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(54) **NOVEL PHOSPHATE-BINDING PROTEIN, PHARMACEUTICAL COMPOSITIONS CONTAINING SAME AND USE THEREOF**

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(57) **ABSTRACT**

A protein includes or is formed by: (i) SEQ ID NO: 1; (ii) any sequence that is derived from sequence SEQ ID NO: 1, for example, by the substitution, removal or addition of one or more amino acids, on the condition that the derivative sequence binds to the phosphate; (iii) any sequence that is homologous to sequence SEQ ID NO: 1, preferably having a homology of at least approximately 80% with sequence SEQ ID NO: 1, on the condition that the homologous sequence binds to the phosphate; or (iv) any fragment of one of the aforementioned sequences on the condition that the fragment binds to the phosphate, such as any fragment comprising at least approximately 20 contiguous amino acids in sequence SEQ ID NO: 1.

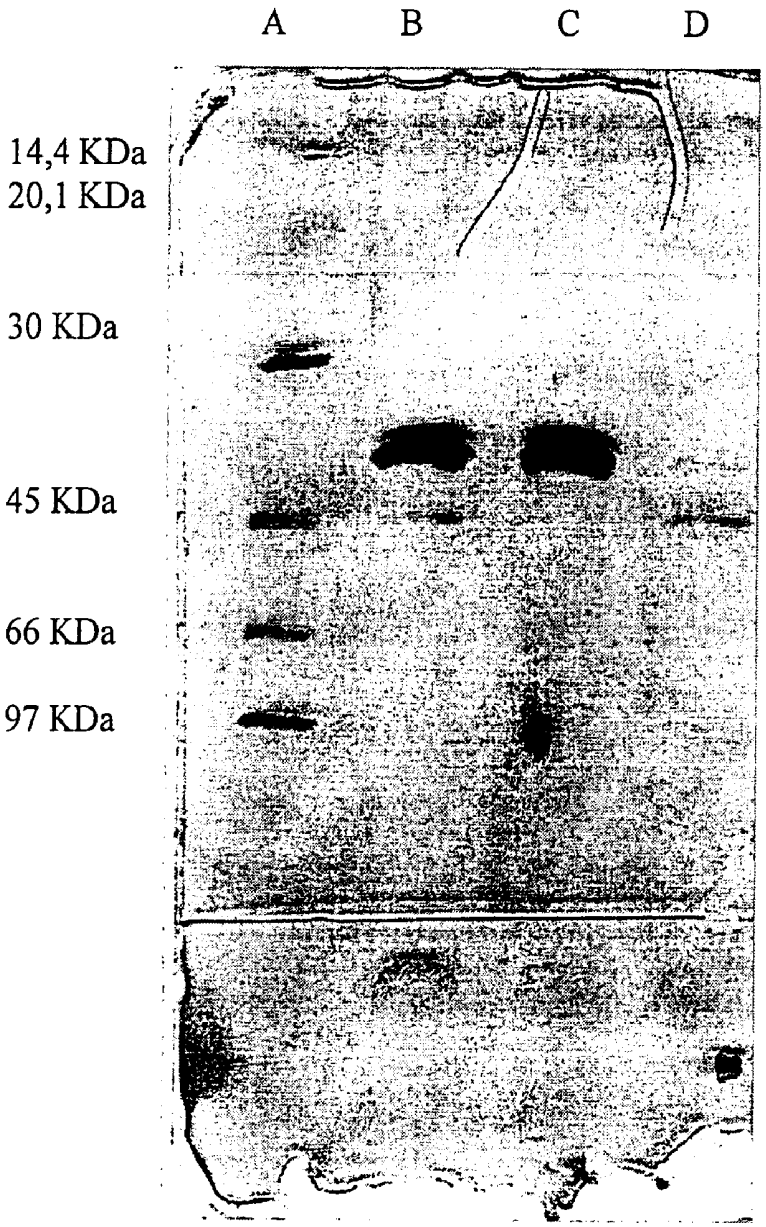

FIGURE 1

FIGURE 2

FIGURE 3

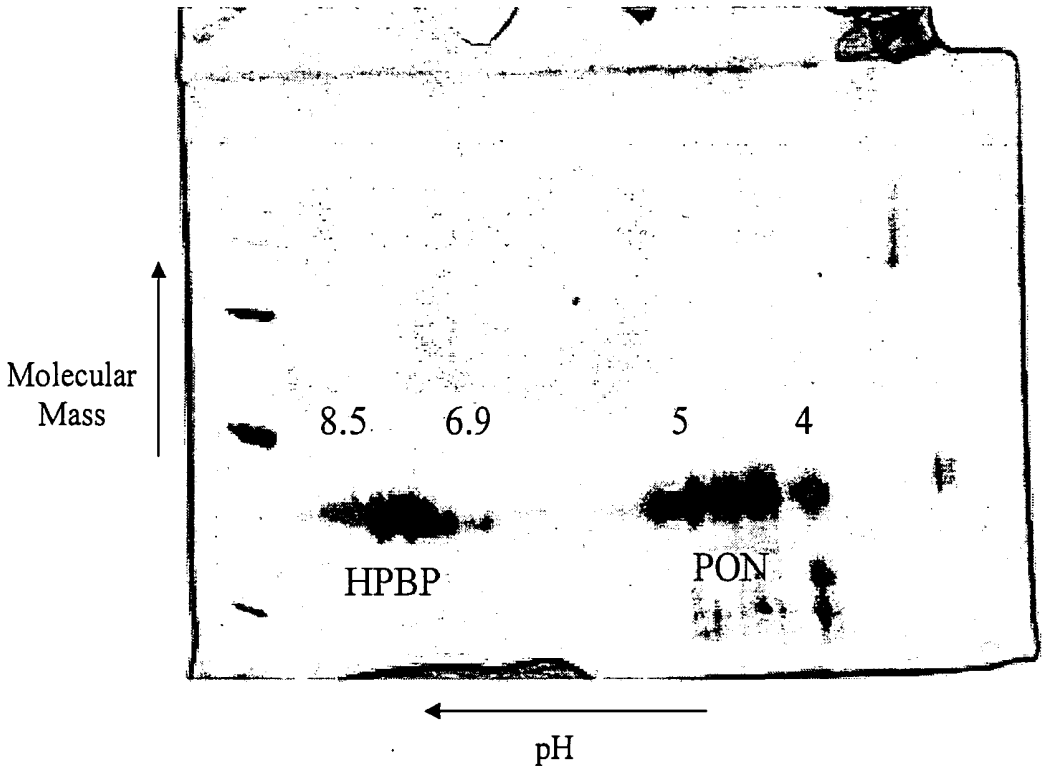

FIGURE 4

ATOM	1	CB	SER	A	1	24.666	45.653	14.370	1.00	26.15	A
ATOM	2	OG	SER	A	1	25.258	46.028	13.130	1.00	38.82	A
ATOM	3	C	SER	A	1	22.519	45.324	15.622	1.00	20.30	A
ATOM	4	O	SER	A	1	21.889	46.093	16.367	1.00	18.83	A
ATOM	5	N	SER	A	1	22.817	47.273	14.074	1.00	22.37	A
ATOM	6	CA	SER	A	1	23.146	45.831	14.317	1.00	22.87	A
ATOM	7	N	ILE	A	2	22.676	44.027	15.878	1.00	14.00	A
ATOM	8	CA	ILE	A	2	22.149	43.401	17.092	1.00	13.36	A
ATOM	9	CB	ILE	A	2	21.747	41.923	16.828	1.00	14.04	A
ATOM	10	CG2	ILE	A	2	21.536	41.191	18.155	1.00	9.05	A
ATOM	11	CG1	ILE	A	2	20.458	41.872	15.988	1.00	13.38	A
ATOM	12	CD1	ILE	A	2	20.173	40.501	15.357	1.00	14.27	A
ATOM	13	C	ILE	A	2	23.303	43.459	18.083	1.00	12.32	A
ATOM	14	O	ILE	A	2	24.376	42.890	17.847	1.00	14.26	A
ATOM	15	N	ASP	A	3	23.075	44.122	19.205	1.00	13.19	A
ATOM	16	CA	ASP	A	3	24.134	44.331	20.193	1.00	11.15	A
ATOM	17	CB	ASP	A	3	24.149	45.830	20.578	1.00	12.52	A
ATOM	18	CG	ASP	A	3	24.268	46.744	19.351	1.00	11.70	A
ATOM	19	OD1	ASP	A	3	25.289	46.618	18.642	1.00	11.97	A
ATOM	20	OD2	ASP	A	3	23.356	47.569	19.094	1.00	13.82	A
ATOM	21	C	ASP	A	3	23.981	43.508	21.456	1.00	11.88	A
ATOM	22	O	ASP	A	3	22.947	43.577	22.116	1.00	11.48	A
ATOM	23	N	GLY	A	4	25.022	42.763	21.800	1.00	9.46	A
ATOM	24	CA	GLY	A	4	24.973	41.947	23.007	1.00	10.97	A
ATOM	25	C	GLY	A	4	26.303	41.966	23.740	1.00	8.48	A
ATOM	26	O	GLY	A	4	27.314	42.413	23.200	1.00	9.87	A
ATOM	27	N	GLY	A	5	26.296	41.496	24.987	1.00	11.77	A
ATOM	28	CA	GLY	A	5	27.511	41.489	25.785	1.00	4.85	A
ATOM	29	C	GLY	A	5	27.163	41.000	27.186	1.00	8.06	A
ATOM	30	O	GLY	A	5	26.009	40.610	27.447	1.00	9.13	A
ATOM	31	N	GLY	A	6	28.144	41.021	28.089	1.00	9.80	A
ATOM	32	CA	GLY	A	6	27.898	40.589	29.458	1.00	9.86	A
ATOM	33	C	GLY	A	6	28.970	39.679	30.014	1.00	7.11	A
ATOM	34	O	GLY	A	6	30.150	40.030	30.000	1.00	8.89	A
ATOM	35	N	ALA	A	7	28.567	38.518	30.525	1.00	9.08	A
ATOM	36	CA	ALA	A	7	29.509	37.540	31.079	1.00	8.69	A
ATOM	37	CB	ALA	A	7	28.814	36.168	31.195	1.00	7.94	A
ATOM	38	C	ALA	A	7	30.811	37.363	30.277	1.00	9.69	A
ATOM	39	O	ALA	A	7	30.781	37.212	29.050	1.00	7.30	A
ATOM	40	N	THR	A	8	31.941	37.367	30.981	1.00	7.56	A
ATOM	41	CA	THR	A	8	33.236	37.135	30.338	1.00	7.21	A
ATOM	42	CB	THR	A	8	34.402	37.865	31.065	1.00	8.00	A
ATOM	43	OG1	THR	A	8	34.532	37.344	32.402	1.00	9.83	A
ATOM	44	CG2	THR	A	8	34.123	39.388	31.139	1.00	10.68	A
ATOM	45	C	THR	A	8	33.542	35.624	30.340	1.00	5.67	A
ATOM	46	O	THR	A	8	34.355	35.168	29.552	1.00	8.00	A
ATOM	47	N	LEU	A	9	32.885	34.842	31.195	1.00	6.65	A
ATOM	48	CA	LEU	A	9	33.190	33.389	31.224	1.00	9.98	A
ATOM	49	CB	LEU	A	9	32.275	32.649	32.238	1.00	10.55	A
ATOM	50	CG	LEU	A	9	32.400	31.109	32.271	1.00	11.53	A
ATOM	51	CD1	LEU	A	9	32.200	30.566	33.699	1.00	10.77	A
ATOM	52	CD2	LEU	A	9	31.356	30.503	31.300	1.00	6.94	A
ATOM	53	C	LEU	A	9	33.103	32.755	29.817	1.00	10.91	A
ATOM	54	O	LEU	A	9	33.985	31.970	29.421	1.00	9.67	A
ATOM	55	N	PRO	A	10	32.051	33.088	29.040	1.00	6.59	A
ATOM	56	CD	PRO	A	10	30.763	33.664	29.485	1.00	8.09	A
ATOM	57	CA	PRO	A	10	31.915	32.521	27.686	1.00	7.68	A
ATOM	58	CB	PRO	A	10	30.428	32.218	27.611	1.00	11.73	A
ATOM	59	CG	PRO	A	10	29.845	33.467	28.251	1.00	8.40	A
ATOM	60	C	PRO	A	10	32.317	33.504	26.579	1.00	8.72	A
ATOM	61	O	PRO	A	10	32.040	33.263	25.396	1.00	9.01	A
ATOM	62	N	GLU	A	11	33.003	34.589	26.928	1.00	5.35	A
ATOM	63	CA	GLU	A	11	33.325	35.565	25.896	1.00	8.04	A
ATOM	64	CB	GLU	A	11	33.978	36.829	26.493	1.00	12.60	A
ATOM	65	CG	GLU	A	11	35.380	36.672	27.001	1.00	21.32	A
ATOM	66	CD	GLU	A	11	35.994	38.013	27.391	1.00	26.61	A
ATOM	67	OE1	GLU	A	11	35.264	38.873	27.920	1.00	30.93	A
ATOM	68	OE2	GLU	A	11	37.203	38.202	27.176	1.00	31.32	A
ATOM	69	C	GLU	A	11	34.143	35.066	24.709	1.00	10.00	A
ATOM	70	O	GLU	A	11	33.866	35.464	23.563	1.00	8.68	A
ATOM	71	N	LYS	A	12	35.134	34.215	24.957	1.00	8.65	A
ATOM	72	CA	LYS	A	12	35.935	33.678	23.850	1.00	10.43	A
ATOM	73	CB	LYS	A	12	37.081	32.840	24.374	1.00	11.05	A
ATOM	74	CG	LYS	A	12	38.151	33.646	25.090	1.00	9.26	A
ATOM	75	CD	LYS	A	12	39.117	32.622	25.673	1.00	17.64	A

