061	
2	8	-7	5.598	5.716	4.582	-3.418	-.118	
2	8	-6	6.897	7.497	-4.003	6.339	-.600	
2	8	-5	4.040	4.407	-3.431	2.765	-.367	
2	8	-4	13.788	14.495	11.313	-9.063	-.707	
2	8	-3	11.298	11.762	11.735	.796	-.464	
2	8	-2	11.655	12.013	-8.013	0.950	-.358	
2	8	-1	1.860	1.930	-.853	1.731	-.070	
2	8	0	12.777	12.715	12.180	-3.649	.062	
2	8	1	1.652	1.612	1.350	-.881	.040	
2	8	2	8.110	8.155	1.503	-8.016	-.045	
2	8	3	3.821	3.639	.241	-3.631	.183	
2	8	4	14.914	15.199	-3.915	14.686	-.285	
2	8	5	3.688	3.781	3.763	-.367	-.093	
2	8	6	10.676	10.432	4.426	-9.447	.244	
2	8	7	5.971	5.763	-1.923	5.433	.208	
2	8	8	5.325	5.290	-2.092	4.859	.035	
2	9	-8	3.447	3.533	-1.820	-3.028	-.086	
2	9	-7	3.640	3.715	-3.558	1.068	-.075	
2	9	-6	5.650	5.812	3.547	4.604	-.162	
2	9	-5	8.839	9.384	6.162	-7.078	-.544	
2	9	-4	6.366	6.720	1.650	-6.514	-.354	
2	9	-3	11.002	11.429	-.105	11.428	-.427	
2	9	-2	9.299	9.557	-9.230	-2.477	-.258	
2	9	-1	13.091	13.226	-3.003	-12.881	-.135	
2	9	0	16.268	16.168	14.271	7.600	.099	
2	9	1	.780	.863	-.744	.436	-.083	
2	9	2	15.978	15.778	-12.337	-9.835	.200	

SEARLESITE, - FINAL STRUCTURE FACTORS LISTING

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DE
2	9	3	.380 *	.564	-.551	.117	-.184	
2	9	4	8.248	8.326	8.312	-.481	-.078	
2	9	5	6.721	6.818	3.670	-5.746	-.097	
2	9	6	3.754	3.530	-3.387	-.995	.224	
2	9	7	3.360	3.218	-.904	3.088	.142	
2	9	8	3.043	2.811	-1.365	-2.457	.233	
2	10	-7	3.163	3.102	1.496	-2.718	.061	
2	10	-6	3.337	3.737	1.023	3.594	-.400	
2	10	-5	5.107	5.508	2.933	4.662	-.401	
2	10	-4	5.935	6.216	2.036	-5.873	-.281	
2	10	-3	6.193	6.458	-2.590	-5.916	-.265	
2	10	-2	11.555	11.969	5.631	10.561	-.414	
2	10	-1	9.100	9.247	8.534	3.562	-.147	
2	10	0	8.129	8.214	.109	-8.213	-.085	
2	10	1	6.186	6.052	-6.013	.688	.134	
2	10	2	1.461	1.337	-.477	-1.271	.104	
2	10	3	6.728	6.557	6.267	-1.927	.171	
2	10	4	5.343	5.362	-.391	5.347	-.018	
2	10	5	.997	1.016	-.101	1.011	-.019	
2	10	6	3.610	3.596	.853	-3.493	.015	
2	10	7	1.652	1.484	-1.224	.803	.189	
2	11	-7	.848 *	.728	-.728	.014	.120	
2	11	-6	3.675	3.941	3.833	.919	-.267	
2	11	-5	4.256	4.538	-.885	-4.451	-.282	
2	11	-4	3.248	3.534	.949	-3.404	-.287	
2	11	-3	4.976	5.198	2.492	4.561	-.222	
2	11	-2	3.893	3.961	-3.856	.906	-.068	
2	11	-1	2.920	2.973	-.230	-2.963	-.052	
2	11	0	1.821	1.882	1.854	-.318	-.060	
2	11	1	2.532	2.680	.928	-2.514	-.148	
2	11	2	3.387	3.418	-1.943	-2.812	-.031	
2	11	3	3.441	3.456	-1.639	3.043	-.015	
2	11	4	2.024	2.067	1.797	-1.021	-.043	
2	11	5	8.590	8.491	.959	-8.437	.099	
2	11	6	1.728	1.856	1.585	-.966	-.128	
2	11	7	5.219	5.067	-1.481	4.846	.152	
2	12	-6	4.313	4.761	4.139	2.352	-.448	
2	12	-5	3.121	3.315	1.024	3.153	-.194	
2	12	-4	4.616	4.836	-2.274	-4.268	-.220	
2	12	-3	1.663	1.647	1.245	-1.078	.016	
2	12	-2	5.927	6.267	2.779	5.617	-.339	
2	12	-1	7.253	7.520	7.059	-2.595	-.267	
2	12	0	3.921	4.078	.920	-3.973	-.156	
2	12	1	9.247	9.514	-7.950	5.227	-.268	
2	12	2	1.585	1.152	.405	-1.078	.433	
2	12	3	5.518	5.570	4.299	-3.543	-.053	
2	12	4	4.880	4.762	1.691	4.452	.118	
2	12	5	1.280	1.132	-1.087	-.315	.148	
2	12	6	3.357	3.200	-1.159	-2.983	.157	
2	13	-5	5.375	5.728	-1.914	-5.399	-.353	
2	13	-4	4.705	5.037	-1.885	-4.671	-.332	
2	13	-3	7.122	7.554	4.766	5.861	-.432	
2	13	-2	2.725	2.994	.757	2.897	-.269	

PEARLESITE, - FINAL STRUCTURE FACTORS LISTING

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DE
2	13	-1	5.408	5.631	-3.541	-4.378	-.222	
2	13	0	2.772	2.935	2.209	-1.933	-.163	
2	13	1	1.923	1.772	-1.744	.311	.151	
2	13	2	1.278	.902	-.874	-.224	.376	
2	13	3	4.222	4.173	3.895	1.499	.049	
2	13	4	2.464	2.576	-.634	-2.497	-.112	
2	13	5	6.829	6.871	-3.533	-5.893	-.042	
2	14	-4	2.150	2.279	2.274	-.149	-.129	
2	14	-3	1.850	2.044	-.553	1.968	-.194	
2	14	-2	1.513	1.712	1.505	.817	-.199	
2	14	-1	6.042	6.255	1.915	-5.955	-.213	
2	14	0	1.779	1.648	.422	-1.593	.131	
2	14	1	8.277	8.736	-.250	8.732	-.459	
2	14	2	1.384	1.528	-1.389	.637	-.144	
2	14	3	7.473	7.637	.633	-7.611	-.164	
2	15	-1	1.851	2.006	.258	-1.989	-.155	
2	15	0	2.574	2.628	-1.220	2.328	-.054	
2	15	1	.930 *	1.204	-1.197	-.125	-.274	
3	0	-10	3.031	2.922	2.922	.032	.109	
3	0	-9	9.328	8.927	-8.925	-.174	.402	
3	0	-8	2.027	1.942	-1.942	-.031	.085	
3	0	-7	10.502	10.881	10.880	.167	-.379	
3	0	-6	2.799	2.745	2.745	-.012	.053	
3	0	-5	9.745	10.201	-10.200	-.127	-.456	
3	0	-4	23.118	24.775	-24.775	-.059	-1.658	
3	0	-3	2.368	1.682	-1.681	-.054	.686	
3	0	-2	7.956	7.143	7.143	.026	.813	
3	0	-1	28.902	26.380	-26.380	.110	2.522	
3	0	0	15.257	15.062	-15.062	-.131	.195	
3	0	1	21.049	22.017	-22.016	-.228	-.968	
3	0	2	23.618	24.223	24.223	.161	-.605	
3	0	3	24.378	26.823	26.823	.195	-2.445	
3	0	4	15.220	15.886	-15.886	-.134	-.666	
3	0	5	2.893	2.859	-2.858	-.071	.035	
3	0	6	.846	.878	.877	.038	-.032	
3	0	7	2.333	2.475	-2.475	-.017	-.142	
3	0	8	2.359	2.231	2.230	.066	.128	
3	0	9	.691 *	.234	.230	.046	.457	
3	0	10	1.302	1.424	-1.420	-.106	-.122	
3	1	-8	1.363	1.266	.926	-.863	.097	
3	1	-7	6.130	6.227	5.152	3.498	-.098	
3	1	-6	8.096	8.457	-5.966	5.994	-.361	
3	1	-5	11.201	11.922	-4.661	-10.973	-.721	
3	1	-4	13.678	14.260	8.065	11.761	-.582	
3	1	-3	34.488	37.999	3.333	37.852	-3.510	
3	1	-2	13.868	13.149	-1.220	-13.092	.720	
3	1	-1	2.160	2.044	-1.620	1.246	.116	
3	1	0	21.521	20.335	-12.458	16.072	1.185	
3	1	1	18.257	15.955	-7.932	-13.843	2.303	
3	1	2	28.907	29.015	16.881	23.599	-.108	
3	1	3	23.213	24.313	6.557	23.412	-1.100	
3	1	4	17.219	18.076	-17.283	-5.296	-.857	
3	1	5	2.801	2.941	.754	-2.843	-.140	