FIGURE 5

ATOM	76	CE	LYS	A	12	40.293	33.277	26.307	1.00	24.93	A
ATOM	77	NZ	LYS	A	12	41.298	32.237	26.600	1.00	25.96	A
ATOM	78	C	LYS	A	12	35.079	32.830	22.934	1.00	11.17	A
ATOM	79	O	LYS	A	12	35.339	32.726	21.736	1.00	8.79	A
ATOM	80	N	LEU	A	13	34.071	32.176	23.498	1.00	7.67	A
ATOM	81	CA	LEU	A	13	33.189	31.383	22.669	1.00	10.04	A
ATOM	82	CB	LEU	A	13	32.230	30.549	23.534	1.00	8.86	A
ATOM	83	CG	LEU	A	13	31.082	29.888	22.769	1.00	8.97	A
ATOM	84	CD1	LEU	A	13	31.649	28.807	21.805	1.00	12.12	A
ATOM	85	CD2	LEU	A	13	30.101	29.268	23.753	1.00	12.69	A
ATOM	86	C	LEU	A	13	32.371	32.292	21.750	1.00	9.01	A
ATOM	87	O	LEU	A	13	32.293	32.064	20.536	1.00	10.60	A
ATOM	88	N	TYR	A	14	31.761	33.329	22.305	1.00	10.47	A
ATOM	89	CA	TYR	A	14	30.920	34.195	21.482	1.00	9.03	A
ATOM	90	CB	TYR	A	14	30.029	35.087	22.352	1.00	8.38	A
ATOM	91	CG	TYR	A	14	29.091	34.293	23.253	1.00	11.48	A
ATOM	92	CD1	TYR	A	14	28.499	33.109	22.806	1.00	12.01	A
ATOM	93	CE1	TYR	A	14	27.671	32.341	23.642	1.00	10.45	A
ATOM	94	CD2	TYR	A	14	28.824	34.706	24.564	1.00	10.30	A
ATOM	95	CE2	TYR	A	14	27.998	33.948	25.403	1.00	10.35	A
ATOM	96	CZ	TYR	A	14	27.430	32.766	24.933	1.00	8.21	A
ATOM	97	OH	TYR	A	14	26.628	32.014	25.757	1.00	8.65	A
ATOM	98	C	TYR	A	14	31.715	35.036	20.489	1.00	9.67	A
ATOM	99	O	TYR	A	14	31.142	35.538	19.515	1.00	8.36	A
ATOM	100	N	LEU	A	15	33.021	35.184	20.738	1.00	8.53	A
ATOM	101	CA	LEU	A	15	33.904	35.936	19.838	1.00	9.45	A
ATOM	102	CB	LEU	A	15	35.087	36.564	20.601	1.00	8.09	A
ATOM	103	CG	LEU	A	15	34.742	37.802	21.433	1.00	14.85	A
ATOM	104	CD1	LEU	A	15	35.932	38.141	22.306	1.00	16.07	A
ATOM	105	CD2	LEU	A	15	34.364	38.990	20.510	1.00	12.61	A
ATOM	106	C	LEU	A	15	34.467	35.018	18.756	1.00	16.00	A
ATOM	107	O	LEU	A	15	35.174	35.466	17.859	1.00	16.13	A
ATOM	108	N	THR	A	16	34.178	33.729	18.848	1.00	11.70	A
ATOM	109	CA	THR	A	16	34.681	32.791	17.853	1.00	11.09	A
ATOM	110	CB	THR	A	16	34.523	31.334	18.371	1.00	11.33	A
ATOM	111	OG1	THR	A	16	35.406	31.142	19.484	1.00	13.08	A
ATOM	112	CG2	THR	A	16	34.848	30.314	17.291	1.00	11.23	A
ATOM	113	C	THR	A	16	33.906	32.997	16.549	1.00	12.10	A
ATOM	114	O	THR	A	16	32.671	32.996	16.540	1.00	12.20	A
ATOM	115	N	PRO	A	17	34.620	33.158	15.420	1.00	14.18	A
ATOM	116	CD	PRO	A	17	36.085	33.162	15.251	1.00	14.83	A
ATOM	117	CA	PRO	A	17	33.933	33.367	14.137	1.00	17.90	A
ATOM	118	CB	PRO	A	17	35.068	33.292	13.113	1.00	20.97	A
ATOM	119	CG	PRO	A	17	36.251	33.842	13.890	1.00	21.64	A
ATOM	120	C	PRO	A	17	32.830	32.341	13.854	1.00	14.42	A
ATOM	121	O	PRO	A	17	33.027	31.143	14.066	1.00	14.18	A
ATOM	122	N	ASP	A	18	31.673	32.836	13.414	1.00	15.17	A
ATOM	123	CA	ASP	A	18	30.515	32.020	13.058	1.00	19.19	A
ATOM	124	CB	ASP	A	18	30.932	30.829	12.169	1.00	23.04	A
ATOM	125	CG	ASP	A	18	31.649	31.260	10.885	1.00	30.30	A
ATOM	126	OD1	ASP	A	18	31.214	32.238	10.239	1.00	30.86	A
ATOM	127	OD2	ASP	A	18	32.645	30.599	10.511	1.00	39.65	A
ATOM	128	C	ASP	A	18	29.657	31.479	14.212	1.00	13.08	A
ATOM	129	O	ASP	A	18	28.651	30.833	13.958	1.00	13.28	A
ATOM	130	N	VAL	A	19	30.041	31.709	15.466	1.00	13.07	A
ATOM	131	CA	VAL	A	19	29.199	31.221	16.570	1.00	8.94	A
ATOM	132	CB	VAL	A	19	29.976	31.225	17.911	1.00	9.65	A
ATOM	133	CG1	VAL	A	19	29.014	31.123	19.098	1.00	11.73	A
ATOM	134	CG2	VAL	A	19	30.930	30.026	17.923	1.00	11.99	A
ATOM	135	C	VAL	A	19	27.971	32.126	16.613	1.00	11.81	A
ATOM	136	O	VAL	A	19	26.829	31.655	16.707	1.00	11.21	A
ATOM	137	N	LEU	A	20	28.198	33.434	16.567	1.00	10.93	A
ATOM	138	CA	LEU	A	20	27.077	34.363	16.486	1.00	8.58	A
ATOM	139	CB	LEU	A	20	27.439	35.730	17.084	1.00	13.44	A
ATOM	140	CG	LEU	A	20	27.677	35.767	18.601	1.00	14.24	A
ATOM	141	CD1	LEU	A	20	27.863	37.222	19.084	1.00	13.26	A
ATOM	142	CD2	LEU	A	20	26.480	35.130	19.315	1.00	11.94	A
ATOM	143	C	LEU	A	20	26.857	34.470	14.969	1.00	15.21	A
ATOM	144	O	LEU	A	20	27.836	34.550	14.196	1.00	11.72	A
ATOM	145	N	THR	A	21	25.596	34.455	14.540	1.00	14.05	A
ATOM	146	CA	THR	A	21	25.268	34.511	13.114	1.00	12.27	A
ATOM	147	CB	THR	A	21	24.006	33.653	12.865	1.00	16.46	A
ATOM	148	OG1	THR	A	21	22.966	34.044	13.774	1.00	13.53	A
ATOM	149	CG2	THR	A	21	24.326	32.173	13.121	1.00	17.80	A
ATOM	150	C	THR	A	21	25.121	35.937	12.509	1.00	14.67	A
ATOM	151	O	THR	A	21	25.452	36.928	13.148	1.00	12.04	A

FIGURE 5 (continued)

ATOM	152	N	ALA	A	22	24.663	36.037	11.265	1.00	12.98	A
ATOM	153	CA	ALA	A	22	24.523	37.335	10.594	1.00	12.25	A
ATOM	154	CB	ALA	A	22	23.913	37.146	9.208	1.00	15.06	A
ATOM	155	C	ALA	A	22	23.749	38.418	11.337	1.00	10.99	A
ATOM	156	O	ALA	A	22	22.688	38.174	11.916	1.00	15.12	A
ATOM	157	N	GLY	A	23	24.285	39.636	11.292	1.00	13.67	A
ATOM	158	CA	GLY	A	23	23.631	40.753	11.951	1.00	14.86	A
ATOM	159	C	GLY	A	23	24.068	41.057	13.371	1.00	14.29	A
ATOM	160	O	GLY	A	23	23.775	42.138	13.894	1.00	15.41	A
ATOM	161	N	PHE	A	24	24.760	40.116	14.001	1.00	12.44	A
ATOM	162	CA	PHE	A	24	25.238	40.283	15.363	1.00	14.48	A
ATOM	163	CB	PHE	A	24	25.424	38.899	16.020	1.00	9.89	A
ATOM	164	CG	PHE	A	24	24.156	38.276	16.527	1.00	12.35	A
ATOM	165	CD1	PHE	A	24	23.225	37.734	15.644	1.00	6.46	A
ATOM	166	CD2	PHE	A	24	23.888	38.237	17.898	1.00	12.73	A
ATOM	167	CE1	PHE	A	24	22.035	37.153	16.125	1.00	11.12	A
ATOM	168	CE2	PHE	A	24	22.695	37.662	18.397	1.00	7.42	A
ATOM	169	CZ	PHE	A	24	21.772	37.118	17.502	1.00	11.79	A
ATOM	170	C	PHE	A	24	26.584	41.030	15.444	1.00	14.36	A
ATOM	171	O	PHE	A	24	27.569	40.592	14.850	1.00	12.41	A
ATOM	172	N	ALA	A	25	26.630	42.141	16.183	1.00	14.60	A
ATOM	173	CA	ALA	A	25	27.881	42.875	16.378	1.00	13.54	A
ATOM	174	CB	ALA	A	25	27.606	44.233	17.024	1.00	15.19	A
ATOM	175	C	ALA	A	25	28.752	42.031	17.315	1.00	12.48	A
ATOM	176	O	ALA	A	25	28.240	41.155	18.023	1.00	12.61	A
ATOM	177	N	PRO	A	26	30.067	42.289	17.348	1.00	11.27	A
ATOM	178	CD	PRO	A	26	30.837	43.202	16.476	1.00	13.96	A
ATOM	179	CA	PRO	A	26	30.952	41.507	18.231	1.00	12.70	A
ATOM	180	CB	PRO	A	26	32.334	42.117	17.989	1.00	14.99	A
ATOM	181	CG	PRO	A	26	32.241	42.582	16.519	1.00	19.22	A
ATOM	182	C	PRO	A	26	30.536	41.602	19.699	1.00	10.57	A
ATOM	183	O	PRO	A	26	30.222	42.681	20.192	1.00	10.54	A
ATOM	184	N	TYR	A	27	30.529	40.456	20.367	1.00	8.04	A
ATOM	185	CA	TYR	A	27	30.161	40.345	21.793	1.00	9.13	A
ATOM	186	CB	TYR	A	27	30.294	38.886	22.231	1.00	8.74	A
ATOM	187	CG	TYR	A	27	29.824	38.612	23.648	1.00	5.12	A
ATOM	188	CD1	TYR	A	27	28.469	38.512	23.938	1.00	6.81	A
ATOM	189	CE1	TYR	A	27	28.024	38.224	25.247	1.00	9.00	A
ATOM	190	CD2	TYR	A	27	30.741	38.423	24.682	1.00	5.70	A
ATOM	191	CE2	TYR	A	27	30.310	38.131	25.992	1.00	7.78	A
ATOM	192	CZ	TYR	A	27	28.948	38.032	26.259	1.00	9.36	A
ATOM	193	OH	TYR	A	27	28.502	37.709	27.532	1.00	8.37	A
ATOM	194	C	TYR	A	27	31.081	41.207	22.675	1.00	10.49	A
ATOM	195	O	TYR	A	27	32.297	41.207	22.494	1.00	9.91	A
ATOM	196	N	ILE	A	28	30.510	41.931	23.635	1.00	8.97	A
ATOM	197	CA	ILE	A	28	31.324	42.765	24.517	1.00	12.31	A
ATOM	198	CB	ILE	A	28	30.801	44.225	24.521	1.00	13.61	A
ATOM	199	CG2	ILE	A	28	31.657	45.098	25.459	1.00	13.95	A
ATOM	200	CG1	ILE	A	28	30.871	44.793	23.095	1.00	11.91	A
ATOM	201	CD1	ILE	A	28	30.192	46.146	22.915	1.00	12.92	A
ATOM	202	C	ILE	A	28	31.333	42.191	25.942	1.00	13.14	A
ATOM	203	O	ILE	A	28	30.315	42.189	26.622	1.00	8.79	A
ATOM	204	N	GLY	A	29	32.499	41.706	26.373	1.00	13.23	A
ATOM	205	CA	GLY	A	29	32.630	41.105	27.695	1.00	15.83	A
ATOM	206	C	GLY	A	29	32.868	42.127	28.791	1.00	16.10	A
ATOM	207	O	GLY	A	29	33.915	42.794	28.826	1.00	12.27	A
ATOM	208	N	THR	A	30	31.900	42.234	29.697	1.00	8.70	A
ATOM	209	CA	THR	A	30	31.966	43.200	30.783	1.00	10.71	A
ATOM	210	CB	THR	A	30	31.061	44.442	30.473	1.00	11.83	A
ATOM	211	OG1	THR	A	30	29.703	44.014	30.222	1.00	16.91	A
ATOM	212	CG2	THR	A	30	31.607	45.235	29.249	1.00	8.83	A
ATOM	213	C	THR	A	30	31.538	42.640	32.147	1.00	11.78	A
ATOM	214	O	THR	A	30	31.532	43.378	33.135	1.00	11.34	A
ATOM	215	N	GLY	A	31	31.187	41.352	32.210	1.00	10.41	A
ATOM	216	CA	GLY	A	31	30.729	40.789	33.473	1.00	8.40	A
ATOM	217	C	GLY	A	31	29.208	40.604	33.467	1.00	9.64	A
ATOM	218	O	GLY	A	31	28.478	41.396	32.862	1.00	8.01	A
ATOM	219	N	SER	A	32	28.718	39.566	34.138	1.00	7.93	A
ATOM	220	CA	SER	A	32	27.274	39.297	34.143	1.00	4.39	A
ATOM	221	CB	SER	A	32	26.961	37.954	34.832	1.00	2.86	A
ATOM	222	OG	SER	A	32	27.538	36.876	34.125	1.00	6.73	A
ATOM	223	C	SER	A	32	26.440	40.386	34.793	1.00	7.61	A
ATOM	224	O	SER	A	32	25.321	40.626	34.354	1.00	9.70	A
ATOM	225	N	GLY	A	33	26.984	41.052	35.811	1.00	8.20	A
ATOM	226	CA	GLY	A	33	26.256	42.121	36.506	1.00	6.91	A

FIGURE 5 (continued)

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ATOM    227  C   GLY A  33      25.942  43.235  35.524  1.00  9.16      A
ATOM    228  O   GLY A  33      24.799  43.708  35.429  1.00  9.95      A
ATOM    229  N   LYS A  34      26.943  43.633  34.749  1.00 10.60      A
ATOM    230  CA  LYS A  34      26.710  44.681  33.758  1.00  8.52      A
ATOM    231  CB  LYS A  34      28.040  45.240  33.250  1.00  7.07      A
ATOM    232  CG  LYS A  34      28.667  46.220  34.250  1.00 12.80      A
ATOM    233  CD  LYS A  34      29.957  46.854  33.703  1.00 10.66      A
ATOM    234  CE  LYS A  34      30.597  47.768  34.748  1.00 10.90      A
ATOM    235  NZ  LYS A  34      29.700  48.890  35.066  1.00 23.47      A
ATOM    236  C   LYS A  34      25.848  44.201  32.601  1.00 12.94      A
ATOM    237  O   LYS A  34      25.070  44.977  32.043  1.00  9.59      A
ATOM    238  N   GLY A  35      25.983  42.928  32.236  1.00  9.69      A
ATOM    239  CA  GLY A  35      25.158  42.386  31.162  1.00  7.50      A
ATOM    240  C   GLY A  35      23.677  42.414  31.542  1.00  9.68      A
ATOM    241  O   GLY A  35      22.831  42.767  30.717  1.00  9.00      A
ATOM    242  N   LYS A  36      23.340  42.077  32.787  1.00  8.56      A
ATOM    243  CA  LYS A  36      21.929  42.089  33.173  1.00  7.26      A
ATOM    244  CB  LYS A  36      21.709  41.393  34.533  1.00  9.15      A
ATOM    245  CG  LYS A  36      21.954  39.861  34.445  1.00  5.28      A
ATOM    246  CD  LYS A  36      21.394  39.069  35.662  1.00  6.85      A
ATOM    247  CE  LYS A  36      21.990  39.576  36.986  1.00 11.53      A
ATOM    248  NZ  LYS A  36      21.397  38.945  38.221  1.00 11.99      A
ATOM    249  C   LYS A  36      21.409  43.527  33.204  1.00 11.18      A
ATOM    250  O   LYS A  36      20.311  43.787  32.724  1.00 14.03      A
ATOM    251  N   ILE A  37      22.190  44.459  33.749  1.00  9.12      A
ATOM    252  CA  ILE A  37      21.752  45.854  33.766  1.00 11.15      A
ATOM    253  CB  ILE A  37      22.778  46.779  34.462  1.00 10.46      A
ATOM    254  CG2 ILE A  37      22.424  48.252  34.197  1.00 11.32      A
ATOM    255  CG1 ILE A  37      22.774  46.522  35.972  1.00  9.50      A
ATOM    256  CD1 ILE A  37      24.024  47.029  36.669  1.00 15.62      A
ATOM    257  C   ILE A  37      21.563  46.368  32.325  1.00 11.78      A
ATOM    258  O   ILE A  37      20.570  47.017  32.018  1.00 11.36      A
ATOM    259  N   ALA A  38      22.518  46.071  31.452  1.00  9.31      A
ATOM    260  CA  ALA A  38      22.438  46.539  30.063  1.00 10.19      A
ATOM    261  CB  ALA A  38      23.650  46.016  29.269  1.00 10.93      A
ATOM    262  C   ALA A  38      21.129  46.102  29.375  1.00  9.69      A
ATOM    263  O   ALA A  38      20.447  46.899  28.712  1.00  8.41      A
ATOM    264  N   PHE A  39      20.771  44.831  29.541  1.00  8.70      A
ATOM    265  CA  PHE A  39      19.566  44.327  28.914  1.00  9.40      A
ATOM    266  CB  PHE A  39      19.549  42.787  28.888  1.00  9.06      A
ATOM    267  CG  PHE A  39      18.287  42.214  28.270  1.00  7.16      A
ATOM    268  CD1 PHE A  39      18.223  41.953  26.896  1.00  8.56      A
ATOM    269  CD2 PHE A  39      17.146  42.000  29.051  1.00  8.19      A
ATOM    270  CE1 PHE A  39      17.035  41.481  26.306  1.00  9.12      A
ATOM    271  CE2 PHE A  39      15.947  41.530  28.479  1.00  9.01      A
ATOM    272  CZ  PHE A  39      15.888  41.269  27.101  1.00  8.28      A
ATOM    273  C   PHE A  39      18.304  44.790  29.608  1.00 12.15      A
ATOM    274  O   PHE A  39      17.398  45.313  28.972  1.00 10.76      A
ATOM    275  N   LEU A  40      18.246  44.602  30.920  1.00  8.71      A
ATOM    276  CA  LEU A  40      17.034  44.938  31.678  1.00  8.94      A
ATOM    277  CB  LEU A  40      17.204  44.513  33.144  1.00  7.80      A
ATOM    278  CG  LEU A  40      17.342  43.005  33.400  1.00 10.06      A
ATOM    279  CD1 LEU A  40      17.809  42.781  34.887  1.00  6.45      A
ATOM    280  CD2 LEU A  40      16.006  42.296  33.132  1.00 12.55      A
ATOM    281  C   LEU A  40      16.626  46.403  31.632  1.00 10.63      A
ATOM    282  O   LEU A  40      15.430  46.730  31.629  1.00 11.89      A
ATOM    283  N   GLU A  41      17.604  47.291  31.586  1.00 10.88      A
ATOM    284  CA  GLU A  41      17.294  48.717  31.551  1.00  9.10      A
ATOM    285  CB  GLU A  41      18.053  49.436  32.669  1.00 13.20      A
ATOM    286  CG  GLU A  41      17.802  48.829  34.036  1.00 11.00      A
ATOM    287  CD  GLU A  41      18.671  49.429  35.131  1.00 22.54      A
ATOM    288  OE1 GLU A  41      18.975  48.713  36.103  1.00 27.36      A
ATOM    289  OE2 GLU A  41      19.037  50.616  35.043  1.00 22.49      A
ATOM    290  C   GLU A  41      17.633  49.361  30.218  1.00 12.72      A
ATOM    291  O   GLU A  41      17.505  50.576  30.066  1.00 13.60      A
ATOM    292  N   ASN A  42      18.010  48.537  29.238  1.00 11.74      A
ATOM    293  CA  ASN A  42      18.463  49.008  27.923  1.00 11.79      A
ATOM    294  CB  ASN A  42      17.322  49.494  27.022  1.00 14.08      A
ATOM    295  CG  ASN A  42      17.824  49.897  25.642  1.00 16.54      A
ATOM    296  OD1 ASN A  42      18.885  49.428  25.189  1.00 15.67      A
ATOM    297  ND2 ASN A  42      17.076  50.763  24.960  1.00 14.22      A
ATOM    298  C   ASN A  42      19.486  50.126  28.091  1.00 16.68      A
ATOM    299  O   ASN A  42      19.300  51.260  27.631  1.00 14.27      A
ATOM    300  N   SER A  43      20.578  49.789  28.767  1.00 14.51      A
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FIGURE 5 (continued)