SEARLESITE, - FINAL STRUCTURE FACTORS LISTING

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F
3	1	6	18.142	18.609	10.612	15.287	-.468
3	1	7	8.947	9.055	-1.723	8.890	-.108
3	1	8	9.159	9.186	-3.490	-8.497	-.027
3	2	-8	1.165	1.084	1.083	0.049	.081
3	2	-7	10.709	11.311	9.061	-6.771	-.603
3	2	-6	7.964	8.290	-7.260	-4.003	-.326
3	2	-5	10.270	10.859	-9.247	5.694	-.589
3	2	-4	8.364	8.528	4.147	7.451	-.163
3	2	-3	13.937	14.796	-14.634	2.185	-.659
3	2	-2	29.302	29.845	-28.199	-9.774	-.542
3	2	-1	2.940	3.164	3.128	-.475	-.224
3	2	0	21.503	19.316	11.201	15.736	2.188
3	2	1	30.588	30.191	-30.064	2.769	.397
3	2	2	11.665	11.742	3.364	-11.249	.123
3	2	3	28.277	29.807	27.922	-10.432	-1.530
3	2	4	8.756	8.846	-8.768	1.167	-.089
3	2	5	7.331	7.332	-5.726	4.579	-.001
3	2	6	5.249	5.420	4.896	2.324	-.171
3	2	7	5.095	5.160	-5.066	.980	-.065
3	3	-8	4.443	4.628	2.158	-4.095	-.186
3	3	-7	6.905	7.036	-1.766	6.810	-.130
3	3	-6	5.331	5.629	1.667	5.376	-.298
3	3	-5	11.923	12.256	-6.795	-10.200	-.333
3	3	-4	12.174	12.472	-2.019	12.308	-.299
3	3	-3	34.560	37.084	22.414	29.543	-2.523
3	3	-2	18.068	18.267	2.213	-18.132	-.199
3	3	-1	29.219	28.338	-28.022	-4.220	.881
3	3	0	40.663	39.171	-11.944	37.305	1.492
3	3	1	15.327	14.764	14.016	-4.639	.563
3	3	2	7.054	6.729	6.539	-1.585	.326
3	3	3	19.847	20.185	-6.325	19.169	-.338
3	3	4	5.066	4.844	-.642	4.801	.222
3	3	5	3.158	3.085	-2.172	2.191	.073
3	3	6	7.792	7.831	2.988	7.239	-.039
3	3	7	8.061	7.931	7.694	1.924	.130
3	4	-7	6.109	6.385	-.211	-6.382	-.276
3	4	-6	8.131	8.453	-7.879	-3.061	-.322
3	4	-5	1.348	1.154	.570	1.003	.195
3	4	-4	10.496	11.063	2.784	10.708	-.568
3	4	-3	8.704	9.149	-8.388	3.655	-.445
3	4	-2	22.099	22.475	-21.827	-5.356	-.376
3	4	-1	9.683	9.192	-7.663	-5.076	.490
3	4	0	16.458	15.294	13.720	6.758	1.164
3	4	1	22.576	21.840	-10.667	19.058	.736
3	4	2	15.009	14.651	.157	-14.650	.358
3	4	3	21.221	21.443	6.021	-20.581	-.223
3	4	4	10.026	9.822	-8.717	4.526	.204
3	4	5	9.777	9.761	6.391	7.377	.016
3	4	6	5.558	5.696	4.967	2.788	-.138
3	4	7	6.543	6.497	-5.788	-2.952	.046
3	5	-7	4.639	4.627	3.229	-3.315	.012
3	5	-6	11.878	12.755	-2.571	12.494	-.878
3	5	-5	5.755	5.856	-5.218	2.659	-.101

EARLESITE, - FINAL STRUCTURE FACTORS LISTING

H	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DE
3	5	-4	7.762	7.885	7.882	-.194	-.123	
3	5	-3	9.902	10.318	9.388	4.281	-.416	
3	5	-2	14.210	14.461	-10.143	-10.308	-.251	
3	5	-1	26.216	26.118	-6.481	25.301	.098	
3	5	0	24.894	24.472	1.248	24.440	.422	
3	5	1	21.314	20.999	-8.140	-19.357	.315	
3	5	2	4.047	3.731	2.087	-3.093	.316	
3	5	3	19.867	19.587	6.051	18.629	.280	
3	5	4	12.238	12.269	-3.868	11.643	-.031	
3	5	5	2.853	2.731	-.046	-2.731	.121	
3	5	6	5.691	5.563	5.499	.843	.128	
3	5	7	3.448	3.209	1.078	3.022	.239	
3	6	-7	2.562	2.876	.966	-2.709	-.314	
3	6	-6	8.380	8.769	-8.238	3.004	-.389	
3	6	-5	3.485	3.571	-3.371	-1.178	-.086	
3	6	-4	10.154	10.509	8.814	-5.723	-.355	
3	6	-3	10.597	10.780	-2.549	10.474	-.183	
3	6	-2	20.983	21.001	-19.858	6.833	-.018	
3	6	-1	7.911	7.852	-5.601	-5.503	.059	
3	6	0	11.063	10.620	10.158	3.096	.443	
3	6	1	2.810	2.695	-2.542	.896	.115	
3	6	2	7.448	7.372	.373	-7.362	.076	
3	6	3	4.903	4.701	-2.724	-3.832	.202	
3	6	4	11.305	11.112	-10.640	3.206	.193	
3	6	5	9.785	9.720	9.301	-2.824	.064	
3	6	6	9.907	9.688	9.458	-2.097	.219	
3	7	-6	9.862	10.429	8.152	6.506	-.567	
3	7	-5	1.907	2.045	.853	-1.858	-.138	
3	7	-4	5.746	5.952	-5.750	1.537	-.206	
3	7	-3	5.399	5.501	4.344	3.375	-.101	
3	7	-2	5.760	5.594	-.383	-5.581	.166	
3	7	-1	11.703	11.853	-6.004	10.220	-.150	
3	7	0	23.078	22.342	3.537	22.060	.737	
3	7	1	8.923	8.850	-2.154	-8.584	.073	
3	7	2	11.416	11.090	-8.736	-6.832	.325	
3	7	3	15.806	15.485	2.227	15.324	.321	
3	7	4	8.329	8.267	7.450	3.582	.062	
3	7	5	1.441	1.263	1.026	-.737	.177	
3	7	6	3.024	3.072	-1.745	2.528	-.048	
3	8	-6	7.608	8.063	-7.052	3.908	-.455	
3	8	-5	2.692	2.985	-1.576	-2.535	-.293	
3	8	-4	8.603	8.964	7.508	-4.898	-.361	
3	8	-3	4.029	4.233	-3.839	1.785	-.204	
3	8	-2	16.895	17.429	-12.507	12.138	-.534	
3	8	-1	4.224	4.169	1.497	3.891	.055	
3	8	0	11.966	11.835	7.168	-9.417	.131	
3	8	1	4.741	4.684	-4.393	-1.623	.058	
3	8	2	5.859	5.818	-5.014	-2.950	.041	
3	8	3	2.497	2.418	.162	2.413	.079	
3	8	4	5.161	5.126	-2.099	4.676	.035	
3	8	5	8.925	8.989	3.123	-8.429	-.004	
3	9	-5	5.643	5.951	2.783	-5.260	-.307	
3	9	-4	2.932	3.055	-1.321	2.754	-.122	

SEARLESITE, - FINAL STRUCTURE FACTORS LISTING

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F
3	9	-3	9.373	9.764	-3.207	9.222	-.391
3	9	-2	9.560	10.064	-7.370	-6.854	-.505
3	9	-1	8.743	8.937	8.750	1.816	-.194
3	9	0	14.094	14.193	7.196	12.234	-.100
3	9	1	12.200	12.424	-12.390	.915	-.224
3	9	2	6.996	7.087	-7.085	.147	-.091
3	9	3	6.838	6.865	5.697	3.830	-.026
3	9	4	7.098	7.189	5.958	1.806	-.091
3	9	5	1.977	1.975	-.857	-1.780	.002
3	10	-4	7.301	7.850	-2.277	-7.513	-.549
3	10	-3	7.172	7.642	.856	7.594	-.471
3	10	-2	6.855	7.278	-.323	7.271	-.423
3	10	-1	5.558	5.861	3.212	-4.903	-.303
3	10	0	.688 *	.787	-.514	-.596	-.099
3	10	1	11.591	11.966	-11.922	1.027	-.375
3	10	2	5.759	5.842	2.991	-5.018	-.083
3	10	3	7.014	7.158	7.031	1.339	-.144
3	10	4	7.536	7.676	-5.683	5.160	-.140
3	11	-3	6.560	7.091	3.690	6.056	-.532
3	11	-2	2.831	2.915	-2.325	-1.766	-.089
3	11	-1	5.135	5.364	-5.354	.324	-.229
3	11	0	8.276	8.645	7.386	4.492	-.369
3	11	1	.413 *	.502	.308	-.397	-.089
3	11	2	9.396	9.953	-8.772	4.702	-.557
4	0	-8	9.435	9.356	9.355	.127	.079
4	0	-7	14.228	14.706	14.705	.182	-.478
4	0	-6	5.904	6.307	-6.306	-.108	-.403
4	0	-5	5.158	5.270	-5.269	-.070	-.112
4	0	-4	11.197	12.199	12.199	.084	-1.002
4	0	-3	6.950	7.234	7.234	.019	-.284
4	0	-2	1.883	1.559	-1.557	.066	.324
4	0	-1	7.232	6.139	-6.138	.054	1.093
4	0	0	23.014	23.195	-23.194	-.198	-.181
4	0	1	6.676	6.799	-6.799	-.084	-.123
4	0	2	28.901	32.450	32.449	.262	-3.549
4	0	3	4.867	5.389	5.388	.047	-.521
4	0	4	17.937	19.967	-19.966	-.224	-2.030
4	0	5	1.812	2.094	2.094	-.003	-.282
4	0	6	4.147	4.613	4.612	.068	-.465
4	0	7	6.333	6.746	-6.746	-.033	-.413
4	1	-8	1.533	1.446	-.510	-1.353	.088
4	1	-7	2.597	2.658	-2.259	-1.400	-.061
4	1	-6	5.446	5.777	2.417	-5.247	-.331
4	1	-5	10.140	10.796	-3.599	-10.179	-.656
4	1	-4	9.070	9.482	-2.724	9.082	-.412
4	1	-3	24.252	25.783	22.983	11.686	-1.531
4	1	-2	27.573	28.598	-5.068	-28.146	-1.026
4	1	-1	40.093	39.660	-32.897	-22.152	.433
4	1	0	19.414	18.455	13.332	-12.761	.959
4	1	1	30.006	30.133	21.069	-21.543	-.128
4	1	2	8.359	8.671	-8.619	-.945	-.312
4	1	3	17.654	18.239	-14.084	-11.589	-.585
4	1	4	17.290	18.691	4.804	-18.063	-1.401