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ATOM    301  CA  SER A  43      21.665  50.740  29.001  1.00 14.54      A
ATOM    302  CB  SER A  43      21.920  50.874  30.520  1.00 19.90      A
ATOM    303  OG  SER A  43      20.922  51.662  31.162  1.00 26.26      A
ATOM    304  C   SER A  43      22.965  50.327  28.302  1.00 13.78      A
ATOM    305  O   SER A  43      23.790  49.633  28.891  1.00 10.60      A
ATOM    306  N   TYR A  44      23.168  50.755  27.056  1.00  9.73      A
ATOM    307  CA  TYR A  44      24.396  50.401  26.361  1.00 10.86      A
ATOM    308  CB  TYR A  44      24.330  50.880  24.904  1.00 10.54      A
ATOM    309  CG  TYR A  44      25.414  50.311  24.034  1.00 12.22      A
ATOM    310  CD1 TYR A  44      26.631  50.983  23.857  1.00 12.57      A
ATOM    311  CE1 TYR A  44      27.625  50.469  23.011  1.00 10.91      A
ATOM    312  CD2 TYR A  44      25.217  49.106  23.357  1.00 10.34      A
ATOM    313  CE2 TYR A  44      26.201  48.587  22.517  1.00 11.21      A
ATOM    314  CZ  TYR A  44      27.394  49.267  22.347  1.00 14.12      A
ATOM    315  OH  TYR A  44      28.357  48.725  21.524  1.00 11.54      A
ATOM    316  C   TYR A  44      25.650  50.971  27.026  1.00  8.02      A
ATOM    317  O   TYR A  44      26.775  50.515  26.756  1.00 10.36      A
ATOM    318  N   ASN A  45      25.484  51.941  27.917  1.00  8.55      A
ATOM    319  CA  ASN A  45      26.657  52.547  28.535  1.00 14.36      A
ATOM    320  CB  ASN A  45      26.271  53.811  29.337  1.00  8.69      A
ATOM    321  CG  ASN A  45      25.707  53.503  30.708  1.00 11.69      A
ATOM    322  OD1 ASN A  45      25.048  52.488  30.910  1.00 13.56      A
ATOM    323  ND2 ASN A  45      25.934  54.411  31.655  1.00 14.48      A
ATOM    324  C   ASN A  45      27.423  51.535  29.388  1.00 13.91      A
ATOM    325  O   ASN A  45      28.573  51.781  29.755  1.00 11.13      A
ATOM    326  N   GLN A  46      26.788  50.393  29.681  1.00  8.83      A
ATOM    327  CA  GLN A  46      27.462  49.337  30.435  1.00 11.62      A
ATOM    328  CB  GLN A  46      26.421  48.390  31.080  1.00 10.13      A
ATOM    329  CG  GLN A  46      25.487  49.076  32.083  1.00 14.66      A
ATOM    330  CD  GLN A  46      26.259  49.792  33.170  1.00 18.72      A
ATOM    331  OE1 GLN A  46      26.983  49.165  33.937  1.00 18.65      A
ATOM    332  NE2 GLN A  46      26.133  51.116  33.228  1.00 16.99      A
ATOM    333  C   GLN A  46      28.408  48.543  29.491  1.00 10.06      A
ATOM    334  O   GLN A  46      29.275  47.818  29.956  1.00 10.43      A
ATOM    335  N   PHE A  47      28.232  48.691  28.174  1.00  8.72      A
ATOM    336  CA  PHE A  47      29.055  48.025  27.148  1.00  7.46      A
ATOM    337  CB  PHE A  47      28.191  47.487  25.992  1.00  7.56      A
ATOM    338  CG  PHE A  47      27.271  46.349  26.366  1.00 12.11      A
ATOM    339  CD1 PHE A  47      27.433  45.651  27.559  1.00 11.35      A
ATOM    340  CD2 PHE A  47      26.268  45.945  25.474  1.00 14.21      A
ATOM    341  CE1 PHE A  47      26.616  44.567  27.861  1.00  9.31      A
ATOM    342  CE2 PHE A  47      25.442  44.859  25.761  1.00  9.84      A
ATOM    343  CZ  PHE A  47      25.617  44.167  26.959  1.00 10.19      A
ATOM    344  C   PHE A  47      30.053  48.988  26.484  1.00 12.94      A
ATOM    345  O   PHE A  47      31.109  48.580  26.022  1.00 14.11      A
ATOM    346  N   GLY A  48      29.677  50.257  26.378  1.00 11.49      A
ATOM    347  CA  GLY A  48      30.551  51.222  25.731  1.00 13.51      A
ATOM    348  C   GLY A  48      30.027  52.642  25.833  1.00 15.44      A
ATOM    349  O   GLY A  48      28.999  52.908  26.459  1.00 16.60      A
ATOM    350  N   THR A  49      30.722  53.566  25.187  1.00 14.37      A
ATOM    351  CA  THR A  49      30.333  54.967  25.256  1.00 13.58      A
ATOM    352  CB  THR A  49      31.576  55.843  25.161  1.00 14.46      A
ATOM    353  OG1 THR A  49      32.234  55.567  23.924  1.00 15.00      A
ATOM    354  CG2 THR A  49      32.558  55.524  26.322  1.00 13.17      A
ATOM    355  C   THR A  49      29.301  55.436  24.216  1.00 14.30      A
ATOM    356  O   THR A  49      28.716  56.511  24.370  1.00 12.47      A
ATOM    357  N   ASN A  50      29.062  54.659  23.162  1.00 13.09      A
ATOM    358  CA  ASN A  50      28.076  55.116  22.173  1.00 14.85      A
ATOM    359  CB  ASN A  50      28.324  54.519  20.785  1.00 15.63      A
ATOM    360  CG  ASN A  50      27.379  55.096  19.739  1.00 18.88      A
ATOM    361  OD1 ASN A  50      26.472  55.883  20.059  1.00 19.28      A
ATOM    362  ND2 ASN A  50      27.574  54.707  18.489  1.00 19.28      A
ATOM    363  C   ASN A  50      26.669  54.751  22.615  1.00 14.82      A
ATOM    364  O   ASN A  50      26.099  53.739  22.187  1.00 14.58      A
ATOM    365  N   THR A  51      26.097  55.608  23.443  1.00 13.25      A
ATOM    366  CA  THR A  51      24.782  55.377  23.988  1.00 15.77      A
ATOM    367  CB  THR A  51      24.595  56.210  25.242  1.00 17.96      A
ATOM    368  OG1 THR A  51      24.937  57.574  24.973  1.00 16.18      A
ATOM    369  CG2 THR A  51      25.506  55.684  26.332  1.00 18.64      A
ATOM    370  C   THR A  51      23.581  55.539  23.053  1.00 18.71      A
ATOM    371  O   THR A  51      22.440  55.436  23.512  1.00 19.68      A
ATOM    372  N   THR A  52      23.820  55.795  21.761  1.00 16.82      A
ATOM    373  CA  THR A  52      22.702  55.865  20.827  1.00 19.67      A
ATOM    374  CB  THR A  52      23.017  56.666  19.524  1.00 22.55      A
ATOM    375  OG1 THR A  52      24.028  56.006  18.744  1.00 22.57      A
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FIGURE 5 (continued)

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ATOM    376  CG2 THR A  52      23.460  58.081  19.875  1.00 21.07      A
ATOM    377  C   THR A  52      22.342  54.428  20.446  1.00 17.92      A
ATOM    378  O   THR A  52      21.270  54.175  19.905  1.00 17.96      A
ATOM    379  N   LYS A  53      23.238  53.488  20.740  1.00 14.41      A
ATOM    380  CA  LYS A  53      22.978  52.080  20.427  1.00 12.53      A
ATOM    381  CB  LYS A  53      24.292  51.292  20.406  1.00 14.33      A
ATOM    382  CG  LYS A  53      25.207  51.573  19.213  1.00 17.93      A
ATOM    383  CD  LYS A  53      26.478  50.731  19.324  1.00 18.20      A
ATOM    384  CE  LYS A  53      27.477  51.052  18.214  1.00 21.01      A
ATOM    385  NZ  LYS A  53      26.908  50.784  16.865  1.00 22.67      A
ATOM    386  C   LYS A  53      22.045  51.470  21.474  1.00 12.72      A
ATOM    387  O   LYS A  53      22.075  51.869  22.635  1.00 11.93      A
ATOM    388  N   ASP A  54      21.223  50.499  21.064  1.00 13.58      A
ATOM    389  CA  ASP A  54      20.298  49.826  21.982  1.00 10.96      A
ATOM    390  CB  ASP A  54      18.887  49.745  21.380  1.00 12.81      A
ATOM    391  CG  ASP A  54      18.249  51.107  21.218  1.00 19.07      A
ATOM    392  OD1 ASP A  54      18.010  51.529  20.059  1.00 17.31      A
ATOM    393  OD2 ASP A  54      17.997  51.759  22.260  1.00 15.46      A
ATOM    394  C   ASP A  54      20.819  48.416  22.246  1.00  8.44      A
ATOM    395  O   ASP A  54      21.505  47.837  21.407  1.00 14.56      A
ATOM    396  N   VAL A  55      20.485  47.875  23.411  1.00 12.75      A
ATOM    397  CA  VAL A  55      20.919  46.541  23.799  1.00 12.22      A
ATOM    398  CB  VAL A  55      21.150  46.486  25.328  1.00  7.89      A
ATOM    399  CG1 VAL A  55      21.596  45.057  25.775  1.00  7.35      A
ATOM    400  CG2 VAL A  55      22.229  47.518  25.707  1.00  6.23      A
ATOM    401  C   VAL A  55      19.840  45.540  23.386  1.00  9.36      A
ATOM    402  O   VAL A  55      18.659  45.768  23.630  1.00 11.95      A
ATOM    403  N   HIS A  56      20.258  44.441  22.755  1.00  9.82      A
ATOM    404  CA  HIS A  56      19.323  43.432  22.285  1.00  8.89      A
ATOM    405  CB  HIS A  56      19.552  43.218  20.782  1.00  8.33      A
ATOM    406  CG  HIS A  56      19.455  44.485  19.985  1.00  9.48      A
ATOM    407  CD2 HIS A  56      20.414  45.264  19.430  1.00 11.14      A
ATOM    408  ND1 HIS A  56      18.255  45.121  19.738  1.00 13.82      A
ATOM    409  CE1 HIS A  56      18.483  46.236  19.064  1.00 12.14      A
ATOM    410  NE2 HIS A  56      19.783  46.345  18.866  1.00 12.83      A
ATOM    411  C   HIS A  56      19.389  42.097  23.033  1.00  9.87      A
ATOM    412  O   HIS A  56      18.419  41.331  23.039  1.00  8.84      A
ATOM    413  N   TRP A  57      20.531  41.797  23.649  1.00 10.03      A
ATOM    414  CA  TRP A  57      20.618  40.535  24.385  1.00 12.07      A
ATOM    415  CB  TRP A  57      20.753  39.340  23.430  1.00  7.72      A
ATOM    416  CG  TRP A  57      22.078  39.288  22.673  1.00  9.96      A
ATOM    417  CD2 TRP A  57      23.188  38.398  22.935  1.00  8.55      A
ATOM    418  CE2 TRP A  57      24.161  38.642  21.945  1.00  7.37      A
ATOM    419  CE3 TRP A  57      23.442  37.413  23.914  1.00  9.79      A
ATOM    420  CD1 TRP A  57      22.430  40.021  21.570  1.00  9.43      A
ATOM    421  NE1 TRP A  57      23.685  39.637  21.124  1.00  7.89      A
ATOM    422  CZ2 TRP A  57      25.381  37.936  21.895  1.00  8.66      A
ATOM    423  CZ3 TRP A  57      24.647  36.713  23.862  1.00  7.59      A
ATOM    424  CH2 TRP A  57      25.605  36.982  22.852  1.00 13.66      A
ATOM    425  C   TRP A  57      21.830  40.575  25.286  1.00  9.35      A
ATOM    426  O   TRP A  57      22.648  41.481  25.179  1.00  9.06      A
ATOM    427  N   ALA A  58      21.945  39.579  26.159  1.00  6.35      A
ATOM    428  CA  ALA A  58      23.081  39.523  27.061  1.00  8.26      A
ATOM    429  CB  ALA A  58      22.755  40.280  28.362  1.00 10.03      A
ATOM    430  C   ALA A  58      23.471  38.101  27.407  1.00  7.97      A
ATOM    431  O   ALA A  58      22.638  37.207  27.401  1.00  9.27      A
ATOM    432  N   GLY A  59      24.749  37.908  27.702  1.00  9.58      A
ATOM    433  CA  GLY A  59      25.213  36.608  28.184  1.00  7.09      A
ATOM    434  C   GLY A  59      25.342  36.791  29.695  1.00  9.23      A
ATOM    435  O   GLY A  59      25.779  37.846  30.159  1.00 10.14      A
ATOM    436  N   SER A  60      24.938  35.801  30.484  1.00  5.73      A
ATOM    437  CA  SER A  60      25.058  35.917  31.938  1.00  5.95      A
ATOM    438  CB  SER A  60      23.815  36.613  32.535  1.00 10.17      A
ATOM    439  OG  SER A  60      23.896  36.707  33.966  1.00  9.12      A
ATOM    440  C   SER A  60      25.161  34.540  32.566  1.00  8.54      A
ATOM    441  O   SER A  60      24.437  33.632  32.146  1.00  9.12      A
ATOM    442  N   ASP A  61      26.067  34.376  33.536  1.00  9.30      A
ATOM    443  CA  ASP A  61      26.132  33.124  34.292  1.00  8.23      A
ATOM    444  CB  ASP A  61      27.543  32.485  34.381  1.00  6.13      A
ATOM    445  CG  ASP A  61      28.600  33.266  33.649  1.00 13.41      A
ATOM    446  OD1 ASP A  61      28.869  32.961  32.449  1.00 10.15      A
ATOM    447  OD2 ASP A  61      29.150  34.191  34.281  1.00 13.11      A
ATOM    448  C   ASP A  61      25.597  33.456  35.710  1.00 10.77      A
ATOM    449  O   ASP A  61      25.818  32.716  36.658  1.00 11.14      A
ATOM    450  N   SER A  62      24.914  34.595  35.833  1.00  7.59      A
ATOM    451  CA  SER A  62      24.213  34.995  37.067  1.00 10.29      A
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FIGURE 5 (continued)

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ATOM    452  CB  SER A  62      24.522  36.437  37.497  1.00 11.42      A
ATOM    453  OG  SER A  62      23.631  36.832  38.549  1.00 11.94      A
ATOM    454  C   SER A  62      22.721  34.944  36.706  1.00 10.70      A
ATOM    455  O   SER A  62      22.274  35.605  35.745  1.00  9.88      A
ATOM    456  N   LYS A  63      21.944  34.168  37.449  1.00  8.95      A
ATOM    457  CA  LYS A  63      20.519  34.089  37.137  1.00 10.67      A
ATOM    458  CB  LYS A  63      19.834  32.996  37.959  1.00 16.43      A
ATOM    459  CG  LYS A  63      20.046  31.605  37.461  1.00 15.34      A
ATOM    460  CD  LYS A  63      19.148  30.619  38.201  1.00 19.94      A
ATOM    461  CE  LYS A  63      17.702  30.671  37.728  1.00 16.96      A
ATOM    462  NZ  LYS A  63      16.903  29.498  38.239  1.00 14.00      A
ATOM    463  C   LYS A  63      19.786  35.392  37.399  1.00 12.40      A
ATOM    464  O   LYS A  63      20.192  36.183  38.257  1.00 10.37      A
ATOM    465  N   LEU A  64      18.699  35.604  36.659  1.00  7.10      A
ATOM    466  CA  LEU A  64      17.863  36.778  36.842  1.00  9.01      A
ATOM    467  CB  LEU A  64      16.824  36.871  35.716  1.00  6.27      A
ATOM    468  CG  LEU A  64      17.447  37.378  34.405  1.00  7.74      A
ATOM    469  CD1 LEU A  64      16.586  37.016  33.190  1.00  8.96      A
ATOM    470  CD2 LEU A  64      17.619  38.883  34.510  1.00  9.78      A
ATOM    471  C   LEU A  64      17.168  36.569  38.197  1.00 10.06      A
ATOM    472  O   LEU A  64      16.712  35.465  38.508  1.00 11.86      A
ATOM    473  N   THR A  65      17.120  37.614  39.012  1.00  6.99      A
ATOM    474  CA  THR A  65      16.503  37.481  40.334  1.00 11.54      A
ATOM    475  CB  THR A  65      17.097  38.472  41.341  1.00 13.33      A
ATOM    476  OG1 THR A  65      16.736  39.811  40.952  1.00 13.29      A
ATOM    477  CG2 THR A  65      18.644  38.331  41.395  1.00 11.42      A
ATOM    478  C   THR A  65      15.009  37.751  40.239  1.00 13.06      A
ATOM    479  O   THR A  65      14.530  38.268  39.233  1.00  9.78      A
ATOM    480  N   ALA A  66      14.272  37.374  41.281  1.00 11.93      A
ATOM    481  CA  ALA A  66      12.831  37.607  41.287  1.00 16.82      A
ATOM    482  CB  ALA A  66      12.231  37.106  42.601  1.00 17.23      A
ATOM    483  C   ALA A  66      12.527  39.104  41.105  1.00 14.69      A
ATOM    484  O   ALA A  66      11.587  39.467  40.409  1.00 12.67      A
ATOM    485  N   SER A  67      13.322  39.962  41.744  1.00 15.98      A
ATOM    486  CA  SER A  67      13.150  41.417  41.640  1.00 12.48      A
ATOM    487  CB  SER A  67      14.108  42.166  42.579  1.00 18.87      A
ATOM    488  OG  SER A  67      13.662  42.081  43.921  1.00 28.18      A
ATOM    489  C   SER A  67      13.403  41.890  40.212  1.00 12.05      A
ATOM    490  O   SER A  67      12.630  42.671  39.666  1.00 12.31      A
ATOM    491  N   GLN A  68      14.495  41.426  39.616  1.00  8.93      A
ATOM    492  CA  GLN A  68      14.796  41.803  38.237  1.00  8.58      A
ATOM    493  CB  GLN A  68      16.123  41.176  37.768  1.00 11.33      A
ATOM    494  CG  GLN A  68      17.343  41.749  38.524  1.00 12.20      A
ATOM    495  CD  GLN A  68      18.656  41.026  38.242  1.00 15.53      A
ATOM    496  OE1 GLN A  68      18.690  39.815  38.034  1.00 11.56      A
ATOM    497  NE2 GLN A  68      19.743  41.770  38.255  1.00 14.33      A
ATOM    498  C   GLN A  68      13.673  41.385  37.290  1.00 12.61      A
ATOM    499  O   GLN A  68      13.270  42.158  36.423  1.00 10.84      A
ATOM    500  N   LEU A  69      13.163  40.164  37.455  1.00 13.81      A
ATOM    501  CA  LEU A  69      12.093  39.687  36.576  1.00 13.47      A
ATOM    502  CB  LEU A  69      11.809  38.189  36.829  1.00 13.08      A
ATOM    503  CG  LEU A  69      12.989  37.268  36.496  1.00 14.83      A
ATOM    504  CD1 LEU A  69      12.772  35.862  37.071  1.00 16.18      A
ATOM    505  CD2 LEU A  69      13.140  37.233  34.981  1.00 11.50      A
ATOM    506  C   LEU A  69      10.810  40.484  36.778  1.00 13.14      A
ATOM    507  O   LEU A  69      10.138  40.860  35.814  1.00 13.07      A
ATOM    508  N   ALA A  70      10.465  40.728  38.034  1.00 12.61      A
ATOM    509  CA  ALA A  70       9.227  41.443  38.328  1.00 12.01      A
ATOM    510  CB  ALA A  70       8.951  41.453  39.841  1.00 13.19      A
ATOM    511  C   ALA A  70       9.275  42.852  37.785  1.00 12.44      A
ATOM    512  O   ALA A  70       8.297  43.334  37.240  1.00 16.48      A
ATOM    513  N   THR A  71      10.419  43.512  37.928  1.00 12.49      A
ATOM    514  CA  THR A  71      10.574  44.865  37.436  1.00 11.47      A
ATOM    515  CB  THR A  71      11.914  45.463  37.941  1.00 18.09      A
ATOM    516  OG1 THR A  71      11.834  45.621  39.370  1.00 19.27      A
ATOM    517  CG2 THR A  71      12.225  46.811  37.267  1.00 13.43      A
ATOM    518  C   THR A  71      10.501  44.905  35.902  1.00 11.57      A
ATOM    519  O   THR A  71       9.881  45.800  35.337  1.00 15.24      A
ATOM    520  N   TYR A  72      11.116  43.941  35.223  1.00 13.13      A
ATOM    521  CA  TYR A  72      11.049  43.941  33.760  1.00 12.95      A
ATOM    522  CB  TYR A  72      11.927  42.839  33.174  1.00 11.21      A
ATOM    523  CG  TYR A  72      12.194  43.011  31.682  1.00 12.14      A
ATOM    524  CD1 TYR A  72      13.122  43.936  31.224  1.00 11.17      A
ATOM    525  CE1 TYR A  72      13.376  44.101  29.841  1.00 11.35      A
ATOM    526  CD2 TYR A  72      11.515  42.239  30.736  1.00 14.03      A
ATOM    527  CE2 TYR A  72      11.765  42.378  29.372  1.00  8.40      A
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FIGURE 5 (continued)

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ATOM    528  CZ  TYR A  72      12.689  43.303  28.928  1.00 10.19      A
ATOM    529  OH  TYR A  72      12.949  43.425  27.585  1.00 10.75      A
ATOM    530  C   TYR A  72       9.604  43.705  33.313  1.00 13.42      A
ATOM    531  O   TYR A  72       9.111  44.346  32.394  1.00 14.74      A
ATOM    532  N   ALA A  73       8.943  42.763  33.970  1.00 14.68      A
ATOM    533  CA  ALA A  73       7.563  42.423  33.650  1.00 15.37      A
ATOM    534  CB  ALA A  73       7.090  41.293  34.556  1.00 10.74      A
ATOM    535  C   ALA A  73       6.631  43.626  33.791  1.00 14.04      A
ATOM    536  O   ALA A  73       5.711  43.811  32.992  1.00 13.32      A
ATOM    537  N   ALA A  74       6.856  44.436  34.815  1.00 16.88      A
ATOM    538  CA  ALA A  74       6.006  45.602  35.032  1.00 17.08      A
ATOM    539  CB  ALA A  74       6.082  46.052  36.505  1.00 13.94      A
ATOM    540  C   ALA A  74       6.354  46.768  34.118  1.00 20.94      A
ATOM    541  O   ALA A  74       5.475  47.357  33.476  1.00 17.04      A
ATOM    542  N   ASN A  75       7.645  47.061  34.014  1.00 15.74      A
ATOM    543  CA  ASN A  75       8.125  48.203  33.241  1.00 17.76      A
ATOM    544  CB  ASN A  75       9.439  48.712  33.839  1.00 19.52      A
ATOM    545  CG  ASN A  75       9.308  49.152  35.289  1.00 24.86      A
ATOM    546  OD1 ASN A  75      10.308  49.485  35.929  1.00 26.13      A
ATOM    547  ND2 ASN A  75       8.084  49.150  35.816  1.00 27.41      A
ATOM    548  C   ASN A  75       8.356  48.070  31.741  1.00 18.90      A
ATOM    549  O   ASN A  75       8.049  48.996  30.986  1.00 16.37      A
ATOM    550  N   LYS A  76       8.910  46.944  31.304  1.00 13.20      A
ATOM    551  CA  LYS A  76       9.235  46.810  29.888  1.00 14.05      A
ATOM    552  CB  LYS A  76      10.709  46.412  29.730  1.00 11.81      A
ATOM    553  CG  LYS A  76      11.706  47.189  30.561  1.00 15.12      A
ATOM    554  CD  LYS A  76      11.710  48.673  30.208  1.00 18.17      A
ATOM    555  CE  LYS A  76      12.942  49.342  30.783  1.00 21.75      A
ATOM    556  NZ  LYS A  76      12.858  50.832  30.665  1.00 23.76      A
ATOM    557  C   LYS A  76       8.414  45.835  29.064  1.00 14.89      A
ATOM    558  O   LYS A  76       8.184  46.053  27.874  1.00 15.18      A
ATOM    559  N   GLN A  77       7.996  44.746  29.686  1.00 13.65      A
ATOM    560  CA  GLN A  77       7.240  43.718  28.978  1.00 15.70      A
ATOM    561  CB  GLN A  77       6.865  42.625  29.964  1.00 14.98      A
ATOM    562  CG  GLN A  77       6.139  41.438  29.381  1.00 18.91      A
ATOM    563  CD  GLN A  77       5.848  40.392  30.441  1.00 26.71      A
ATOM    564  OE1 GLN A  77       6.747  39.965  31.167  1.00 25.14      A
ATOM    565  NE2 GLN A  77       4.593  39.968  30.534  1.00 21.79      A
ATOM    566  C   GLN A  77       5.989  44.205  28.222  1.00 16.81      A
ATOM    567  O   GLN A  77       5.718  43.746  27.114  1.00 17.54      A
ATOM    568  N   PRO A  78       5.216  45.142  28.800  1.00 19.48      A
ATOM    569  CD  PRO A  78       5.255  45.765  30.134  1.00 12.68      A
ATOM    570  CA  PRO A  78       4.023  45.575  28.056  1.00 15.54      A
ATOM    571  CB  PRO A  78       3.428  46.654  28.958  1.00 19.25      A
ATOM    572  CG  PRO A  78       3.787  46.150  30.342  1.00 17.82      A
ATOM    573  C   PRO A  78       4.325  46.080  26.646  1.00 20.10      A
ATOM    574  O   PRO A  78       3.614  45.748  25.692  1.00 18.30      A
ATOM    575  N   GLY A  79       5.393  46.860  26.512  1.00 15.27      A
ATOM    576  CA  GLY A  79       5.745  47.379  25.210  1.00 17.02      A
ATOM    577  C   GLY A  79       6.802  46.616  24.427  1.00 20.02      A
ATOM    578  O   GLY A  79       6.839  46.731  23.199  1.00 15.38      A
ATOM    579  N   TRP A  80       7.639  45.830  25.111  1.00 13.75      A
ATOM    580  CA  TRP A  80       8.723  45.092  24.440  1.00 14.43      A
ATOM    581  CB  TRP A  80      10.062  45.359  25.136  1.00 11.39      A
ATOM    582  CG  TRP A  80      10.549  46.780  25.071  1.00 15.13      A
ATOM    583  CD2 TRP A  80      11.672  47.329  25.767  1.00 13.37      A
ATOM    584  CE2 TRP A  80      11.823  48.666  25.332  1.00 13.52      A
ATOM    585  CE3 TRP A  80      12.573  46.817  26.716  1.00 12.51      A
ATOM    586  CD1 TRP A  80      10.068  47.779  24.271  1.00 19.04      A
ATOM    587  NE1 TRP A  80      10.831  48.919  24.418  1.00 16.58      A
ATOM    588  CZ2 TRP A  80      12.840  49.502  25.812  1.00 15.28      A
ATOM    589  CZ3 TRP A  80      13.586  47.645  27.197  1.00 13.05      A
ATOM    590  CH2 TRP A  80      13.710  48.979  26.739  1.00 16.82      A
ATOM    591  C   TRP A  80       8.560  43.580  24.349  1.00 16.83      A
ATOM    592  O   TRP A  80       9.361  42.909  23.685  1.00 16.92      A
ATOM    593  N   GLY A  81       7.562  43.031  25.033  1.00 15.56      A
ATOM    594  CA  GLY A  81       7.380  41.584  25.001  1.00 11.72      A
ATOM    595  C   GLY A  81       8.071  40.921  26.186  1.00 13.05      A
ATOM    596  O   GLY A  81       8.856  41.557  26.894  1.00  8.85      A
ATOM    597  N   LYS A  82       7.784  39.638  26.395  1.00 10.46      A
ATOM    598  CA  LYS A  82       8.374  38.882  27.499  1.00 11.96      A
ATOM    599  CB  LYS A  82       7.702  37.506  27.608  1.00 11.82      A
ATOM    600  CG  LYS A  82       6.341  37.497  28.315  1.00 12.27      A
ATOM    601  CD  LYS A  82       5.578  36.167  28.137  1.00 15.83      A
ATOM    602  CE  LYS A  82       6.296  34.971  28.782  1.00 21.44      A
ATOM    603  NZ  LYS A  82       6.571  35.179  30.234  1.00 18.30      A
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FIGURE 5 (continued)