PEARLESITE, - FINAL STRUCTURE FACTORS LISTING

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DE
						4.818	-.334	
						11.477	-.962	
4	1	5	6.619	6.953	5.013			
4	1	6	10.572	11.534	-1.141		-.246	
4	1	7	3.204	3.451	3.045		-.150	
4	2	-8	6.698	6.848	6.110		-.668	
4	2	-7	12.024	12.692	10.152		-.480	
4	2	-6	7.918	8.398	-7.935		-.452	
4	2	-5	9.906	10.358	8.360		-.710	
4	2	-4	9.383	10.093	10.078		-.308	
4	2	-3	14.088	14.396	-11.511		-.565	
4	2	-2	1.770	2.334	1.982		.489	
4	2	-1	16.392	15.903	11.258		-.993	
4	2	0	10.017	11.010	-10.287		.097	
4	2	1	27.227	27.130	-26.967		-1.309	
4	2	2	23.747	25.057	23.871		-.960	
4	2	3	18.671	19.631	16.625		-1.466	
4	2	4	21.626	23.092	-22.537		-.284	
4	2	5	6.233	6.517	3.802		-.208	
4	2	6	4.023	4.231	4.229		-.349	
4	2	7	8.117	8.466	-7.874		.056	
4	3	-7	1.439	1.383	.073		-.559	
4	3	-6	9.117	9.677	-9.498		-.358	
4	3	-5	6.446	6.804	-.826		-1.864	
4	3	-4	18.055	19.918	19.676		-.512	
4	3	-3	5.951	6.463	4.020		-1.770	
4	3	-2	31.085	32.856	-13.186		.277	
4	3	-1	6.256	5.989	-.832		.416	
4	3	0	6.557	6.141	-2.415		-.448	
4	3	1	31.450	31.898	-2.002		-.482	
4	3	2	14.734	15.216	7.974		-.297	
4	3	3	3.888	4.185	-4.164		-.568	
4	3	4	13.448	14.016	-13.511		-.294	
4	3	5	6.576	6.870	6.639		-.652	
4	3	6	12.941	13.593	13.591		-.063	
4	3	7	3.658	3.721	-3.110		-.446	
4	4	-7	4.645	5.091	3.282		-.396	
4	4	-6	4.585	4.981	-4.413		-.578	
4	4	-5	10.003	10.581	10.279		-.684	
4	4	4	12.739	13.423	12.672		-.736	
4	4	3	14.271	15.006	-14.640		-.605	
4	4	2	14.470	15.075	-8.527		-.115	
4	4	1	19.382	19.497	18.426		.047	
4	4	0	26.870	26.823	.344		-.217	
4	4	1	15.909	16.126	-15.833		-.635	
4	4	2	24.121	24.756	8.519		.073	
4	4	3	2.914	2.841	1.456		-.507	
4	4	4	12.615	13.122	-9.576		-.515	
4	4	5	8.252	8.767	8.509		.038	
4	4	6	4.109	4.071	2.242		-.241	
4	4	7	10.629	10.869	-10.865		.790	
4	5	-3	17.272	16.483	14.476		.627	
4	5	-2	10.149	9.521	-8.845		1.050	
4	5	-1	14.344	13.294	-10.411		.904	
4	5	0	16.428	15.524	9.298			

SEARLESITE, - FINAL STRUCTURE FACTORS LISTING

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DE
4	5	1	32.078	29.747	-2.615	-29.632	2.351	
4	5	2	8.704	8.312	-7.969	-2.362	.392	
4	5	3	11.504	10.859	1.492	10.756	.645	
4	5	4	7.358	7.009	2.023	-6.711	.349	
4	5	5	6.362	6.149	-.689	-6.110	.213	
4	5	6	3.847	3.744	3.619	.959	.102	
4	5	7	5.803	5.565	5.178	-2.039	.238	
4	6	-7	4.975	4.784	1.712	-4.467	.191	
4	6	-6	6.389	6.059	-5.677	2.118	.331	
4	6	-5	10.110	9.749	8.678	-4.443	.360	
4	6	-4	12.994	12.704	12.252	-3.358	.290	
4	6	-3	11.998	11.449	-10.634	4.243	.549	
4	6	-2	11.492	10.898	-10.168	3.922	.594	
4	6	-1	12.793	11.974	11.904	1.294	.816	
4	6	0	10.342	9.461	8.395	-4.363	.881	
4	6	1	9.545	8.807	-5.721	6.696	.738	
4	6	2	1.616	1.506	-1.263	-.821	.109	
4	6	3	11.181	10.877	-6.942	-8.374	.304	
4	6	4	5.149	5.049	-4.305	2.638	.100	
4	6	5	13.365	13.147	13.027	-1.772	.217	
4	6	6	.873	.505	-.447	.237	.368	
4	7	-6	5.661	5.572	2.623	4.916	.089	
4	7	-5	6.295	5.989	-2.566	-5.411	.306	
4	7	-4	9.310	9.192	2.346	-8.888	.117	
4	7	-3	5.191	5.030	5.011	.442	.161	
4	7	-2	9.407	9.120	-4.402	-7.988	.286	
4	7	-1	5.897	5.508	5.157	1.934	.389	
4	7	0	3.412	3.211	2.771	1.622	.201	
4	7	1	24.432	23.594	-14.357	-18.724	.837	
4	7	2	4.218	4.167	-.820	-4.086	.051	
4	7	3	7.772	7.651	6.188	4.500	.121	
4	7	4	1.035	.649	-.636	-.131	.386	
4	7	5	4.458	4.315	1.411	-4.078	.143	
4	7	6	5.757	5.684	2.346	-5.177	.073	
4	8	-5	10.393	10.113	6.298	-7.913	.280	
4	8	-4	9.927	9.679	8.807	-4.014	.249	
4	8	-3	13.201	12.842	-9.455	8.690	.359	
4	8	-2	7.893	7.702	-4.921	5.924	.191	
4	8	-1	14.949	14.671	13.753	-5.110	.277	
4	8	0	5.745	5.609	5.341	-1.714	.135	
4	8	1	12.801	12.520	-12.430	-1.504	.280	
4	8	2	1.879	1.871	.073	1.746	.008	
4	8	3	7.104	7.003	3.173	6.243	.101	
4	8	4	8.430	8.354	-6.779	-4.883	.075	
4	8	5	8.932	9.014	3.173	-8.436	-.081	
4	9	-5	4.632	4.387	-2.895	-3.296	.245	
4	9	-4	4.737	4.535	-3.321	3.087	.202	
4	9	-3	5.135	5.153	2.195	-4.662	-.018	
4	9	-2	9.834	9.655	1.221	-9.577	.180	
4	9	-1	5.530	5.417	5.103	1.817	.113	
4	9	0	3.402	3.265	2.414	2.198	.137	
4	9	1	14.441	14.141	-12.510	-6.593	.300	
4	9	2	6.917	6.834	-6.239	-2.789	.083	

SEARLESITE, - FINAL STRUCTURE FACTORS LISTING

H	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DE
4	9	3	12.555	12.361	12.148	2.288	.193	
4	9	4	5.268	5.351	3.365	-4.160	-.082	
4	10	-4	4.049	4.010	2.155	-3.382	.039	
4	10	-3	5.743	5.599	.465	5.579	.144	
4	10	-2	5.794	5.651	4.167	3.816	.143	
4	10	-1	6.609	6.336	5.534	-3.087	.272	
4	10	0	10.337	10.071	-9.128	-4.255	.266	
4	10	1	3.879	3.749	-2.070	3.126	.130	
4	10	2	10.506	10.108	10.026	1.284	.399	
4	10	3	3.329	3.247	-3.150	-.791	.082	
4	11	-2	8.793	8.532	-6.697	-5.287	.261	
4	11	-1	6.123	6.047	3.910	-4.613	.076	
4	11	0	6.850	6.767	6.766	.139	.082	
4	11	1	10.370	10.281	-10.211	1.195	.090	
4	11	2	3.485	3.371	-1.762	2.874	.114	
5	0	-8	10.854	10.128	10.126	.174	.727	
5	0	-7	3.581	3.614	3.613	.034	-.033	
5	0	-6	19.784	19.284	-19.283	-.213	.500	
5	0	-5	8.063	8.135	8.135	.014	-.072	
5	0	-4	14.469	14.308	14.307	.118	.161	
5	0	-3	8.923	8.903	-8.903	-.021	.020	
5	0	-2	8.483	8.387	8.387	.044	.076	
5	0	-1	15.703	14.770	-14.770	-.034	.933	
5	0	0	22.094	20.410	-20.409	-.174	1.684	
5	0	1	17.420	16.543	16.543	.103	.877	
5	0	2	27.120	25.974	25.972	.257	1.146	
5	0	3	3.777	3.256	-3.255	-.097	.521	
5	0	4	12.275	12.255	-12.254	-.166	.020	
5	0	5	17.336	17.384	17.383	.143	-.048	
5	0	6	6.811	6.760	6.760	.096	.051	
5	0	7	6.482	6.385	-6.384	-.035	.098	
5	1	-7	2.844	2.771	-2.691	-.665	.072	
5	1	-6	7.131	6.957	-6.865	-1.128	.174	
5	1	-5	3.531	3.449	2.973	1.750	.082	
5	1	-4	24.933	25.198	15.005	20.244	-.266	
5	1	-3	23.958	24.268	-8.139	22.863	-.311	
5	1	-2	19.990	19.233	-13.220	-13.970	.757	
5	1	-1	14.298	12.949	10.992	6.845	1.348	
5	1	0	37.152	35.489	3.104	35.353	1.663	
5	1	1	3.177	2.608	1.688	-1.988	.569	
5	1	2	4.766	4.794	-3.332	-3.447	-.029	
5	1	3	9.588	9.419	-9.385	-.809	.169	
5	1	4	2.968	3.142	.883	-3.016	-.174	
5	1	5	13.576	13.584	7.146	11.552	-.008	
5	1	6	8.646	8.647	2.209	8.360	-.002	
5	1	7	6.289	6.263	-5.823	-2.305	.026	
5	2	-7	1.189	.897	-.879	.176	.292	
5	2	-6	9.130	9.092	-7.345	5.358	.038	
5	2	-5	9.009	9.008	8.984	.649	.001	
5	2	-4	5.201	5.012	.078	-5.012	.189	
5	2	-3	8.245	7.908	-6.042	-5.101	.338	
5	2	-2	11.692	11.151	10.755	2.947	.541	
5	2	-1	9.943	9.365	-3.777	8.569	.579	

SEARLESITE, - FINAL STRUCTURE FACTORS LISTING

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DE
5	2	0	23.242	21.934	-20.470	7.877	1.309	
5	2	1	6.322	6.212	6.064	-1.349	.110	
5	2	2	28.154	27.371	25.013	-11.113	.784	
5	2	3	2.910	2.686	-2.644	-.470	.224	
5	2	4	8.025	7.755	-4.603	6.242	.269	
5	2	5	12.468	12.342	12.313	.842	.127	
5	2	6	5.189	5.010	2.678	-4.235	.179	
5	2	7	3.975	3.774	-1.593	-3.422	.201	
5	3	-7	4.911	4.691	-4.661	.532	.219	
5	3	-6	3.517	3.321	-2.089	2.581	.196	
5	3	-5	2.392	2.422	2.362	.536	-.030	
5	3	-4	14.874	14.558	7.198	12.654	.316	
5	3	-3	14.408	14.125	8.834	11.021	.283	
5	3	-2	14.611	14.243	-13.860	-3.281	.368	
5	3	-1	25.072	23.738	-9.668	21.680	1.334	
5	3	0	27.323	25.902	20.473	15.867	1.421	
5	3	1	15.183	14.198	2.212	-14.024	.985	
5	3	2	14.488	14.130	-13.301	4.769	.358	
5	3	3	15.084	14.376	-8.254	11.771	.707	
5	3	4	2.672	2.667	.200	-2.659	.005	
5	3	5	8.173	7.970	7.957	-.465	.203	
5	3	6	7.553	7.350	3.301	6.567	.203	
5	3	7	2.136	1.899	-1.143	1.517	.237	
5	4	-7	6.168	5.922	-.430	-5.906	.246	
5	4	-6	8.821	8.497	-5.647	6.350	.323	
5	4	-5	14.481	14.061	13.284	4.610	.420	
5	4	-4	7.372	7.212	-1.145	-7.121	.160	
5	4	-3	21.900	21.708	-20.310	-7.646	.193	
5	4	-2	13.847	13.638	13.628	.511	.209	
5	4	-1	23.408	21.984	10.588	19.266	1.424	
5	4	0	17.845	17.053	-14.061	9.648	.792	
5	4	1	10.550	10.342	.547	-10.328	.207	
5	4	2	17.020	16.284	12.510	-10.425	.736	
5	4	3	2.203	2.130	-1.787	1.158	.073	
5	4	4	10.407	10.426	-.001	10.426	-.019	
5	4	5	16.770	16.400	15.618	-5.004	.370	
5	4	6	8.690	8.529	-2.162	-8.250	.160	
5	4	7	9.551	9.325	-8.858	2.913	.226	
5	5	-7	9.682	9.212	-3.322	8.593	.470	
5	5	-6	7.816	7.710	-5.370	5.533	.106	
5	5	-5	8.167	7.879	3.451	-7.083	.288	
5	5	-4	10.028	9.697	9.552	-1.668	.331	
5	5	-3	19.696	19.283	-3.391	18.982	.414	
5	5	-2	9.398	9.150	-5.364	7.413	.248	
5	5	-1	13.220	12.386	11.187	5.317	.834	
5	5	0	8.357	7.578	-1.881	7.341	.779	
5	5	1	17.021	16.115	-10.420	-12.293	.906	
5	5	2	12.854	12.140	5.015	11.055	.714	
5	5	3	16.822	16.567	-3.213	16.252	.255	
5	5	4	10.947	10.869	-8.676	-6.546	.079	
5	5	5	7.465	7.251	6.344	-3.512	.214	
5	5	6	7.594	7.419	7.037	2.349	.176	
5	6	-6	4.222	4.066	-4.059	-.238	.156	

EARLESITE, - FINAL STRUCTURE FACTORS LISTING

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DE
5	6	-5	12.402	11.979	10.586	-5.607	.423	
5	6	-4	1.910	1.627	.496	1.550	.283	
5	6	-3	18.425	17.657	-17.159	4.164	.769	
5	6	-2	2.034	1.997	1.970	.328	.037	
5	6	-1	15.996	15.619	14.955	-1.385	.976	
5	6	0	8.478	7.895	3.222	7.207	.583	
5	6	1	7.982	7.393	-5.841	4.532	.589	
5	6	2	7.071	6.846	-2.360	-6.426	.225	
5	6	3	1.893	1.726	1.726	.008	.167	
5	6	4	8.356	8.213	8.058	-1.591	.143	
5	6	5	9.110	9.012	8.006	-4.138	.098	
5	6	6	6.733	6.592	-6.512	1.022	.142	
5	7	-6	4.332	4.142	.372	4.125	.190	
5	7	-5	9.125	8.794	-6.761	-5.623	.330	
5	7	-4	4.358	4.196	2.963	2.972	.162	
5	7	-3	10.790	10.420	7.891	6.804	.370	
5	7	-2	3.946	3.744	-3.226	1.900	.202	
5	7	-1	11.249	10.550	2.433	10.266	.698	
5	7	0	3.756	3.599	3.088	1.849	.157	
5	7	1	12.183	11.609	-9.942	-5.994	.574	
5	7	2	7.445	7.170	-3.517	6.248	.275	
5	7	3	12.740	12.396	5.517	11.101	.344	
5	7	4	.381 *	.384	-.328	-.199	-.003	
5	7	5	6.351	6.278	-2.934	-5.550	.073	
5	8	-5	10.417	10.095	8.354	-5.668	.322	
5	8	-4	4.933	4.835	-3.869	-2.900	.098	
5	8	-3	17.529	17.233	-12.287	12.084	.296	
5	8	-2	9.049	8.690	8.349	2.410	.359	
5	8	-1	15.283	14.652	12.100	-8.262	.632	
5	8	0	8.927	8.530	-8.234	-2.226	.397	
5	8	1	10.881	10.463	-1.978	10.274	.419	
5	8	2	10.845	10.345	9.162	4.803	.501	
5	8	3	9.074	8.983	-3.598	-8.231	.091	
5	8	4	3.482	3.382	-.815	-3.283	.100	
5	8	5	7.546	7.391	7.002	-2.367	.154	
5	9	-4	2.232	2.047	-1.263	1.611	.185	
5	9	-3	3.381	3.284	2.067	2.552	.097	
5	9	-2	5.262	5.093	3.983	-3.173	.169	
5	9	-1	8.906	8.600	7.040	4.939	.306	
5	9	0	11.356	11.050	-6.046	9.250	.306	
5	9	1	15.905	15.530	-14.633	-5.204	.375	
5	9	2	10.011	9.796	9.371	2.857	.215	
5	9	3	11.474	11.231	7.733	8.144	.243	
5	9	4	9.623	9.464	-9.038	-2.807	.159	
5	10	-3	6.268	6.224	-.579	6.197	.044	
5	10	-2	3.675	3.573	3.475	-.835	.102	
5	10	-1	4.739	4.711	-2.221	-4.154	.028	
5	10	0	3.589	3.455	-2.653	2.212	.134	
5	10	1	7.244	7.266	6.679	2.862	-.022	
5	10	2	4.947	4.723	4.655	-.799	.224	
5	10	3	4.045	4.074	-3.722	1.657	-.030	
5	11	-1	6.327	6.110	6.075	-.652	.217	
5	11	0	6.065	6.051	-.696	6.011	.014	

SEARLESITE, - FINAL STRUCTURE FACTORS LISTING

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DE
5	11	1	9.328	9.289	-7.407	5.606	.039	
6	0	-7	5.529	5.133	-5.132	-.086	.396	
6	0	-6	9.665	9.381	-9.380	-.165	.284	
6	0	-5	12.943	12.706	12.706	.118	.237	
6	0	-4	6.027	6.101	6.101	.100	-.075	
6	0	-3	1.247	1.107	1.106	-.054	.140	
6	0	-2	9.064	8.515	-8.515	-.026	.549	
6	0	-1	27.842	26.411	-26.411	-.111	1.431	
6	0	0	.910	.343	-.331	-.088	.567	
6	0	1	3.103	2.680	2.676	.141	.423	
6	0	2	9.914	9.802	-9.802	.045	.112	
6	0	3	13.605	13.312	-13.310	-.231	.293	
6	0	4	3.672	3.571	-3.570	-.079	.102	
6	0	5	8.190	8.067	8.065	.157	.124	
6	0	6	.767 *	.896	.896	.019	-.129	
6	0	7	.803 *	.298	-.289	-.070	.506	
6	1	-7	4.304	4.197	-.593	-4.155	.106	
6	1	-6	8.268	8.164	-1.310	-8.058	.104	
6	1	-5	3.658	3.643	3.223	-1.697	.015	
6	1	-4	10.093	9.835	4.075	8.951	.259	
6	1	-3	10.902	10.517	-3.557	-9.898	.384	
6	1	-2	30.145	30.195	-3.354	-28.709	-.050	
6	1	-1	19.163	18.121	4.396	17.579	1.042	
6	1	0	26.887	25.364	20.567	14.844	1.523	
6	1	1	33.910	32.833	-9.777	-31.343	1.077	
6	1	2	18.982	18.677	-16.594	-8.571	.305	
6	1	3	7.904	7.834	7.344	-2.729	.070	
6	1	4	8.826	8.704	4.766	-7.283	.122	
6	1	5	8.588	8.682	-1.043	8.619	-.094	
6	1	6	3.378	3.377	-1.695	2.921	.001	
6	1	7	6.289	6.284	.409	-6.271	.005	
6	2	-7	4.016	3.974	-2.964	2.647	.042	
6	2	-6	9.149	8.935	-7.360	5.065	.214	
6	2	-5	12.708	12.941	12.105	-4.576	-.233	
6	2	-4	9.866	9.689	2.295	-9.414	.177	
6	2	-3	10.612	10.540	-10.469	1.223	.073	
6	2	-2	11.523	11.528	11.335	2.101	-.006	
6	2	-1	18.213	17.592	-16.907	4.861	.621	
6	2	0	28.210	26.820	-25.904	6.953	1.389	
6	2	1	12.695	12.246	10.098	-6.927	.449	
6	2	2	6.534	6.262	1.440	-6.095	.272	
6	2	3	19.008	18.640	-17.654	5.980	.368	
6	2	4	9.644	9.542	-5.939	7.469	.101	
6	2	5	12.521	12.502	11.412	-5.107	.018	
6	2	6	8.377	8.405	.935	-8.353	-.029	
6	2	7	7.696	7.631	-7.342	2.080	.064	
6	3	-7	7.761	7.558	-7.316	1.895	.203	
6	3	-6	7.654	7.609	-1.103	-7.529	.045	
6	3	-5	11.251	11.119	8.872	-6.701	.132	
6	3	-4	5.424	5.384	3.765	3.848	.040	
6	3	-3	11.698	11.474	-10.529	-4.561	.224	
6	3	-2	15.001	14.709	-5.014	-13.828	.291	
6	3	-1	18.886	18.352	15.650	9.584	.534	