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ATOM    604  C   LYS A  82       9.868  38.658  27.275  1.00 12.45      A
ATOM    605  O   LYS A  82      10.313  38.530  26.126  1.00 11.99      A
ATOM    606  N   LEU A  83      10.649  38.598  28.357  1.00 10.87      A
ATOM    607  CA  LEU A  83      12.057  38.305  28.161  1.00 10.47      A
ATOM    608  CB  LEU A  83      12.955  38.929  29.248  1.00 16.59      A
ATOM    609  CG  LEU A  83      13.059  38.501  30.707  1.00 13.98      A
ATOM    610  CD1 LEU A  83      13.627  37.083  30.856  1.00 13.97      A
ATOM    611  CD2 LEU A  83      14.010  39.508  31.412  1.00 12.95      A
ATOM    612  C   LEU A  83      12.191  36.790  28.142  1.00  8.84      A
ATOM    613  O   LEU A  83      11.288  36.062  28.604  1.00 12.14      A
ATOM    614  N   ILE A  84      13.294  36.330  27.567  1.00  9.04      A
ATOM    615  CA  ILE A  84      13.606  34.912  27.467  1.00  7.94      A
ATOM    616  CB  ILE A  84      13.734  34.492  25.986  1.00 11.27      A
ATOM    617  CG2 ILE A  84      14.322  33.075  25.875  1.00 15.02      A
ATOM    618  CG1 ILE A  84      12.356  34.567  25.306  1.00 13.46      A
ATOM    619  CD1 ILE A  84      12.407  34.310  23.806  1.00 10.66      A
ATOM    620  C   ILE A  84      14.957  34.682  28.151  1.00  9.44      A
ATOM    621  O   ILE A  84      15.918  35.410  27.891  1.00  9.33      A
ATOM    622  N   GLU A  85      15.018  33.686  29.023  1.00  7.70      A
ATOM    623  CA  GLU A  85      16.269  33.331  29.683  1.00  8.79      A
ATOM    624  CB  GLU A  85      16.211  33.631  31.196  1.00  7.98      A
ATOM    625  CG  GLU A  85      17.532  33.291  31.922  1.00  8.35      A
ATOM    626  CD  GLU A  85      17.472  33.466  33.442  1.00  9.44      A
ATOM    627  OE1 GLU A  85      16.520  32.969  34.103  1.00 13.35      A
ATOM    628  OE2 GLU A  85      18.408  34.077  33.998  1.00 10.18      A
ATOM    629  C   GLU A  85      16.452  31.832  29.442  1.00  9.15      A
ATOM    630  O   GLU A  85      15.614  31.047  29.870  1.00 10.73      A
ATOM    631  N   VAL A  86      17.513  31.438  28.733  1.00  9.15      A
ATOM    632  CA  VAL A  86      17.772  30.021  28.458  1.00  9.61      A
ATOM    633  CB  VAL A  86      17.394  29.631  26.987  1.00  8.48      A
ATOM    634  CG1 VAL A  86      15.866  29.641  26.795  1.00 11.82      A
ATOM    635  CG2 VAL A  86      18.062  30.587  25.998  1.00  8.25      A
ATOM    636  C   VAL A  86      19.247  29.653  28.653  1.00 12.36      A
ATOM    637  O   VAL A  86      20.135  30.490  28.488  1.00  7.65      A
ATOM    638  N   PRO A  87      19.530  28.392  29.034  1.00  7.50      A
ATOM    639  CD  PRO A  87      18.611  27.261  29.245  1.00 11.19      A
ATOM    640  CA  PRO A  87      20.927  27.986  29.213  1.00  8.03      A
ATOM    641  CB  PRO A  87      20.806  26.551  29.747  1.00 11.47      A
ATOM    642  CG  PRO A  87      19.531  26.065  29.123  1.00 18.08      A
ATOM    643  C   PRO A  87      21.551  28.031  27.803  1.00 12.05      A
ATOM    644  O   PRO A  87      20.845  27.799  26.798  1.00 11.64      A
ATOM    645  N   SER A  88      22.844  28.346  27.739  1.00 10.05      A
ATOM    646  CA  SER A  88      23.607  28.427  26.480  1.00  8.91      A
ATOM    647  CB  SER A  88      24.472  29.695  26.471  1.00  6.92      A
ATOM    648  OG  SER A  88      25.266  29.787  25.294  1.00 11.36      A
ATOM    649  C   SER A  88      24.484  27.177  26.379  1.00  7.85      A
ATOM    650  O   SER A  88      24.385  26.432  25.401  1.00  7.71      A
ATOM    651  N   VAL A  89      25.365  26.993  27.368  1.00  7.73      A
ATOM    652  CA  VAL A  89      26.218  25.802  27.481  1.00  8.66      A
ATOM    653  CB  VAL A  89      27.639  26.010  26.874  1.00  5.11      A
ATOM    654  CG1 VAL A  89      27.522  26.503  25.400  1.00  7.72      A
ATOM    655  CG2 VAL A  89      28.444  27.016  27.744  1.00  8.02      A
ATOM    656  C   VAL A  89      26.407  25.527  28.980  1.00 10.90      A
ATOM    657  O   VAL A  89      26.037  26.356  29.809  1.00  9.82      A
ATOM    658  N   ALA A  90      26.982  24.369  29.325  1.00 10.64      A
ATOM    659  CA  ALA A  90      27.242  24.059  30.722  1.00  8.29      A
ATOM    660  CB  ALA A  90      26.792  22.616  31.077  1.00  8.16      A
ATOM    661  C   ALA A  90      28.764  24.190  30.863  1.00  7.63      A
ATOM    662  O   ALA A  90      29.498  24.095  29.880  1.00  7.66      A
ATOM    663  N   THR A  91      29.233  24.345  32.091  1.00  7.77      A
ATOM    664  CA  THR A  91      30.651  24.559  32.300  1.00  9.18      A
ATOM    665  CB  THR A  91      30.945  26.074  32.165  1.00 10.09      A
ATOM    666  OG1 THR A  91      32.337  26.323  32.365  1.00 11.79      A
ATOM    667  CG2 THR A  91      30.156  26.862  33.214  1.00 11.41      A
ATOM    668  C   THR A  91      31.116  24.140  33.686  1.00 10.91      A
ATOM    669  O   THR A  91      30.326  24.055  34.614  1.00  9.96      A
ATOM    670  N   SER A  92      32.409  23.858  33.811  1.00 11.52      A
ATOM    671  CA  SER A  92      32.972  23.598  35.122  1.00  9.75      A
ATOM    672  CB  SER A  92      34.167  22.642  35.011  1.00 12.03      A
ATOM    673  OG  SER A  92      35.213  23.181  34.186  1.00 10.62      A
ATOM    674  C   SER A  92      33.490  24.962  35.601  1.00 10.73      A
ATOM    675  O   SER A  92      33.397  25.974  34.883  1.00  8.53      A
ATOM    676  N   VAL A  93      33.980  25.003  36.837  1.00  8.68      A
ATOM    677  CA  VAL A  93      34.640  26.197  37.369  1.00  7.08      A
ATOM    678  CB  VAL A  93      34.010  26.736  38.667  1.00  7.09      A
ATOM    679  CG1 VAL A  93      34.896  27.906  39.215  1.00 10.40      A
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FIGURE 5 (continued)

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ATOM    680  CG2 VAL A  93      32.592  27.269  38.376  1.00 10.45      A
ATOM    681  C   VAL A  93      36.033  25.643  37.694  1.00  9.49      A
ATOM    682  O   VAL A  93      36.162  24.745  38.527  1.00 12.26      A
ATOM    683  N   ALA A  94      37.064  26.148  37.025  1.00  8.00      A
ATOM    684  CA  ALA A  94      38.425  25.645  37.236  1.00  8.64      A
ATOM    685  CB  ALA A  94      39.204  25.722  35.921  1.00  7.88      A
ATOM    686  C   ALA A  94      39.197  26.374  38.329  1.00  7.97      A
ATOM    687  O   ALA A  94      38.906  27.530  38.625  1.00  8.61      A
ATOM    688  N   ILE A  95      40.210  25.709  38.894  1.00  5.77      A
ATOM    689  CA  ILE A  95      41.016  26.290  39.963  1.00  7.30      A
ATOM    690  CB  ILE A  95      40.870  25.486  41.307  1.00  9.66      A
ATOM    691  CG2 ILE A  95      41.522  26.261  42.465  1.00  6.29      A
ATOM    692  CG1 ILE A  95      39.401  25.218  41.641  1.00 10.13      A
ATOM    693  CD1 ILE A  95      38.566  26.491  41.909  1.00 13.60      A
ATOM    694  C   ILE A  95      42.496  26.263  39.572  1.00  8.10      A
ATOM    695  O   ILE A  95      43.261  25.373  40.001  1.00 10.23      A
ATOM    696  N   PRO A  96      42.923  27.216  38.742  1.00  6.65      A
ATOM    697  CD  PRO A  96      42.133  28.263  38.063  1.00  6.16      A
ATOM    698  CA  PRO A  96      44.330  27.265  38.326  1.00  7.43      A
ATOM    699  CB  PRO A  96      44.275  28.107  37.054  1.00  9.06      A
ATOM    700  CG  PRO A  96      43.207  29.147  37.446  1.00  8.84      A
ATOM    701  C   PRO A  96      45.133  27.938  39.434  1.00 10.94      A
ATOM    702  O   PRO A  96      44.574  28.645  40.277  1.00  8.21      A
ATOM    703  N   PHE A  97      46.441  27.715  39.447  1.00  9.05      A
ATOM    704  CA  PHE A  97      47.276  28.302  40.480  1.00  8.97      A
ATOM    705  CB  PHE A  97      47.259  27.414  41.732  1.00 10.70      A
ATOM    706  CG  PHE A  97      47.748  26.015  41.477  1.00  9.86      A
ATOM    707  CD1 PHE A  97      49.114  25.720  41.524  1.00 10.13      A
ATOM    708  CD2 PHE A  97      46.862  25.010  41.121  1.00  7.97      A
ATOM    709  CE1 PHE A  97      49.589  24.436  41.211  1.00  9.97      A
ATOM    710  CE2 PHE A  97      47.326  23.704  40.802  1.00  8.94      A
ATOM    711  CZ  PHE A  97      48.709  23.433  40.852  1.00  7.63      A
ATOM    712  C   PHE A  97      48.698  28.418  39.949  1.00  9.55      A
ATOM    713  O   PHE A  97      49.054  27.761  38.962  1.00  9.51      A
ATOM    714  N   ARG A  98      49.498  29.260  40.597  1.00  8.26      A
ATOM    715  CA  ARG A  98      50.900  29.457  40.205  1.00 11.26      A
ATOM    716  CB  ARG A  98      51.149  30.927  39.808  1.00 13.41      A
ATOM    717  CG  ARG A  98      52.624  31.218  39.452  1.00 12.41      A
ATOM    718  CD  ARG A  98      52.902  32.648  39.002  1.00 15.00      A
ATOM    719  NE  ARG A  98      54.350  32.871  38.907  1.00 20.95      A
ATOM    720  CZ  ARG A  98      55.048  33.714  39.670  1.00 19.61      A
ATOM    721  NH1 ARG A  98      54.454  34.446  40.606  1.00 16.05      A
ATOM    722  NH2 ARG A  98      56.361  33.824  39.500  1.00 22.95      A
ATOM    723  C   ARG A  98      51.765  29.079  41.415  1.00  9.82      A
ATOM    724  O   ARG A  98      51.955  29.881  42.327  1.00 12.72      A
ATOM    725  N   LYS A  99      52.258  27.838  41.417  1.00 13.72      A
ATOM    726  CA  LYS A  99      53.081  27.314  42.510  1.00 14.88      A
ATOM    727  CB  LYS A  99      52.179  26.922  43.688  1.00 10.80      A
ATOM    728  CG  LYS A  99      52.899  26.401  44.919  1.00  8.32      A
ATOM    729  CD  LYS A  99      53.744  27.518  45.557  1.00 10.62      A
ATOM    730  CE  LYS A  99      54.525  27.007  46.790  1.00 10.76      A
ATOM    731  NZ  LYS A  99      55.346  28.125  47.368  1.00 13.56      A
ATOM    732  C   LYS A  99      53.809  26.095  41.956  1.00 14.43      A
ATOM    733  O   LYS A  99      53.200  25.056  41.701  1.00 15.34      A
ATOM    734  N   ALA A 100      55.120  26.226  41.769  1.00 12.67      A
ATOM    735  CA  ALA A 100      55.911  25.143  41.202  1.00 14.53      A
ATOM    736  CB  ALA A 100      57.354  25.629  40.914  1.00 14.12      A
ATOM    737  C   ALA A 100      55.960  23.900  42.072  1.00 14.42      A
ATOM    738  O   ALA A 100      55.929  23.987  43.303  1.00 16.53      A
ATOM    739  N   GLY A 101      56.061  22.751  41.409  1.00 10.16      A
ATOM    740  CA  GLY A 101      56.133  21.476  42.096  1.00 11.78      A
ATOM    741  C   GLY A 101      55.786  20.360  41.136  1.00 17.78      A
ATOM    742  O   GLY A 101      54.853  20.479  40.338  1.00 14.78      A
ATOM    743  N   GLY A 102      56.543  19.274  41.195  1.00 13.81      A
ATOM    744  CA  GLY A 102      56.273  18.156  40.313  1.00 20.81      A
ATOM    745  C   GLY A 102      55.051  17.348  40.720  1.00 16.58      A
ATOM    746  O   GLY A 102      54.498  16.627  39.898  1.00 16.24      A
ATOM    747  N   ASN A 103      54.624  17.451  41.976  1.00 17.72      A
ATOM    748  CA  ASN A 103      53.465  16.675  42.434  1.00 16.85      A
ATOM    749  CB  ASN A 103      53.372  16.694  43.963  1.00 15.22      A
ATOM    750  CG  ASN A 103      54.365  15.760  44.615  1.00 23.02      A
ATOM    751  OD1 ASN A 103      55.279  15.249  43.955  1.00 19.32      A
ATOM    752  ND2 ASN A 103      54.205  15.535  45.916  1.00 15.75      A
ATOM    753  C   ASN A 103      52.145  17.197  41.885  1.00 15.38      A
ATOM    754  O   ASN A 103      51.991  18.390  41.666  1.00 11.02      A
ATOM    755  N   ALA A 104      51.183  16.306  41.693  1.00 16.02      A
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FIGURE 5 (continued)