BARLESITE, - FINAL STRUCTURE FACTORS LISTING

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DE
6	3	0	4.893	4.648	4.630	.408	.245	
6	3	1	30.858	29.672	-4.919	-29.262	1.186	
6	3	2	8.175	7.752	-5.283	5.674	.422	
6	3	3	12.650	12.744	-10.512	7.205	-.094	
6	3	4	18.771	18.754	4.004	-18.322	.016	
6	3	5	10.387	10.287	9.990	2.454	.099	
6	3	6	7.631	7.840	-1.565	7.682	-.009	
6	3	7	6.283	6.108	-5.369	-2.914	.174	
6	4	-7	2.294	1.970	1.146	1.602	.324	
6	4	-6	6.541	6.250	.006	6.250	.291	
6	4	-5	7.574	7.479	-5.612	-4.944	.095	
6	4	-4	11.382	11.218	-7.153	-8.642	.165	
6	4	-3	8.544	8.352	-3.410	-7.623	.192	
6	4	-2	10.123	9.638	6.576	7.046	.485	
6	4	-1	17.573	17.562	-8.084	15.590	.011	
6	4	0	8.731	8.184	-7.138	-4.004	.547	
6	4	1	13.062	12.796	-7.226	-10.561	.265	
6	4	2	7.902	7.810	-7.772	.768	.092	
6	4	3	12.590	12.435	-1.075	12.389	.154	
6	4	4	3.255	3.114	3.113	-.109	.141	
6	4	5	11.378	11.309	.004	-11.309	.069	
6	4	6	6.956	6.815	-6.754	-.911	.140	
6	5	-6	6.354	6.002	-.136	-6.001	.352	
6	5	-5	13.436	13.022	-.656	-13.005	.415	
6	5	-4	3.327	3.257	1.729	2.760	.070	
6	5	-3	7.218	6.988	2.643	6.469	.230	
6	5	-2	11.558	10.925	-2.523	-10.629	.634	
6	5	-1	2.640	2.158	2.158	.003	.482	
6	5	0	12.991	12.174	7.212	-9.808	.816	
6	5	1	13.596	13.137	-3.570	-12.643	.459	
6	5	2	15.042	14.703	-5.527	13.624	.339	
6	5	3	3.411	3.217	-3.217	-.047	.194	
6	5	4	13.157	13.108	-1.410	-13.032	.049	
6	5	5	5.107	4.945	4.864	-.892	.162	
6	5	6	5.029	4.976	1.783	4.645	.053	
6	6	-6	2.448	2.248	1.078	1.972	.200	
6	6	-5	11.875	11.630	10.171	-5.639	.246	
6	6	-4	11.648	11.402	-10.363	-4.754	.246	
6	6	-3	16.517	16.317	-14.954	6.527	.301	
6	6	-2	16.367	15.594	14.350	-6.103	.773	
6	6	-1	8.448	8.057	7.376	-3.244	.390	
6	6	0	20.065	19.173	-15.144	11.758	.892	
6	6	1	9.871	9.651	-9.525	1.554	.220	
6	6	2	3.809	3.786	-.310	-3.774	.023	
6	6	3	1.003	.527	.240	-.469	.476	
6	6	4	2.905	2.769	2.015	1.900	.136	
6	6	5	3.637	3.807	-.615	-3.757	-.170	
6	6	6	9.020	8.859	-8.246	-3.236	.161	
6	7	-6	9.781	9.468	-6.172	-7.180	.313	
6	7	-5	8.255	8.077	-.125	-8.076	.178	
6	7	-4	6.048	5.907	4.034	4.315	.141	
6	7	-3	1.243	.740	-.518	-.529	.502	
6	7	-2	8.761	8.558	1.402	-8.443	.203	

EARLESITE, - FINAL STRUCTURE FACTORS LISTING

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DE
					6.840	1.864	.307	
6	7	-1	7.397	7.090	-3.794	-2.342	.184	
6	7	0	4.643	4.459	-8.782	-16.479	.845	
6	7	1	19.518	18.673	6.232	9.028	.273	
6	7	2	11.244	10.970	2.150	11.682	.338	
6	7	3	12.216	11.878	-7.068	-14.651	-.016	
6	7	4	16.251	16.267	.354	-3.991	.042	
6	7	5	4.049	4.007	.910	-7.701	.102	
6	8	-3	7.857	7.755	-5.402	6.157	.179	
6	8	-4	8.369	8.191	-4.579	4.891	.144	
6	8	-3	6.843	6.700	6.634	-10.104	.389	
6	8	-2	12.477	12.088	-.391	-5.327	.116	
6	8	-1	5.457	5.341	-6.621	8.712	.290	
6	8	0	11.232	10.942	-.828	8.595	.101	
6	8	1	8.736	8.635	-1.376	-3.896	.011	
6	8	2	4.142	4.131	-.942	-3.015	.114	
6	8	3	3.273	3.158	-1.220	-1.930	.211	
6	8	4	2.494	2.283	.079	-1.089	-.028	
6	9	-4	1.063	1.092	8.046	-2.942	-.062	
6	9	-3	8.505	8.567	2.189	-5.559	.018	
6	9	-2	5.992	5.974	-1.169	3.154	.072	
6	9	-1	3.436	3.363	-6.753	-3.803	.178	
6	9	0	7.928	7.750	-1.347	-5.930	.141	
6	9	1	6.222	6.081	8.516	5.904	.039	
6	9	2	10.401	10.363	-.877	.032	.040	
6	9	3	.918	.878	-6.439	-4.379	.060	
6	9	4	7.846	7.787	-.881	6.324	.066	
6	10	-3	6.451	6.385	-.863	-5.125	-.013	
6	10	-2	5.184	5.197	-4.792	-5.789	.070	
6	10	-1	7.585	7.515	.836	5.984	.197	
6	10	0	6.240	6.042	5.342	3.606	.104	
6	10	1	6.549	6.446	-.806	-1.174	.065	
6	10	2	1.489	1.424	-11.234	-.174	.306	
7	0	-7	11.540	11.235	-4.009	-.066	-.097	
7	0	-6	3.913	4.010	21.841	.233	-.137	
7	0	-5	21.706	21.842	6.500	.049	-.010	
7	0	-4	6.490	6.500	-10.699	-.103	.155	
7	0	-3	10.855	10.700	14.188	.053	.015	
7	0	-2	14.204	14.189	5.623	-.003	.133	
7	0	-1	5.756	5.623	-4.794	.017	.097	
7	0	0	4.891	4.794	17.883	.196	.874	
7	0	1	18.758	17.884	1.374	-.020	-.263	
7	0	2	1.111	1.374	-15.809	-.209	.133	
7	0	3	15.943	15.810	7.313	.097	.031	
7	0	4	7.344	7.314	18.039	.226	-.199	
7	0	5	17.842	18.041	1.803	-.047	.384	
7	0	6	2.187	1.803	-5.054	-.384	.147	
7	1	-7	5.215	5.069	3.035	-3.394	-.015	
7	1	-6	4.538	4.553	7.298	10.225	.125	
7	1	-5	12.687	12.562	-6.918	6.033	.123	
7	1	-4	9.302	9.179	-8.420	-13.413	.304	
7	1	-3	16.141	15.837	5.367	5.295	.510	
7	1	-2	8.049	7.539	15.115	35.175	.830	
7	1	-1	39.116	38.285				

SEARLESITE, - FINAL STRUCTURE FACTORS LISTING

STRUCTURE

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DE
7	1	0	5.105	4.929	-3.754	3.195	.176	
7	1	1	24.619	23.960	-12.462	-20.464	.659	
7	1	2	8.826	8.354	3.701	7.489	.472	
7	1	3	1.991	1.897	1.896	-.049	.095	
7	1	4	6.873	6.938	.958	-6.872	-.065	
7	1	5	8.147	8.094	-.551	8.075	.053	
7	1	6	4.998	5.017	-3.041	-3.991	-.019	
7	2	-7	4.642	4.321	-1.032	4.196	.321	
7	2	-6	5.962	5.954	-5.736	1.593	.009	
7	2	-5	12.605	12.512	10.757	-6.390	.092	
7	2	-4	7.150	7.188	6.873	-2.103	-.038	
7	2	-3	3.209	3.183	3.182	.060	.026	
7	2	-2	6.102	5.937	5.716	1.605	.165	
7	2	-1	10.043	9.586	-4.072	8.679	.456	
7	2	0	12.943	12.640	11.976	-4.044	.303	
7	2	1	11.361	11.075	7.166	-8.445	.286	
7	2	2	6.306	6.086	-4.140	4.460	.220	
7	2	3	10.871	10.781	-.092	10.781	.089	
7	2	4	3.017	3.025	3.017	.213	-.008	
7	2	5	14.720	14.534	10.155	-10.398	.186	
7	2	6	3.621	3.471	2.531	-2.376	.150	
7	3	-7	1.055	.680	.428	.528	.375	
7	3	-6	4.733	4.713	2.444	-4.030	.020	
7	3	-5	4.569	4.484	1.118	4.342	.085	
7	3	-4	4.990	4.824	-1.633	4.539	.166	
7	3	-3	6.902	6.812	-6.750	.917	.090	
7	3	-2	4.572	4.724	1.021	4.612	-.152	
7	3	-1	21.468	20.950	13.055	16.385	.519	
7	3	0	10.527	10.009	9.187	-3.974	.518	
7	3	1	12.915	12.254	-10.316	-6.615	.661	
7	3	2	21.103	20.599	-11.707	16.949	.504	
7	3	3	9.772	9.660	4.470	-8.563	.112	
7	3	4	11.610	11.647	4.735	-10.641	-.036	
7	3	5	9.571	9.386	-.452	9.375	.185	
7	3	6	4.254	4.286	-3.990	-1.565	-.032	
7	4	-6	5.397	5.173	-1.969	4.784	.224	
7	4	-5	13.084	12.851	9.640	-8.499	.233	
7	4	-4	10.114	9.883	-2.817	-9.473	.231	
7	4	-3	7.438	7.288	-3.437	6.426	.151	
7	4	-2	23.071	22.515	21.143	7.739	.556	
7	4	-1	4.831	4.650	4.375	-1.577	.180	
7	4	0	14.523	13.889	-13.065	-4.712	.634	
7	4	1	8.907	8.638	7.507	-4.273	.269	
7	4	2	14.611	14.266	8.998	11.071	.346	
7	4	3	8.787	8.667	-1.298	8.569	.120	
7	4	4	8.779	8.718	3.546	-7.964	.061	
7	4	5	7.795	7.883	4.697	-6.331	-.088	
7	4	6	2.194	2.414	-2.406	.199	-.220	
7	5	-6	11.632	11.310	-1.877	-11.153	.322	
7	5	-5	1.954	1.864	1.548	1.038	.090	
7	5	-4	15.860	15.741	-.073	15.741	.119	
7	5	-3	2.227	2.073	-2.039	-.373	.154	
7	5	-2	1.729	1.597	.409	-1.544	.132	

EARLESITE, - FINAL STRUCTURE FACTORS LISTING

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DE
7	5	-1	11.986	11.619	9.074	7.256	.367	
7	5	0	5.682	5.532	4.097	-3.717	.150	
7	5	1	5.481	5.307	-5.301	-.252	.174	
7	5	2	15.622	15.343	-1.997	15.213	.279	
7	5	3	4.966	4.981	-3.799	-3.221	-.014	
7	5	4	16.174	15.967	-.336	-15.964	.207	
7	5	5	7.163	7.127	3.298	6.318	.036	
7	5	6	6.757	6.644	-3.149	5.850	.113	
7	6	-6	2.257	2.028	1.534	1.326	.229	
7	6	-5	4.942	4.929	.963	-4.834	.012	
7	6	-4	7.119	6.923	-5.675	3.965	.196	
7	6	-3	2.086	1.981	1.217	-1.563	.105	
7	6	-2	18.739	18.432	16.054	-9.055	.307	
7	6	-1	9.350	9.169	4.351	8.072	.181	
7	6	0	9.698	9.368	-8.059	4.775	.331	
7	6	1	2.905	2.844	-1.990	-2.032	.061	
7	6	2	9.518	9.317	9.281	.817	.201	
7	6	3	9.703	9.612	9.156	2.924	.091	
7	6	4	1.872	1.713	-1.713	.003	.159	
7	6	5	6.009	6.081	-3.507	-4.967	-.072	
7	7	-5	3.316	3.278	-1.286	3.015	.039	
7	7	-4	4.853	4.821	1.984	4.393	.032	
7	7	-3	4.062	3.932	2.847	2.712	.130	
7	7	-2	1.392	1.257	.296	1.221	.136	
7	7	-1	4.989	4.914	3.512	3.437	.079	
7	7	0	7.817	7.603	-.477	-7.588	.214	
7	7	1	3.406	3.521	-3.519	.087	-.115	
7	7	2	18.025	18.140	5.661	17.234	-.114	
7	7	3	6.052	5.946	-.703	-5.904	.106	
7	7	4	12.860	12.889	-8.273	-9.884	-.030	
7	7	5	5.952	5.735	-1.411	5.558	.217	
7	8	-4	7.429	7.287	-4.788	5.493	.142	
7	8	-3	.630	.676	-.671	.083	-.047	
7	8	-2	17.712	17.291	11.772	-12.665	.420	
7	8	-1	1.621	1.527	-.966	1.182	.094	
7	8	0	15.797	15.599	-4.808	14.840	.197	
7	8	1	6.822	6.793	6.635	-1.456	.029	
7	8	2	7.850	7.927	6.452	-4.606	-.077	
7	8	3	2.325	2.315	-1.764	1.500	.009	
7	8	4	1.284	1.163	.114	-1.158	.121	
7	9	-3	5.136	5.127	3.752	-3.494	.009	
7	9	-2	1.081	.793	-.793	.009	.288	
7	9	-1	6.474	6.351	-2.403	5.879	.123	
7	9	0	4.039	3.942	-1.406	-3.683	.096	
7	9	1	4.476	4.315	3.488	-2.540	.161	
7	9	2	8.855	8.982	5.309	7.245	-.127	
7	9	3	3.908	3.882	-3.868	.336	.026	
7	10	-2	8.936	8.878	-3.073	-8.355	.058	
7	10	-1	5.681	5.812	5.439	1.911	-.131	
7	10	0	6.735	7.021	4.354	5.508	-.286	
7	10	1	2.470	2.420	2.378	.448	.051	
8	0	-7	5.140	5.199	-5.196	-.168	-.059	
8	0	-6	3.697	3.840	-3.840	.034	-.143	

SEARLESITE, - FINAL STRUCTURE FACTORS LISTING

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DEL
8	0	-5	10.846	10.932	10.930	.170	-.085	
8	0	-4	4.419	4.336	-4.335	-.100	.083	
8	0	-3	14.482	14.127	-14.126	-.147	.355	
8	0	-2	4.946	5.081	5.081	.032	-.135	
8	0	-1	6.321	6.328	-6.328	-.027	-.007	
8	0	0	.556 *	.287	.286	.019	.270	
8	0	1	2.752	2.624	-2.624	.049	.128	
8	0	2	23.004	22.866	-22.865	-.197	.138	
8	0	3	7.085	7.041	-7.040	-.138	.044	
8	0	4	5.576	5.759	5.757	.173	-.183	
8	0	5	5.976	5.864	5.863	.086	.112	
8	0	6	3.491	3.408	-3.405	-.152	.083	
8	1	-7	3.030	3.012	1.342	-2.696	.018	
8	1	-6	4.814	4.863	4.328	-2.217	-.049	
8	1	-5	4.208	3.860	-2.775	2.684	.348	
8	1	-4	14.445	14.671	-5.689	-13.523	-.226	
8	1	-3	10.216	10.178	-2.741	-9.802	.038	
8	1	-2	16.137	16.123	9.580	12.968	.014	
8	1	-1	14.812	14.264	5.639	13.102	.548	
8	1	0	13.403	13.004	-10.272	-7.974	.399	
8	1	1	9.617	9.056	-1.403	-8.946	.561	
8	1	2	10.606	10.484	4.072	9.661	.122	
8	1	3	2.163	2.186	2.180	-.165	-.023	
8	1	4	2.804	2.754	-1.507	-2.306	.050	
8	1	5	3.625	3.806	-2.769	2.611	-.181	
8	1	6	7.902	7.937	.853	-7.891	-.035	
8	2	-7	13.540	12.966	-12.487	3.493	.573	
8	2	-6	1.951	2.030	-.748	-1.887	-.078	
8	2	-5	14.629	14.423	13.703	-4.499	.206	
8	2	-4	12.557	12.531	-12.513	-.673	.027	
8	2	-3	10.114	10.110	-9.990	1.550	.004	
8	2	-2	13.937	13.947	13.567	3.232	-.009	
8	2	-1	11.079	10.470	-10.422	-1.003	.609	
8	2	0	16.699	16.308	-14.297	-7.845	.391	
8	2	1	10.119	9.855	9.448	-2.802	.264	
8	2	2	16.705	16.725	-11.752	11.900	-.019	
8	2	3	21.596	21.705	-20.232	7.860	-.109	
8	2	4	13.241	13.564	10.016	-9.146	-.323	
8	2	5	9.845	9.959	7.575	-6.465	-.114	
8	2	6	9.395	9.569	-8.948	3.389	-.174	
8	3	-6	7.718	7.699	1.006	-7.633	.020	
8	3	-5	1.861	1.843	.213	1.831	.018	
8	3	-4	8.911	8.832	-8.804	-.697	.079	
8	3	-3	9.584	9.620	-4.360	-8.575	-.035	
8	3	-2	8.469	8.124	7.586	2.909	.344	
8	3	-1	13.783	13.275	11.357	6.872	.509	
8	3	0	6.049	5.869	-1.360	-5.709	.180	
8	3	1	13.502	13.218	-13.100	1.765	.283	
8	3	2	8.567	8.506	2.838	8.018	.062	
8	3	3	9.625	9.519	6.716	-6.746	.106	
8	3	4	4.264	4.207	-.682	-4.151	.057	
8	3	5	6.586	6.626	-2.986	5.915	-.040	
8	3	6	5.839	5.885	-5.497	-2.103	-.046	