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ATOM    756  CA  ALA A 104      49.880  16.744  41.219  1.00 16.65      A
ATOM    757  CB  ALA A 104      49.068  15.538  40.741  1.00 20.27      A
ATOM    758  C   ALA A 104      49.170  17.427  42.395  1.00 15.98      A
ATOM    759  O   ALA A 104      49.298  16.986  43.531  1.00 15.25      A
ATOM    760  N   VAL A 105      48.470  18.530  42.127  1.00 13.62      A
ATOM    761  CA  VAL A 105      47.701  19.227  43.157  1.00 13.77      A
ATOM    762  CB  VAL A 105      47.708  20.756  42.945  1.00 15.80      A
ATOM    763  CG1 VAL A 105      46.645  21.409  43.814  1.00 16.24      A
ATOM    764  CG2 VAL A 105      49.081  21.310  43.295  1.00 15.48      A
ATOM    765  C   VAL A 105      46.273  18.699  43.026  1.00 13.93      A
ATOM    766  O   VAL A 105      45.634  18.867  41.982  1.00 11.00      A
ATOM    767  N   ASP A 106      45.781  18.059  44.085  1.00 11.30      A
ATOM    768  CA  ASP A 106      44.446  17.447  44.087  1.00 13.33      A
ATOM    769  CB  ASP A 106      44.594  15.914  44.007  1.00 15.23      A
ATOM    770  CG  ASP A 106      43.266  15.181  43.763  1.00 18.75      A
ATOM    771  OD1 ASP A 106      43.294  13.932  43.636  1.00 20.08      A
ATOM    772  OD2 ASP A 106      42.201  15.832  43.705  1.00 16.37      A
ATOM    773  C   ASP A 106      43.748  17.854  45.371  1.00 13.44      A
ATOM    774  O   ASP A 106      44.013  17.312  46.441  1.00 12.47      A
ATOM    775  N   LEU A 107      42.838  18.809  45.256  1.00 12.47      A
ATOM    776  CA  LEU A 107      42.126  19.322  46.424  1.00 10.60      A
ATOM    777  CB  LEU A 107      41.608  20.743  46.139  1.00  9.94      A
ATOM    778  CG  LEU A 107      42.656  21.830  45.874  1.00 15.11      A
ATOM    779  CD1 LEU A 107      41.992  23.049  45.233  1.00 12.77      A
ATOM    780  CD2 LEU A 107      43.332  22.222  47.191  1.00 15.50      A
ATOM    781  C   LEU A 107      40.936  18.504  46.860  1.00 11.58      A
ATOM    782  O   LEU A 107      40.118  18.134  46.029  1.00 11.26      A
ATOM    783  N   SER A 108      40.840  18.205  48.157  1.00 10.03      A
ATOM    784  CA  SER A 108      39.632  17.555  48.632  1.00  9.49      A
ATOM    785  CB  SER A 108      39.823  16.938  50.026  1.00 11.45      A
ATOM    786  OG  SER A 108      40.112  17.944  50.988  1.00 10.62      A
ATOM    787  C   SER A 108      38.686  18.762  48.734  1.00 13.88      A
ATOM    788  O   SER A 108      39.137  19.909  48.733  1.00  9.31      A
ATOM    789  N   VAL A 109      37.384  18.528  48.795  1.00 11.62      A
ATOM    790  CA  VAL A 109      36.456  19.648  48.915  1.00 12.52      A
ATOM    791  CB  VAL A 109      34.997  19.149  48.822  1.00 14.25      A
ATOM    792  CG1 VAL A 109      34.022  20.273  49.172  1.00 10.43      A
ATOM    793  CG2 VAL A 109      34.738  18.624  47.385  1.00  9.95      A
ATOM    794  C   VAL A 109      36.705  20.397  50.228  1.00  8.60      A
ATOM    795  O   VAL A 109      36.646  21.622  50.265  1.00  9.21      A
ATOM    796  N   LYS A 110      36.995  19.666  51.301  1.00  9.28      A
ATOM    797  CA  LYS A 110      37.307  20.306  52.593  1.00  7.04      A
ATOM    798  CB  LYS A 110      37.597  19.237  53.650  1.00  7.60      A
ATOM    799  CG  LYS A 110      38.038  19.793  55.030  1.00  9.51      A
ATOM    800  CD  LYS A 110      36.987  20.726  55.655  1.00  7.71      A
ATOM    801  CE  LYS A 110      37.436  21.170  57.033  1.00 15.09      A
ATOM    802  NZ  LYS A 110      36.482  22.129  57.688  1.00 11.10      A
ATOM    803  C   LYS A 110      38.532  21.234  52.452  1.00  8.55      A
ATOM    804  O   LYS A 110      38.588  22.313  53.040  1.00  9.65      A
ATOM    805  N   GLU A 111      39.530  20.803  51.696  1.00  8.56      A
ATOM    806  CA  GLU A 111      40.711  21.640  51.495  1.00 11.39      A
ATOM    807  CB  GLU A 111      41.817  20.836  50.800  1.00 13.45      A
ATOM    808  CG  GLU A 111      42.582  19.940  51.784  1.00 15.25      A
ATOM    809  CD  GLU A 111      43.527  18.960  51.098  1.00 16.99      A
ATOM    810  OE1 GLU A 111      44.310  18.296  51.808  1.00 12.70      A
ATOM    811  OE2 GLU A 111      43.477  18.851  49.860  1.00 13.80      A
ATOM    812  C   GLU A 111      40.342  22.881  50.663  1.00 12.16      A
ATOM    813  O   GLU A 111      40.751  23.998  50.983  1.00  8.45      A
ATOM    814  N   LEU A 112      39.586  22.680  49.587  1.00 11.50      A
ATOM    815  CA  LEU A 112      39.157  23.802  48.753  1.00 11.60      A
ATOM    816  CB  LEU A 112      38.127  23.339  47.728  1.00 12.29      A
ATOM    817  CG  LEU A 112      37.520  24.486  46.906  1.00 13.68      A
ATOM    818  CD1 LEU A 112      38.486  24.835  45.793  1.00 14.87      A
ATOM    819  CD2 LEU A 112      36.183  24.067  46.307  1.00 23.81      A
ATOM    820  C   LEU A 112      38.491  24.845  49.648  1.00 11.64      A
ATOM    821  O   LEU A 112      38.782  26.036  49.569  1.00  9.35      A
ATOM    822  N   CYS A 113      37.598  24.370  50.511  1.00  9.13      A
ATOM    823  CA  CYS A 113      36.869  25.251  51.407  1.00 10.02      A
ATOM    824  C   CYS A 113      37.806  26.040  52.332  1.00 10.42      A
ATOM    825  O   CYS A 113      37.620  27.243  52.550  1.00  9.94      A
ATOM    826  CB  CYS A 113      35.881  24.414  52.215  1.00  7.06      A
ATOM    827  SG  CYS A 113      34.495  23.714  51.225  1.00 12.97      A
ATOM    828  N   GLY A 114      38.815  25.357  52.854  1.00  8.53      A
ATOM    829  CA  GLY A 114      39.774  25.979  53.746  1.00  8.15      A
ATOM    830  C   GLY A 114      40.615  27.023  53.048  1.00  8.58      A
ATOM    831  O   GLY A 114      40.974  28.045  53.660  1.00  9.42      A
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FIGURE 5 (continued)

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ATOM    832  N   VAL A 115      40.929  26.780  51.773  1.00  8.91      A
ATOM    833  CA  VAL A 115      41.724  27.727  51.001  1.00 11.99      A
ATOM    834  CB  VAL A 115      42.142  27.154  49.611  1.00 10.97      A
ATOM    835  CG1 VAL A 115      42.754  28.274  48.736  1.00 12.08      A
ATOM    836  CG2 VAL A 115      43.175  26.034  49.794  1.00  9.96      A
ATOM    837  C   VAL A 115      40.933  28.999  50.769  1.00 10.50      A
ATOM    838  O   VAL A 115      41.450  30.107  50.958  1.00 10.53      A
ATOM    839  N   PHE A 116      39.672  28.856  50.383  1.00 10.04      A
ATOM    840  CA  PHE A 116      38.885  30.046  50.123  1.00 12.53      A
ATOM    841  CB  PHE A 116      37.891  29.774  49.000  1.00  8.51      A
ATOM    842  CG  PHE A 116      38.564  29.656  47.664  1.00  8.77      A
ATOM    843  CD1 PHE A 116      39.041  28.429  47.220  1.00  7.52      A
ATOM    844  CD2 PHE A 116      38.792  30.791  46.892  1.00 10.79      A
ATOM    845  CE1 PHE A 116      39.742  28.319  46.019  1.00 11.26      A
ATOM    846  CE2 PHE A 116      39.494  30.708  45.682  1.00 12.98      A
ATOM    847  CZ  PHE A 116      39.971  29.463  45.244  1.00 12.19      A
ATOM    848  C   PHE A 116      38.236  30.713  51.319  1.00 11.72      A
ATOM    849  O   PHE A 116      37.688  31.802  51.180  1.00 10.01      A
ATOM    850  N   SER A 117      38.323  30.077  52.493  1.00  7.36      A
ATOM    851  CA  SER A 117      37.802  30.669  53.722  1.00 12.12      A
ATOM    852  CB  SER A 117      37.217  29.605  54.654  1.00 11.41      A
ATOM    853  OG  SER A 117      38.251  28.827  55.231  1.00 12.73      A
ATOM    854  C   SER A 117      38.935  31.372  54.474  1.00 12.93      A
ATOM    855  O   SER A 117      38.693  32.241  55.316  1.00  9.90      A
ATOM    856  N   GLY A 118      40.169  30.988  54.174  1.00 14.10      A
ATOM    857  CA  GLY A 118      41.312  31.576  54.860  1.00 13.07      A
ATOM    858  C   GLY A 118      41.850  30.640  55.931  1.00 15.32      A
ATOM    859  O   GLY A 118      42.935  30.873  56.484  1.00 15.65      A
ATOM    860  N   ARG A 119      41.107  29.575  56.241  1.00 15.32      A
ATOM    861  CA  ARG A 119      41.550  28.622  57.266  1.00 15.10      A
ATOM    862  CB  ARG A 119      40.503  27.518  57.485  1.00 17.52      A
ATOM    863  CG  ARG A 119      40.986  26.359  58.390  1.00 19.04      A
ATOM    864  CD  ARG A 119      39.880  25.325  58.628  1.00 17.23      A
ATOM    865  NE  ARG A 119      39.338  24.771  57.377  1.00 11.41      A
ATOM    866  CZ  ARG A 119      39.828  23.717  56.727  1.00 13.77      A
ATOM    867  NH1 ARG A 119      40.895  23.061  57.188  1.00  9.19      A
ATOM    868  NH2 ARG A 119      39.239  23.317  55.607  1.00 10.56      A
ATOM    869  C   ARG A 119      42.896  27.990  56.896  1.00 14.09      A
ATOM    870  O   ARG A 119      43.749  27.784  57.757  1.00 12.49      A
ATOM    871  N   ILE A 120      43.074  27.672  55.620  1.00 14.25      A
ATOM    872  CA  ILE A 120      44.327  27.088  55.134  1.00 11.87      A
ATOM    873  CB  ILE A 120      44.066  25.956  54.113  1.00 13.86      A
ATOM    874  CG2 ILE A 120      45.373  25.443  53.529  1.00 12.88      A
ATOM    875  CG1 ILE A 120      43.349  24.796  54.812  1.00 12.97      A
ATOM    876  CD1 ILE A 120      42.920  23.638  53.863  1.00 12.93      A
ATOM    877  C   ILE A 120      45.042  28.241  54.445  1.00 16.50      A
ATOM    878  O   ILE A 120      44.606  28.704  53.391  1.00 15.43      A
ATOM    879  N   ALA A 121      46.131  28.706  55.051  1.00 15.30      A
ATOM    880  CA  ALA A 121      46.884  29.848  54.529  1.00 14.70      A
ATOM    881  CB  ALA A 121      47.111  30.850  55.640  1.00 21.39      A
ATOM    882  C   ALA A 121      48.211  29.482  53.904  1.00 15.45      A
ATOM    883  O   ALA A 121      48.868  30.329  53.284  1.00 16.44      A
ATOM    884  N   ASN A 122      48.608  28.227  54.056  1.00 12.07      A
ATOM    885  CA  ASN A 122      49.887  27.789  53.507  1.00 12.53      A
ATOM    886  CB  ASN A 122      50.853  27.467  54.660  1.00 13.64      A
ATOM    887  CG  ASN A 122      52.279  27.293  54.188  1.00 16.68      A
ATOM    888  OD1 ASN A 122      52.666  26.224  53.725  1.00 18.01      A
ATOM    889  ND2 ASN A 122      53.063  28.363  54.279  1.00 14.68      A
ATOM    890  C   ASN A 122      49.681  26.568  52.608  1.00 11.32      A
ATOM    891  O   ASN A 122      48.809  25.737  52.865  1.00 11.94      A
ATOM    892  N   TRP A 123      50.454  26.499  51.528  1.00 12.38      A
ATOM    893  CA  TRP A 123      50.365  25.390  50.580  1.00 10.94      A
ATOM    894  CB  TRP A 123      51.330  25.597  49.406  1.00 10.33      A
ATOM    895  CG  TRP A 123      50.761  26.503  48.337  1.00 12.83      A
ATOM    896  CD2 TRP A 123      49.900  26.108  47.261  1.00 10.58      A
ATOM    897  CE2 TRP A 123      49.568  27.279  46.533  1.00 12.26      A
ATOM    898  CE3 TRP A 123      49.381  24.884  46.841  1.00 12.52      A
ATOM    899  CD1 TRP A 123      50.916  27.862  48.227  1.00 15.24      A
ATOM    900  NE1 TRP A 123      50.198  28.334  47.140  1.00 12.70      A
ATOM    901  CZ2 TRP A 123      48.732  27.256  45.403  1.00 10.92      A
ATOM    902  CZ3 TRP A 123      48.547  24.863  45.710  1.00 16.36      A
ATOM    903  CH2 TRP A 123      48.237  26.043  45.012  1.00  9.72      A
ATOM    904  C   TRP A 123      50.661  24.045  51.213  1.00 13.55      A
ATOM    905  O   TRP A 123      50.284  23.006  50.676  1.00 13.98      A
ATOM    906  N   SER A 124      51.346  24.054  52.349  1.00 13.10      A
ATOM    907  CA  SER A 124      51.654  22.801  53.010  1.00 11.36      A
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FIGURE 5 (continued)

ATOM	908	CB	SER	A	124	52.670	23.038	54.135	1.00	11.89	A
ATOM	909	OG	SER	A	124	52.130	23.884	55.132	1.00	14.19	A
ATOM	910	C	SER	A	124	50.361	22.161	53.564	1.00	17.25	A
ATOM	911	O	SER	A	124	50.354	20.974	53.924	1.00	13.81	A
ATOM	912	N	GLY	A	125	49.273	22.937	53.617	1.00	13.73	A
ATOM	913	CA	GLY	A	125	47.999	22.416	54.117	1.00	13.26	A
ATOM	914	C	GLY	A	125	47.216	21.569	53.101	1.00	19.05	A
ATOM	915	O	GLY	A	125	46.116	21.066	53.404	1.00	15.82	A
ATOM	916	N	ILE	A	126	47.759	21.413	51.892	1.00	11.57	A
ATOM	917	CA	ILE	A	126	47.111	20.590	50.866	1.00	13.57	A
ATOM	918	CB	ILE	A	126	47.116	21.338	49.499	1.00	10.65	A
ATOM	919	CG2	ILE	A	126	46.584	20.440	48.369	1.00	10.73	A
ATOM	920	CG1	ILE	A	126	46.244	22.598	49.639	1.00	14.04	A
ATOM	921	CD1	ILE	A	126	46.355	23.571	48.474	1.00	21.47	A
ATOM	922	C	ILE	A	126	47.886	19.270	50.794	1.00	14.42	A
ATOM	923	O	ILE	A	126	49.012	19.228	50.299	1.00	12.48	A
ATOM	924	N	THR	A	127	47.287	18.199	51.310	1.00	14.33	A
ATOM	925	CA	THR	A	127	47.974	16.918	51.341	1.00	15.70	A
ATOM	926	CB	THR	A	127	47.144	15.848	52.079	1.00	20.78	A
ATOM	927	OG1	THR	A	127	45.978	15.519	51.309	1.00	21.71	A
ATOM	928	CG2	THR	A	127	46.719	16.379	53.462	1.00	19.06	A
ATOM	929	C	THR	A	127	48.389	16.389	49.978	1.00	15.85	A
ATOM	930	O	THR	A	127	47.628	16.442	49.011	1.00	15.48	A
ATOM	931	N	GLY	A	128	49.627	15.907	49.925	1.00	11.25	A
ATOM	932	CA	GLY	A	128	50.202	15.348	48.719	1.00	13.92	A
ATOM	933	C	GLY	A	128	50.726	16.299	47.655	1.00	15.93	A
ATOM	934	O	GLY	A	128	51.360	15.837	46.718	1.00	18.28	A
ATOM	935	N	ALA	A	129	50.491	17.610	47.788	1.00	13.36	A
ATOM	936	CA	ALA	A	129	50.929	18.558	46.765	1.00	14.53	A
ATOM	937	CB	ALA	A	129	50.138	19.873	46.886	1.00	13.51	A
ATOM	938	C	ALA	A	129	52.428	18.856	46.777	1.00	20.08	A
ATOM	939	O	ALA	A	129	52.954	19.427	45.811	1.00	13.92	A
ATOM	940	N	GLY	A	130	53.110	18.489	47.863	1.00	15.72	A
ATOM	941	CA	GLY	A	130	54.552	18.715	47.931	1.00	18.22	A
ATOM	942	C	GLY	A	130	54.937	20.167	47.720	1.00	17.01	A
ATOM	943	O	GLY	A	130	55.944	20.485	47.088	1.00	16.95	A
ATOM	944	N	ARG	A	131	54.130	21.059	48.274	1.00	14.88	A
ATOM	945	CA	ARG	A	131	54.361	22.500	48.142	1.00	14.67	A
ATOM	946	CB	ARG	A	131	53.312	23.102	47.190	1.00	10.65	A
ATOM	947	CG	ARG	A	131	53.506	22.713	45.730	1.00	14.78	A
ATOM	948	CD	ARG	A	131	52.234	22.985	44.895	1.00	13.27	A
ATOM	949	NE	ARG	A	131	52.479	22.959	43.441	1.00	13.40	A
ATOM	950	CZ	ARG	A	131	52.670	21.873	42.695	1.00	12.12	A
ATOM	951	NH1	ARG	A	131	52.880	22.010	41.383	1.00	12.83	A
ATOM	952	NH2	ARG	A	131	52.656	20.660	43.233	1.00	13.76	A
ATOM	953	C	ARG	A	131	54.217	23.171	49.502	1.00	14.12	A
ATOM	954	O	ARG	A	131	53.451	22.703	50.329	1.00	15.12	A
ATOM	955	N	SER	A	132	54.948	24.258	49.730	1.00	12.39	A
ATOM	956	CA	SER	A	132	54.830	24.987	50.990	1.00	15.94	A
ATOM	957	CB	SER	A	132	55.817	24.450	52.046	1.00	22.25	A
ATOM	958	OG	SER	A	132	57.143	24.690	51.644	1.00	25.99	A
ATOM	959	C	SER	A	132	55.070	26.468	50.735	1.00	12.92	A
ATOM	960	O	SER	A	132	55.695	26.857	49.746	1.00	16.84	A
ATOM	961	N	GLY	A	133	54.570	27.300	51.634	1.00	14.33	A
ATOM	962	CA	GLY	A	133	54.695	28.734	51.442	1.00	14.73	A
ATOM	963	C	GLY	A	133	53.295	29.318	51.394	1.00	14.56	A
ATOM	964	O	GLY	A	133	52.320	28.589	51.183	1.00	12.31	A
ATOM	965	N	PRO	A	134	53.162	30.633	51.561	1.00	15.09	A
ATOM	966	CD	PRO	A	134	54.254	31.607	51.743	1.00	16.35	A
ATOM	967	CA	PRO	A	134	51.854	31.291	51.548	1.00	14.55	A
ATOM	968	CB	PRO	A	134	52.196	32.760	51.828	1.00	20.54	A
ATOM	969	CG	PRO	A	134	53.623	32.900	51.266	1.00	21.58	A
ATOM	970	C	PRO	A	134	50.997	31.143	50.299	1.00	16.29	A
ATOM	971	O	PRO	A	134	51.509	31.105	49.180	1.00	12.69	A
ATOM	972	N	ILE	A	135	49.685	31.057	50.527	1.00	13.39	A
ATOM	973	CA	ILE	A	135	48.688	30.973	49.454	1.00	13.74	A
ATOM	974	CB	ILE	A	135	47.523	30.010	49.801	1.00	15.95	A
ATOM	975	CG2	ILE	A	135	46.417	30.115	48.727	1.00	13.97	A
ATOM	976	CG1	ILE	A	135	48.032	28.582	49.918	1.00	15.73	A
ATOM	977	CD1	ILE	A	135	46.988	27.607	50.453	1.00	15.61	A
ATOM	978	C	ILE	A	135	48.077	32.366	49.353	1.00	13.04	A
ATOM	979	O	ILE	A	135	47.757	32.983	50.372	1.00	15.69	A
ATOM	980	N	GLN	A	136	47.918	32.872	48.136	1.00	11.91	A
ATOM	981	CA	GLN	A	136	47.319	34.190	47.958	1.00	11.20	A
ATOM	982	CB	GLN	A	136	48.317	35.145	47.306	1.00	12.71	A
ATOM	983	CG	GLN	A	136	47.892	36.594	47.337	1.00	19.42	A

FIGURE 5 (continued)

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ATOM    984  CD  GLN A 136      48.999  37.566  46.905  1.00 23.10      A
ATOM    985  OE1 GLN A 136      49.620  37.403  45.858  1.00 23.52      A
ATOM    986  NE2 GLN A 136      49.233  38.585  47.714  1.00 30.84      A
ATOM    987  C   GLN A 136      46.105  34.023  47.053  1.00  9.51      A
ATOM    988  O   GLN A 136      46.254  33.639  45.921  1.00  9.81      A
ATOM    989  N   VAL A 137      44.911  34.303  47.552  1.00  8.18      A
ATOM    990  CA  VAL A 137      43.717  34.161  46.733  1.00  4.96      A
ATOM    991  CB  VAL A 137      42.470  33.907  47.657  1.00  8.36      A
ATOM    992  CG1 VAL A 137      41.176  34.014  46.855  1.00  5.20      A
ATOM    993  CG2 VAL A 137      42.589  32.543  48.294  1.00 10.61      A
ATOM    994  C   VAL A 137      43.442  35.380  45.837  1.00  9.91      A
ATOM    995  O   VAL A 137      43.555  36.534  46.284  1.00  9.14      A
ATOM    996  N   VAL A 138      43.124  35.114  44.566  1.00  7.01      A
ATOM    997  CA  VAL A 138      42.735  36.134  43.600  1.00  8.67      A
ATOM    998  CB  VAL A 138      43.437  35.976  42.226  1.00  9.91      A
ATOM    999  CG1 VAL A 138      42.983  37.092  41.301  1.00 11.71      A
ATOM   1000  CG2 VAL A 138      44.947  36.068  42.394  1.00 18.67      A
ATOM   1001  C   VAL A 138      41.237  35.914  43.386  1.00  7.40      A
ATOM   1002  O   VAL A 138      40.791  34.775  43.196  1.00  7.75      A
ATOM   1003  N   TYR A 139      40.452  36.987  43.435  1.00  9.87      A
ATOM   1004  CA  TYR A 139      39.009  36.871  43.256  1.00  9.42      A
ATOM   1005  CB  TYR A 139      38.303  36.902  44.625  1.00  8.26      A
ATOM   1006  CG  TYR A 139      38.509  38.192  45.389  1.00  9.37      A
ATOM   1007  CD1 TYR A 139      37.570  39.211  45.322  1.00  8.61      A
ATOM   1008  CE1 TYR A 139      37.748  40.424  46.013  1.00  9.72      A
ATOM   1009  CD2 TYR A 139      39.659  38.397  46.177  1.00  9.71      A
ATOM   1010  CE2 TYR A 139      39.853  39.616  46.878  1.00 12.90      A
ATOM   1011  CZ  TYR A 139      38.890  40.623  46.786  1.00 15.66      A
ATOM   1012  OH  TYR A 139      39.045  41.829  47.459  1.00  8.23      A
ATOM   1013  C   TYR A 139      38.507  38.006  42.381  1.00  8.45      A
ATOM   1014  O   TYR A 139      39.246  38.947  42.099  1.00  8.15      A
ATOM   1015  N   ARG A 140      37.259  37.899  41.935  1.00  8.93      A
ATOM   1016  CA  ARG A 140      36.660  38.903  41.070  1.00  7.41      A
ATOM   1017  CB  ARG A 140      35.514  38.296  40.243  1.00 10.32      A
ATOM   1018  CG  ARG A 140      35.991  37.317  39.148  1.00  5.86      A
ATOM   1019  CD  ARG A 140      36.556  38.103  37.948  1.00  5.80      A
ATOM   1020  NE  ARG A 140      35.502  38.821  37.218  1.00  7.23      A
ATOM   1021  CZ  ARG A 140      34.659  38.232  36.376  1.00 11.87      A
ATOM   1022  NH1 ARG A 140      34.748  36.918  36.152  1.00  5.93      A
ATOM   1023  NH2 ARG A 140      33.715  38.952  35.769  1.00  8.31      A
ATOM   1024  C   ARG A 140      36.129  40.063  41.895  1.00  8.44      A
ATOM   1025  O   ARG A 140      35.327  39.896  42.832  1.00  8.91      A
ATOM   1026  N   ALA A 141      36.583  41.242  41.523  1.00  8.44      A
ATOM   1027  CA  ALA A 141      36.198  42.471  42.206  1.00  8.99      A
ATOM   1028  CB  ALA A 141      37.121  43.579  41.761  1.00 12.40      A
ATOM   1029  C   ALA A 141      34.748  42.895  41.975  1.00 11.15      A
ATOM   1030  O   ALA A 141      34.091  43.421  42.878  1.00  9.17      A
ATOM   1031  N   GLU A 142      34.258  42.679  40.765  1.00 10.41      A
ATOM   1032  CA  GLU A 142      32.912  43.110  40.401  1.00 11.28      A
ATOM   1033  CB  GLU A 142      32.944  43.735  38.995  1.00 11.17      A
ATOM   1034  CG  GLU A 142      32.968  42.720  37.800  1.00 16.02      A
ATOM   1035  CD  GLU A 142      34.319  41.984  37.551  1.00 14.71      A
ATOM   1036  OE1 GLU A 142      35.102  41.758  38.492  1.00 20.26      A
ATOM   1037  OE2 GLU A 142      34.582  41.608  36.382  1.00 15.07      A
ATOM   1038  C   GLU A 142      31.854  42.001  40.428  1.00 15.45      A
ATOM   1039  O   GLU A 142      32.160  40.827  40.689  1.00 11.17      A
ATOM   1040  N   VAL A 143      30.604  42.399  40.170  1.00 13.82      A
ATOM   1041  CA  VAL A 143      29.474  41.461  40.114  1.00 12.65      A
ATOM   1042  CB  VAL A 143      28.155  42.192  39.792  1.00 12.26      A
ATOM   1043  CG1 VAL A 143      27.052  41.196  39.668  1.00 17.81      A
ATOM   1044  CG2 VAL A 143      27.822  43.174  40.870  1.00 18.80      A
ATOM   1045  C   VAL A 143      29.770  40.456  38.996  1.00 12.06      A
ATOM   1046  O   VAL A 143      29.785  40.814  37.811  1.00 10.75      A
ATOM   1047  N   SER A 144      29.972  39.198  39.388  1.00 10.21      A
ATOM   1048  CA  SER A 144      30.352  38.119  38.462  1.00  6.60      A
ATOM   1049  CB  SER A 144      31.822  37.764  38.758  1.00  8.21      A
ATOM   1050  OG  SER A 144      32.188  36.468  38.328  1.00  8.64      A
ATOM   1051  C   SER A 144      29.499  36.834  38.512  1.00  7.57      A
ATOM   1052  O   SER A 144      29.166  36.346  39.601  1.00  8.05      A
ATOM   1053  N   GLY A 145      29.168  36.303  37.330  1.00  5.34      A
ATOM   1054  CA  GLY A 145      28.437  35.047  37.226  1.00  7.72      A
ATOM   1055  C   GLY A 145      29.335  33.884  37.638  1.00  7.84      A
ATOM   1056  O   GLY A 145      28.873  32.870  38.197  1.00  6.69      A
ATOM   1057  N   THR A 146      30.628  34.001  37.357  1.00  6.57      A
ATOM   1058  CA  THR A 146      31.574  32.953  37.758  1.00  6.39      A
ATOM   1059  CB  THR A 146      33.012  33.263  37.279  1.00  9.37      A
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FIGURE 5 (continued)

ATOM	1060	OG1	THR	A	146	33.026	33.463	35.855	1.00	8.49	A
ATOM	1061	CG2	THR	A	146	33.928	32.087	37.613	1.00	11.25	A
ATOM	1062	C	THR	A	146	31.569	32.892	39.294	1.00	8.02	A
ATOM	1063	O	THR	A	146	31.601	31.802	39.888	1.00	8.00	A
ATOM	1064	N	THR	A	147	31.551	34.064	39.930	1.00	6.33	A
ATOM	1065	CA	THR	A	147	31.483	34.131	41.394	1.00	8.35	A
ATOM	1066	CB	THR	A	147	31.554	35.591	41.921	1.00	6.29	A
ATOM	1067	OG1	THR	A	147	32.834	36.161	41.624	1.00	7.92	A
ATOM	1068	CG2	THR	A	147	31.373	35.602	43.450	1.00	8.46	A
ATOM	1069	C	THR	A	147	30.175	33.486	41.885	1.00	5.86	A
ATOM	1070	O	THR	A	147	30.172	32.745	42.883	1.00	7.90	A
ATOM	1071	N	GLU	A	148	29.059	33.751	41.198	1.00	5.81	A
ATOM	1072	CA	GLU	A	148	27.786	33.131	41.592	1.00	5.50	A
ATOM	1073	CB	GLU	A	148	26.644	33.653	40.710	1.00	6.06	A
ATOM	1074	CG	GLU	A	148	25.284	33.004	41.058	1.00	10.99	A
ATOM	1075	CD	GLU	A	148	24.076	33.737	40.457	1.00	12.04	A
ATOM	1076	OE1	GLU	A	148	23.920	34.966	40.685	1.00	9.92	A
ATOM	1077	OE2	GLU	A	148	23.271	33.078	39.765	1.00	13.03	A
ATOM	1078	C	GLU	A	148	27.846	31.591	41.491	1.00	6.20	A
ATOM	1079	O	GLU	A	148	27.419	30.866	42.408	1.00	7.44	A
ATOM	1080	N	LEU	A	149	28.318	31.077	40.359	1.00	4.66	A
ATOM	1081	CA	LEU	A	149	28.442	29.616	40.196	1.00	6.87	A
ATOM	1082	CB	LEU	A	149	29.011	29.301	38.807	1.00	7.74	A
ATOM	1083	CG	LEU	A	149	28.105	29.569	37.591	1.00	8.75	A
ATOM	1084	CD1	LEU	A	149	28.878	29.218	36.342	1.00	10.50	A
ATOM	1085	CD2	LEU	A	149	26.804	28.721	37.678	1.00	9.52	A
ATOM	1086	C	LEU	A	149	29.376	28.980	41.254	1.00	7.07	A
ATOM	1087	O	LEU	A	149	29.127	27.865	41.754	1.00	7.65	A
ATOM	1088	N	PHE	A	150	30.473	29.670	41.568	1.00	8.71	A
ATOM	1089	CA	PHE	A	150	31.459	29.183	42.540	1.00	7.06	A
ATOM	1090	CB	PHE	A	150	32.752	30.021	42.427	1.00	6.97	A
ATOM	1091	CG	PHE	A	150	33.884	29.551	43.325	1.00	9.24	A
ATOM	1092	CD1	PHE	A	150	34.313	28.225	43.305	1.00	10.27	A
ATOM	1093	CD2	PHE	A	150	34.557	30.455	44.138	1.00	12.03	A
ATOM	1094	CE1	PHE	A	150	35.411	27.803	44.081	1.00	12.21	A
ATOM	1095	CE2	PHE	A	150	35.657	30.050	44.920	1.00	11.31	A
ATOM	1096	CZ	PHE	A	150	36.083	28.721	44.890	1.00	10.56	A
ATOM	1097	C	PHE	A	150	30.936	29.217	43.987	1.00	7.58	A
ATOM	1098	O	PHE	A	150	31.060	28.236	44.709	1.00	6.52	A
ATOM	1099	N	THR	A	151	30.350	30.334	44.409	1.00	7.57	A
ATOM	1100	CA	THR	A	151	29.836	30.437	45.770	1.00	8.97	A
ATOM	1101	CB	THR	A	151	29.548	31.938	46.193	1.00	9.78	A
ATOM	1102	OG1	THR	A	151	28.580	32.526	45.314	1.00	8.77	A
ATOM	1103	CG2	THR	A	151	30.826	32.744	46.152	1.00	7.96	A
ATOM	1104	C	THR	A	151	28.588	29.588	45.988	1.00	7.22	A
ATOM	1105	O	THR	A	151	28.274	29.245	47.131	1.00	7.49	A
ATOM	1106	N	ARG	A	152	27.873	29.229	44.916	1.00	5.13	A
ATOM	1107	CA	ARG	A	152	26.715	28.351	45.099	1.00	9.17	A
ATOM	1108	CB	ARG	A	152	25.914	28.189	43.796	1.00	9.15	A
ATOM	1109	CG	ARG	A	152	24.606	27.376	43.974	1.00	10.79	A
ATOM	1110	CD	ARG	A	152	23.671	27.529	42.755	1.00	17.61	A
ATOM	1111	NE	ARG	A	152	23.071	28.868	42.641	1.00	14.93	A
ATOM	1112	CZ	ARG	A	152	23.188	29.662	41.577	1.00	16.78	A
ATOM	1113	NH1	ARG	A	152	22.605	30.860	41.565	1.00	11.71	A
ATOM	1114	NH2	ARG	A	152	23.885	29.265	40.518	1.00	11.02	A
ATOM	1115	C	ARG	A	152	27.274	27.007	45.557	1.00	7.79	A
ATOM	1116	O	ARG	A	152	26.671	26.313	46.389	1.00	5.08	A
ATOM	1117	N	PHE	A	153	28.436	26.639	45.017	1.00	6.70	A
ATOM	1118	CA	PHE	A	153	29.101	25.395	45.413	1.00	9.70	A
ATOM	1119	CB	PHE	A	153	30.280	25.059	44.478	1.00	7.27	A
ATOM	1120	CG	PHE	A	153	30.974	23.747	44.812	1.00	6.93	A
ATOM	1121	CD1	PHE	A	153	30.451	22.532	44.389	1.00	9.41	A
ATOM	1122	CD2	PHE	A	153	32.134	23.738	45.592	1.00	9.61	A
ATOM	1123	CE1	PHE	A	153	31.069	21.315	44.747	1.00	11.43	A
ATOM	1124	CE2	PHE	A	153	32.764	22.534	45.959	1.00	13.90	A
ATOM	1125	CZ	PHE	A	153	32.229	21.323	45.537	1.00	11.19	A
ATOM	1126	C	PHE	A	153	29.640	25.503	46.842	1.00	8.50	A
ATOM	1127	O	PHE	A	153	29.455	24.586	47.638	1.00	8.41	A
ATOM	1128	N	LEU	A	154	30.320	26.599	47.167	1.00	6.84	A
ATOM	1129	CA	LEU	A	154	30.877	26.752	48.521	1.00	6.20	A
ATOM	1130	CB	LEU	A	154	31.672	28.060	48.657	1.00	6.23	A
ATOM	1131	CG	LEU	A	154	32.876	28.250	47.720	1.00	6.30	A
ATOM	1132	CD1	LEU	A	154	33.543	29.583	48.020	1.00	9.48	A
ATOM	1133	CD2	LEU	A	154	33.893	27.117	47.886	1.00	6.15	A
ATOM	1134	C	LEU	A	154	29.762	26.737	49.564	1.00	6.13	A
ATOM	1135	O	LEU	A	154	29.912	26.170	50.641	1.00	9.16	A