SEARLESITE, - FINAL STRUCTURE FACTORS LISTING

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DE
8	4	-6	5.446	5.380	-5.373	.275	.066	
8	4	-5	10.236	10.250	2.125	-10.027	-.014	
8	4	-4	5.131	5.140	-5.023	-1.094	-.009	
8	4	-3	9.777	9.582	-3.080	9.074	.195	
8	4	-2	9.676	9.429	9.100	-2.466	.248	
8	4	-1	12.886	12.882	-11.245	-6.286	.003	
8	4	0	13.849	13.639	-11.896	-6.673	.209	
8	4	1	6.553	6.594	1.165	6.491	-.041	
8	4	2	12.860	12.771	-2.787	12.463	.089	
8	4	3	4.016	3.981	-2.724	-2.903	.035	
8	4	4	5.920	5.868	-3.986	-4.307	.052	
8	4	5	2.606	2.826	-2.170	-1.810	-.220	
8	5	-6	8.289	8.125	-2.426	-7.754	.164	
8	5	-5	5.420	5.292	-.682	5.248	.128	
8	5	-4	1.731	1.721	-1.691	.321	.010	
8	5	-3	5.153	5.157	-4.900	-1.606	-.003	
8	5	-2	3.940	3.950	1.569	-3.625	-.009	
8	5	-1	10.507	10.296	9.326	-4.369	.209	
8	5	0	3.004	2.950	1.257	2.669	.054	
8	5	1	8.320	8.301	-5.717	6.019	.018	
8	5	2	5.857	5.610	.037	5.610	.246	
8	5	3	10.843	10.836	1.774	-10.690	.007	
8	5	4	3.809	3.700	-.491	-3.667	.109	
8	5	5	9.552	9.657	-1.739	9.499	-.105	
8	6	-5	2.059	2.014	.844	-1.829	.045	
8	6	-4	11.886	11.668	-11.498	1.987	.218	
8	6	-3	5.527	5.468	1.509	-5.250	.058	
8	6	-2	16.688	16.774	16.065	-4.828	-.086	
8	6	-1	17.338	16.917	-16.349	4.346	.420	
8	6	0	19.283	19.289	-19.065	2.928	-.006	
8	6	1	12.833	12.732	11.905	-4.515	.101	
8	6	2	5.771	5.645	4.641	3.214	.126	
8	6	3	11.837	11.886	-9.890	6.594	-.049	
8	6	4	4.553	4.535	-1.959	-4.090	.018	
8	6	5	1.789	1.759	.326	-1.729	.030	
8	7	-5	2.615	2.776	.823	2.651	-.161	
8	7	-4	4.531	4.443	1.051	4.317	.088	
8	7	-3	6.059	5.974	-3.434	-4.888	.086	
8	7	-2	1.520	1.352	.937	-.975	.168	
8	7	-1	3.604	3.704	3.641	-.680	-.100	
8	7	0	7.797	7.709	-3.341	-6.948	.088	
8	7	1	7.576	7.674	2.084	7.386	-.098	
8	7	2	11.265	11.319	8.197	7.806	-.054	
8	7	3	10.608	10.610	-5.846	-8.854	-.001	
8	7	4	10.427	10.543	-9.377	-4.619	-.116	
8	8	-4	3.746	3.743	-3.708	.509	.004	
8	8	-3	6.718	6.602	-1.229	-6.486	.116	
8	8	-2	8.193	8.163	1.951	-7.926	.031	
8	8	-1	10.892	10.857	-5.836	9.155	.035	
8	8	0	7.352	7.357	-6.096	4.117	-.005	
8	8	1	5.602	5.701	3.403	-4.573	-.098	
8	8	2	1.108	.993	.806	.579	.115	
8	8	3	3.681	3.855	-3.852	-.147	-.173	

EARLESITE, - FINAL STRUCTURE FACTORS LISTING

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DEL
8	9	-3	.429 *	.142	.140	-.020	.287	
8	9	-2	5.843	5.836	-5.835	.054	.007	
8	9	-1	2.959	3.158	-1.208	-2.918	-.199	
8	9	0	5.053	5.016	4.931	-.919	.037	
8	9	1	2.888	2.983	2.911	.650	-.095	
8	9	2	2.485	2.560	2.171	1.356	-.075	
9	0	-6	10.322	9.981	9.979	.181	.341	
9	0	-5	11.156	10.990	10.990	.125	.166	
9	0	-4	16.850	16.859	-16.858	-.182	-.009	
9	0	-3	6.323	6.419	6.419	-.008	-.096	
9	0	-2	23.020	23.295	23.294	.178	-.275	
9	0	-1	4.014	3.854	-3.854	.009	.160	
9	0	0	8.318	8.102	8.102	.059	.216	
9	0	1	9.157	9.148	9.148	.050	.009	
9	0	2	17.358	17.233	-17.232	-.178	.125	
9	0	3	2.304	2.278	-2.278	.022	.026	
9	0	4	17.815	18.337	18.336	.247	-.522	
9	0	5	1.568	1.836	-1.835	-.045	-.268	
9	1	-6	1.934	1.914	-1.295	-1.410	.020	
9	1	-5	3.717	3.630	-3.625	-.177	.087	
9	1	-4	9.273	9.342	-3.251	-8.759	-.069	
9	1	-3	4.148	4.240	3.949	-1.544	-.092	
9	1	-2	12.978	12.775	5.960	11.299	.203	
9	1	-1	6.288	6.150	-4.640	4.037	.138	
9	1	0	11.531	11.380	-2.477	-11.107	.151	
9	1	1	3.548	3.543	.188	-3.538	.006	
9	1	2	13.111	12.968	5.046	11.946	.144	
9	1	3	1.898	2.072	1.770	-1.078	-.174	
9	1	4	9.632	9.812	-5.715	-7.977	-.180	
9	1	5	2.790	2.774	.664	-2.693	.016	
9	2	-6	3.477	3.308	3.224	-.744	.168	
9	2	-5	5.851	5.704	5.136	-2.482	.147	
9	2	-4	2.717	2.503	-2.453	.498	.215	
9	2	-3	6.928	6.777	2.513	6.293	.151	
9	2	-2	14.297	14.319	14.261	-1.288	-.022	
9	2	-1	8.432	8.307	-.062	-8.306	.125	
9	2	0	10.444	10.428	8.856	-5.506	.016	
9	2	1	9.318	9.278	6.616	6.504	.040	
9	2	2	18.905	19.273	-15.413	11.571	-.368	
9	2	3	6.186	6.158	4.931	-3.690	.027	
9	2	4	11.267	11.620	8.829	-7.555	-.352	
9	2	5	4.408	4.764	-4.618	1.171	-.356	
9	3	-6	4.121	4.129	1.958	-3.635	-.008	
9	3	-5	6.679	6.524	-3.830	5.282	.154	
9	3	-4	8.255	8.266	-7.603	-3.244	-.011	
9	3	-3	4.668	4.496	1.786	-4.126	.172	
9	3	-2	10.814	10.648	10.180	3.123	.166	
9	3	-1	3.167	3.042	2.892	.945	.125	
9	3	0	9.762	9.892	-9.880	.478	-.130	
9	3	1	1.586	1.354	-.419	-1.288	.231	
9	3	2	8.408	8.433	7.803	3.199	-.026	
9	3	3	4.027	4.024	2.171	-3.389	.003	
9	3	4	5.719	5.910	-1.275	-5.771	-.192	

SEARLESITE, - FINAL STRUCTURE FACTORS LISTING

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DE
9	3	5	6.657	6.787	-6.337	2.428	-.130	
9	4	-6	6.659	6.544	4.336	-4.901	.115	
9	4	-5	6.981	6.911	5.281	-4.457	.070	
9	4	-4	13.033	13.106	-8.715	9.789	-.073	
9	4	-3	12.546	12.455	12.249	2.256	.090	
9	4	-2	18.347	18.970	16.438	-9.469	-.623	
9	4	-1	17.142	15.948	-15.881	-5.920	.194	
9	4	0	2.203	2.158	1.788	1.209	.045	
9	4	1	20.398	20.845	19.752	6.661	-.447	
9	4	2	6.361	6.341	-5.160	3.685	.020	
9	4	3	6.983	7.078	-7.054	-.578	-.095	
9	4	4	6.783	6.875	6.094	-3.182	-.092	
9	4	5	.865 *	.860	-.513	.690	.006	
9	5	-5	8.445	8.381	2.136	8.104	.064	
9	5	-4	4.779	4.821	-4.091	2.550	-.042	
9	5	-3	9.436	9.421	-5.159	-7.883	.015	
9	5	-2	8.032	7.847	6.829	-3.865	.185	
9	5	-1	9.240	9.213	7.002	5.988	.026	
9	5	0	4.601	4.633	-4.632	-.035	-.032	
9	5	1	3.982	4.047	-3.716	1.604	-.065	
9	5	2	7.913	7.813	7.743	1.048	.100	
9	5	3	10.057	10.271	2.454	-9.973	-.214	
9	5	4	5.864	5.902	-5.835	-.882	-.038	
9	6	-5	.485 *	.397	-.395	.041	.088	
9	6	-4	2.785	2.832	1.969	-2.036	-.048	
9	6	-3	10.913	11.045	11.044	.182	-.132	
9	6	-2	5.606	5.784	4.225	-3.949	-.178	
9	6	-1	12.476	12.610	-12.532	1.397	-.134	
9	6	0	4.084	4.123	4.078	-.609	-.039	
9	6	1	14.085	14.292	13.885	-3.390	-.207	
9	6	2	6.614	6.574	-1.647	6.365	.039	
9	6	3	2.425	2.493	-1.771	1.754	-.068	
9	6	4	.547 *	.435	.413	-.136	.112	
9	7	-4	3.127	3.205	-2.333	2.197	-.077	
9	7	-3	1.635	1.455	-.503	-1.141	.181	
9	7	-2	3.524	3.642	2.039	-3.018	-.118	
9	7	-1	4.903	5.039	-2.688	-4.262	-.135	
9	7	0	5.807	5.760	2.304	5.280	.046	
9	7	1	8.799	8.940	8.508	2.746	-.141	
9	7	2	3.644	3.732	.396	-3.710	-.087	
9	7	3	10.719	11.120	-9.271	-6.141	-.401	
9	8	-3	8.176	8.178	4.735	-6.668	-.001	
9	8	-2	7.205	7.265	7.177	-1.124	-.060	
9	8	-1	12.013	12.052	-9.504	7.411	-.039	
9	8	0	2.157	2.237	1.421	-1.727	-.080	
9	8	1	13.123	13.500	12.366	-5.415	-.377	
9	8	2	4.076	4.243	-3.965	1.509	-.166	
9	9	-1	6.752	6.947	6.177	3.178	-.195	
9	9	0	5.045	5.156	1.344	-4.978	-.111	
10	0	-6	1.648	1.597	1.591	.136	.052	
10	0	-5	6.678	6.809	-6.808	-.068	-.131	
10	0	-4	8.569	8.801	-8.799	-.207	-.232	
10	0	-3	1.311	1.454	-1.453	.038	-.143	

SEARLESITE. - FINAL STRUCTURE FACTORS LISTING

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DEL
10	0	-2	6.562	6.719	6.718	.110	-.156	
10	0	-1	1.914	1.720	1.720	-.045	.194	
10	0	0	1.322	1.345	-1.345	-.015	-.022	
10	0	1	8.171	8.060	-8.060	-.070	.110	
10	0	2	10.578	10.557	-10.556	-.119	.021	
10	0	3	10.223	10.603	10.602	.135	-.380	
10	0	4	1.133	1.244	1.239	.107	-.111	
10	0	5	12.408	13.064	-13.062	-.186	-.655	
10	1	-6	4.898	4.840	.372	-4.826	.057	
10	1	-5	4.520	4.741	-4.237	2.127	-.221	
10	1	-4	6.136	6.207	-2.226	-5.795	-.071	
10	1	-3	8.536	8.620	8.619	-.133	-.084	
10	1	-2	11.135	11.374	-1.677	11.250	-.239	
10	1	-1	8.441	8.563	-7.817	-3.495	-.122	
10	1	0	8.094	8.185	1.008	-8.123	-.092	
10	1	1	11.998	12.415	6.677	10.467	-.417	
10	1	2	15.138	15.463	.350	15.459	-.325	
10	1	3	5.092	5.331	-4.382	-3.036	-.240	
10	1	4	6.657	6.694	3.265	-5.844	-.037	
10	1	5	2.919	2.992	-1.460	2.611	-.073	
10	2	-5	3.316	3.699	-3.656	-.561	-.383	
10	2	-4	15.434	15.462	-14.036	6.487	-.028	
10	2	-3	5.867	5.870	5.540	1.940	-.003	
10	2	-2	10.064	9.790	6.820	-7.024	.274	
10	2	-1	13.043	13.010	-11.659	-5.773	.033	
10	2	0	6.376	6.434	6.434	.027	-.058	
10	2	1	8.967	9.193	-.641	9.171	-.226	
10	2	2	14.118	14.396	-14.100	2.866	-.278	
10	2	3	9.094	9.356	4.641	-8.124	-.263	
10	2	4	4.135	4.384	3.710	-2.334	-.249	
10	2	5	9.729	9.983	-7.842	6.178	-.254	
10	3	-5	8.166	8.156	-3.282	7.466	.011	
10	3	-4	7.127	7.358	-.887	-7.304	-.231	
10	3	-3	4.599	4.652	.549	-4.619	-.052	
10	3	-2	9.432	9.491	5.048	8.038	-.066	
10	3	-1	4.675	4.468	-3.416	2.881	.207	
10	3	0	8.764	8.754	-7.262	-4.888	.010	
10	3	1	7.009	7.275	2.744	6.737	-.265	
10	3	2	14.892	15.051	10.554	10.731	-.159	
10	3	3	7.053	7.476	2.833	-6.918	-.423	
10	3	4	9.339	9.684	-9.684	-.004	-.345	
10	4	-5	5.544	5.621	-4.283	3.640	-.077	
10	4	-4	7.053	7.197	-.092	7.196	-.143	
10	4	-3	3.031	2.957	2.798	-.958	.074	
10	4	-2	11.918	12.192	-4.777	-11.218	-.275	
10	4	-1	8.884	9.039	-8.786	-2.123	-.155	
10	4	0	9.280	9.445	6.374	6.971	-.165	
10	4	1	4.263	4.376	4.281	-.905	-.113	
10	4	2	5.787	9.837	-9.812	.707	-.050	
10	4	3	.961	.715	-.713	-.051	.246	
10	4	4	1.427	1.163	-.630	-.977	.265	
10	5	-4	8.848	8.927	-8.547	-2.576	-.079	
10	5	-3	9.941	10.211	2.647	-9.862	-.270	

SEARLESITE, - FINAL STRUCTURE FACTORS LISTING

H	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DE
10	5	-2	7.563	7.766	5.781	5.186	-.204	
10	5	-1	7.784	7.967	-5.941	5.308	-.183	
10	5	0	4.037	4.173	-3.671	1.984	-.136	
10	5	1	6.686	6.925	6.478	2.448	-.239	
10	5	2	4.957	5.203	5.105	-1.000	-.245	
10	5	3	2.430	2.538	-1.819	-1.769	-.107	
10	5	4	3.628	3.811	-1.568	3.474	-.183	
10	6	-4	3.450	3.303	-.940	3.167	.147	
10	6	-3	5.135	5.132	3.999	-3.216	.003	
10	6	-2	5.377	5.447	-5.043	-2.059	-.069	
10	6	-1	13.369	13.690	-13.142	3.835	-.321	
10	6	0	9.885	10.297	7.271	-7.291	-.412	
10	6	1	8.086	8.281	8.217	-1.029	-.196	
10	6	2	11.460	11.719	-9.148	7.325	-.259	
10	6	3	2.895	2.955	-2.954	-.073	-.060	
10	7	-3	7.323	7.294	-4.682	-5.593	.029	
10	7	-2	2.375	2.410	-1.981	1.373	-.035	
10	7	-1	5.597	5.643	1.565	5.422	-.046	
10	7	0	3.521	3.773	3.739	.501	-.252	
10	7	1	3.048	3.039	2.714	1.368	.009	
10	7	2	1.777	1.727	-1.659	.483	.050	
10	8	-1	6.812	7.013	-6.649	2.228	-.200	
10	8	0	4.619	4.857	4.761	-.958	-.238	
10	8	1	6.866	7.163	.306	-7.161	-.302	
11	0	-5	5.229	5.359	-5.357	-.135	-.130	
11	0	-4	7.656	7.666	-7.665	-.111	-.010	
11	0	-3	8.817	8.887	8.885	.183	-.071	
11	0	-2	13.779	14.097	14.097	.110	-.319	
11	0	-1	7.184	7.137	-7.136	-.096	.047	
11	0	0	1.388	1.363	1.363	-.002	.026	
11	0	1	3.542	3.573	3.573	-.002	-.031	
11	0	2	1.797	1.831	-1.831	-.014	-.034	
11	0	3	7.323	7.604	7.602	.145	-.281	
11	0	4	4.603	4.705	-4.705	-.010	-.103	
11	1	-5	4.339	4.552	1.247	4.378	-.213	
11	1	-4	10.959	11.272	6.807	-8.985	-.313	
11	1	-3	5.101	5.077	-4.783	1.704	.024	
11	1	-2	4.522	4.710	-2.958	3.665	-.188	
11	1	-1	16.551	17.357	2.621	-17.158	-.805	
11	1	0	4.497	4.693	-1.548	-4.430	-.196	
11	1	1	13.427	13.910	1.384	13.841	-.482	
11	1	2	3.774	3.721	2.545	2.715	.053	
11	1	3	8.960	9.363	.507	-9.349	-.403	
11	1	4	3.388	3.565	-3.496	-.699	-.177	
11	2	-5	5.086	5.185	-3.788	3.540	-.099	
11	2	-4	6.035	6.045	-1.617	5.824	-.010	
11	2	-3	5.480	5.615	5.093	-2.364	-.135	
11	2	-2	9.337	9.556	4.917	-8.194	-.219	
11	2	-1	2.180	2.370	1.461	-1.865	-.190	
11	2	0	7.919	8.106	2.294	7.775	-.188	
11	2	0	7.919	8.106	2.294	7.775	-.188	

EARLESITE, - FINAL STRUCTURE FACTORS LISTING

ALL REFLECTIONS	NUMERATOR	DENOMINATOR	NUMBER	R
WEIGHTED R	68157.42	35211883.00	1694	.044
UNWEIGHTED R	528.84	15107.58	1694	.035
RANGES OF F(OBS)				
	26922.28	12804210.15	951	.046
	15363.25	14292626.43	519	.033
	5287.73	3314217.75	147	.040
	3522.96	1489207.74	47	.049
	6813.38	1189608.83	17	.076
	2293.88	1322643.76	10	.042
	7937.59	584487.76	2	.117
	16.35	214880.59	1	.009

RANGES OF (SIN(THETA)/LAMBDA)**2				
	27237.01	6026707.98	147	.067
	11243.80	5530608.79	262	.045
	6642.97	6831500.59	318	.031
	8295.43	8678219.18	360	.031
	9579.05	5961750.71	352	.040
	1884.33	1069055.24	89	.042
	1301.62	651719.84	79	.045
	1973.20	462320.66	87	.065

UNREJECTED REFLECTIONS	NUMERATOR	DENOMINATOR	NUMBER	R
WEIGHTED R	68157.42	35211883.00	1694	.044
UNWEIGHTED R	528.84	15107.58	1694	.035

RANGES OF F(OBS)				
	26922.28	12804210.15	951	.046
	15363.25	14292626.43	519	.033
	5287.73	3314217.75	147	.040
	3522.96	1489207.74	47	.049
	6813.38	1189608.83	17	.076
	2293.88	1322643.76	10	.042
	7937.59	584487.76	2	.117
	16.35	214880.59	1	.009

RANGES OF (SIN(THETA)/LAMBDA)**2				
	27237.01	6026707.98	147	.067
	11243.80	5530608.79	262	.045
	6642.97	6831500.59	318	.031
	8295.43	8678219.18	360	.031
	9579.05	5961750.71	352	.040
	1884.33	1069055.24	89	.042
	1301.62	651719.84	79	.045
	1973.20	462320.66	87	.065

SUM FCAL 15063.59
 STANDARD DEV OF UNIT WEIGHT OBS 6.34