FIGURE 5 (continued)

ATOM	1136	N	ASN	A	155	28.652	27.376	49.233	1.00	5.19	A
ATOM	1137	CA	ASN	A	155	27.493	27.430	50.116	1.00	6.32	A
ATOM	1138	CB	ASN	A	155	26.406	28.314	49.486	1.00	11.33	A
ATOM	1139	CG	ASN	A	155	25.093	28.294	50.274	1.00	14.59	A
ATOM	1140	OD1	ASN	A	155	24.149	27.596	49.906	1.00	9.21	A
ATOM	1141	ND2	ASN	A	155	25.034	29.062	51.361	1.00	8.23	A
ATOM	1142	C	ASN	A	155	26.929	26.042	50.363	1.00	8.76	A
ATOM	1143	O	ASN	A	155	26.465	25.712	51.465	1.00	8.00	A
ATOM	1144	N	ALA	A	156	26.965	25.203	49.336	1.00	8.80	A
ATOM	1145	CA	ALA	A	156	26.418	23.867	49.493	1.00	7.63	A
ATOM	1146	CB	ALA	A	156	26.068	23.300	48.119	1.00	8.06	A
ATOM	1147	C	ALA	A	156	27.336	22.882	50.222	1.00	12.23	A
ATOM	1148	O	ALA	A	156	26.854	22.037	50.994	1.00	9.62	A
ATOM	1149	N	LYS	A	157	28.646	23.029	50.015	1.00	9.93	A
ATOM	1150	CA	LYS	A	157	29.623	22.064	50.537	1.00	10.69	A
ATOM	1151	CB	LYS	A	157	30.437	21.527	49.352	1.00	14.97	A
ATOM	1152	CG	LYS	A	157	29.604	20.877	48.227	1.00	13.56	A
ATOM	1153	CD	LYS	A	157	28.855	19.640	48.729	1.00	16.77	A
ATOM	1154	CE	LYS	A	157	28.357	18.784	47.575	1.00	22.67	A
ATOM	1155	NZ	LYS	A	157	27.652	17.546	48.069	1.00	21.73	A
ATOM	1156	C	LYS	A	157	30.611	22.438	51.638	1.00	8.73	A
ATOM	1157	O	LYS	A	157	31.215	21.552	52.245	1.00	11.63	A
ATOM	1158	N	CYS	A	158	30.821	23.725	51.876	1.00	8.12	A
ATOM	1159	CA	CYS	A	158	31.759	24.132	52.916	1.00	8.20	A
ATOM	1160	C	CYS	A	158	30.974	24.252	54.207	1.00	9.14	A
ATOM	1161	O	CYS	A	158	30.648	25.349	54.661	1.00	10.53	A
ATOM	1162	CB	CYS	A	158	32.390	25.464	52.537	1.00	10.13	A
ATOM	1163	SG	CYS	A	158	33.331	25.358	50.982	1.00	11.82	A
ATOM	1164	N	THR	A	159	30.699	23.108	54.822	1.00	8.92	A
ATOM	1165	CA	THR	A	159	29.856	23.091	56.017	1.00	6.75	A
ATOM	1166	CB	THR	A	159	28.850	21.933	55.903	1.00	10.13	A
ATOM	1167	OG1	THR	A	159	29.551	20.690	55.987	1.00	12.88	A
ATOM	1168	CG2	THR	A	159	28.146	21.989	54.527	1.00	14.84	A
ATOM	1169	C	THR	A	159	30.545	23.021	57.361	1.00	8.62	A
ATOM	1170	O	THR	A	159	29.878	22.956	58.398	1.00	7.39	A
ATOM	1171	N	THR	A	160	31.875	23.038	57.358	1.00	8.39	A
ATOM	1172	CA	THR	A	160	32.603	22.980	58.612	1.00	9.53	A
ATOM	1173	CB	THR	A	160	33.194	21.558	58.889	1.00	8.99	A
ATOM	1174	OG1	THR	A	160	34.011	21.140	57.788	1.00	12.55	A
ATOM	1175	CG2	THR	A	160	32.083	20.559	59.114	1.00	11.60	A
ATOM	1176	C	THR	A	160	33.727	24.010	58.712	1.00	10.20	A
ATOM	1177	O	THR	A	160	34.774	23.739	59.314	1.00	8.76	A
ATOM	1178	N	GLN	A	161	33.523	25.189	58.121	1.00	8.66	A
ATOM	1179	CA	GLN	A	161	34.525	26.260	58.254	1.00	9.46	A
ATOM	1180	CB	GLN	A	161	34.564	27.121	56.989	1.00	9.58	A
ATOM	1181	CG	GLN	A	161	34.956	26.309	55.742	1.00	7.83	A
ATOM	1182	CD	GLN	A	161	36.305	25.608	55.936	1.00	10.81	A
ATOM	1183	OE1	GLN	A	161	36.429	24.396	55.758	1.00	12.80	A
ATOM	1184	NE2	GLN	A	161	37.306	26.374	56.313	1.00	10.64	A
ATOM	1185	C	GLN	A	161	34.058	27.096	59.449	1.00	8.71	A
ATOM	1186	O	GLN	A	161	32.979	26.866	59.960	1.00	8.58	A
ATOM	1187	N	PRO	A	162	34.870	28.047	59.928	1.00	11.51	A
ATOM	1188	CD	PRO	A	162	36.316	28.193	59.693	1.00	10.65	A
ATOM	1189	CA	PRO	A	162	34.433	28.869	61.071	1.00	9.23	A
ATOM	1190	CB	PRO	A	162	35.631	29.780	61.326	1.00	11.89	A
ATOM	1191	CG	PRO	A	162	36.786	28.884	60.979	1.00	14.39	A
ATOM	1192	C	PRO	A	162	33.171	29.660	60.727	1.00	10.67	A
ATOM	1193	O	PRO	A	162	32.280	29.838	61.567	1.00	12.32	A
ATOM	1194	N	GLY	A	163	33.112	30.158	59.492	1.00	8.94	A
ATOM	1195	CA	GLY	A	163	31.943	30.903	59.040	1.00	11.83	A
ATOM	1196	C	GLY	A	163	31.307	30.149	57.883	1.00	11.53	A
ATOM	1197	O	GLY	A	163	31.687	28.989	57.628	1.00	9.27	A
ATOM	1198	N	THR	A	164	30.359	30.781	57.178	1.00	7.79	A
ATOM	1199	CA	THR	A	164	29.698	30.140	56.039	1.00	10.06	A
ATOM	1200	CB	THR	A	164	28.213	29.775	56.347	1.00	9.77	A
ATOM	1201	OG1	THR	A	164	27.565	30.914	56.934	1.00	12.97	A
ATOM	1202	CG2	THR	A	164	28.119	28.585	57.328	1.00	7.94	A
ATOM	1203	C	THR	A	164	29.696	31.081	54.837	1.00	10.41	A
ATOM	1204	O	THR	A	164	29.786	32.301	55.001	1.00	7.96	A
ATOM	1205	N	PHE	A	165	29.571	30.507	53.637	1.00	7.32	A
ATOM	1206	CA	PHE	A	165	29.551	31.275	52.395	1.00	9.34	A
ATOM	1207	CB	PHE	A	165	30.321	30.541	51.299	1.00	8.51	A
ATOM	1208	CG	PHE	A	165	31.799	30.451	51.539	1.00	7.69	A
ATOM	1209	CD1	PHE	A	165	32.659	31.455	51.096	1.00	8.05	A
ATOM	1210	CD2	PHE	A	165	32.338	29.338	52.181	1.00	10.52	A
ATOM	1211	CE1	PHE	A	165	34.062	31.349	51.288	1.00	6.48	A

FIGURE 5 (continued)

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ATOM   1212  CE2 PHE A 165      33.720  29.214  52.385  1.00  6.44      A
ATOM   1213  CZ  PHE A 165      34.591  30.221  51.935  1.00  7.86      A
ATOM   1214  C   PHE A 165      28.135  31.467  51.854  1.00 10.39      A
ATOM   1215  O   PHE A 165      27.428  30.485  51.648  1.00 11.83      A
ATOM   1216  N   ALA A 166      27.738  32.712  51.601  1.00  8.80      A
ATOM   1217  CA  ALA A 166      26.424  33.000  51.006  1.00 10.97      A
ATOM   1218  CB  ALA A 166      25.942  34.397  51.423  1.00 10.57      A
ATOM   1219  C   ALA A 166      26.593  32.960  49.483  1.00 10.58      A
ATOM   1220  O   ALA A 166      27.694  33.182  48.968  1.00  7.60      A
ATOM   1221  N   VAL A 167      25.516  32.668  48.766  1.00  9.26      A
ATOM   1222  CA  VAL A 167      25.572  32.658  47.303  1.00  7.71      A
ATOM   1223  CB  VAL A 167      24.384  31.924  46.686  1.00  7.77      A
ATOM   1224  CG1 VAL A 167      24.546  31.870  45.159  1.00  8.04      A
ATOM   1225  CG2 VAL A 167      24.283  30.511  47.265  1.00 10.61      A
ATOM   1226  C   VAL A 167      25.473  34.123  46.875  1.00  8.91      A
ATOM   1227  O   VAL A 167      24.523  34.816  47.244  1.00  7.79      A
ATOM   1228  N   THR A 168      26.408  34.580  46.048  1.00  8.13      A
ATOM   1229  CA  THR A 168      26.411  35.974  45.653  1.00  6.66      A
ATOM   1230  CB  THR A 168      27.060  36.810  46.769  1.00 13.46      A
ATOM   1231  OG1 THR A 168      27.129  38.188  46.370  1.00 12.35      A
ATOM   1232  CG2 THR A 168      28.478  36.311  47.040  1.00 12.28      A
ATOM   1233  C   THR A 168      27.228  36.178  44.375  1.00 11.69      A
ATOM   1234  O   THR A 168      27.960  35.282  43.947  1.00 11.22      A
ATOM   1235  N   THR A 169      27.106  37.352  43.770  1.00  9.36      A
ATOM   1236  CA  THR A 169      27.888  37.641  42.580  1.00  5.90      A
ATOM   1237  CB  THR A 169      27.074  38.484  41.565  1.00 11.79      A
ATOM   1238  OG1 THR A 169      26.724  39.739  42.169  1.00  9.77      A
ATOM   1239  CG2 THR A 169      25.811  37.747  41.128  1.00 12.13      A
ATOM   1240  C   THR A 169      29.156  38.450  42.953  1.00  9.03      A
ATOM   1241  O   THR A 169      30.000  38.712  42.099  1.00  8.64      A
ATOM   1242  N   VAL A 170      29.279  38.848  44.224  1.00 11.21      A
ATOM   1243  CA  VAL A 170      30.430  39.641  44.680  1.00 11.07      A
ATOM   1244  CB  VAL A 170      29.944  41.003  45.248  1.00  8.64      A
ATOM   1245  CG1 VAL A 170      29.433  41.863  44.106  1.00  8.12      A
ATOM   1246  CG2 VAL A 170      28.802  40.805  46.208  1.00 14.20      A
ATOM   1247  C   VAL A 170      31.158  38.830  45.741  1.00 10.94      A
ATOM   1248  O   VAL A 170      30.694  38.747  46.859  1.00 11.12      A
ATOM   1249  N   PHE A 171      32.305  38.247  45.386  1.00 11.66      A
ATOM   1250  CA  PHE A 171      33.003  37.367  46.312  1.00  9.52      A
ATOM   1251  CB  PHE A 171      34.279  36.775  45.677  1.00  8.67      A
ATOM   1252  CG  PHE A 171      34.940  35.686  46.519  1.00 10.69      A
ATOM   1253  CD1 PHE A 171      36.009  35.978  47.358  1.00  9.84      A
ATOM   1254  CD2 PHE A 171      34.457  34.377  46.502  1.00 14.44      A
ATOM   1255  CE1 PHE A 171      36.593  34.986  48.184  1.00  8.85      A
ATOM   1256  CE2 PHE A 171      35.024  33.377  47.311  1.00 12.76      A
ATOM   1257  CZ  PHE A 171      36.096  33.686  48.158  1.00 12.60      A
ATOM   1258  C   PHE A 171      33.353  37.977  47.661  1.00 12.55      A
ATOM   1259  O   PHE A 171      33.292  37.294  48.679  1.00  7.64      A
ATOM   1260  N   ALA A 172      33.704  39.257  47.677  1.00  6.57      A
ATOM   1261  CA  ALA A 172      34.088  39.865  48.946  1.00  9.02      A
ATOM   1262  CB  ALA A 172      34.655  41.279  48.721  1.00  9.26      A
ATOM   1263  C   ALA A 172      32.948  39.885  49.957  1.00 11.22      A
ATOM   1264  O   ALA A 172      33.188  40.071  51.155  1.00 10.96      A
ATOM   1265  N   ASN A 173      31.714  39.677  49.493  1.00  8.23      A
ATOM   1266  CA  ASN A 173      30.563  39.651  50.409  1.00 10.55      A
ATOM   1267  CB  ASN A 173      29.361  40.396  49.822  1.00 11.87      A
ATOM   1268  CG  ASN A 173      29.628  41.862  49.606  1.00 13.88      A
ATOM   1269  OD1 ASN A 173      30.289  42.512  50.412  1.00 13.36      A
ATOM   1270  ND2 ASN A 173      29.098  42.398  48.515  1.00 16.29      A
ATOM   1271  C   ASN A 173      30.062  38.245  50.759  1.00 13.21      A
ATOM   1272  O   ASN A 173      29.077  38.109  51.498  1.00 10.89      A
ATOM   1273  N   SER A 174      30.716  37.212  50.238  1.00  7.67      A
ATOM   1274  CA  SER A 174      30.250  35.859  50.468  1.00  9.24      A
ATOM   1275  CB  SER A 174      30.869  34.905  49.429  1.00  9.01      A
ATOM   1276  OG  SER A 174      30.359  33.580  49.598  1.00  8.15      A
ATOM   1277  C   SER A 174      30.440  35.250  51.863  1.00  7.73      A
ATOM   1278  O   SER A 174      29.480  34.822  52.506  1.00  8.54      A
ATOM   1279  N   TYR A 175      31.684  35.160  52.303  1.00  6.67      A
ATOM   1280  CA  TYR A 175      31.978  34.535  53.599  1.00  6.35      A
ATOM   1281  CB  TYR A 175      33.493  34.371  53.735  1.00  7.83      A
ATOM   1282  CG  TYR A 175      33.928  33.429  54.847  1.00  6.19      A
ATOM   1283  CD1 TYR A 175      34.845  33.842  55.825  1.00  9.13      A
ATOM   1284  CE1 TYR A 175      35.315  32.938  56.811  1.00  7.78      A
ATOM   1285  CD2 TYR A 175      33.481  32.102  54.879  1.00  6.63      A
ATOM   1286  CE2 TYR A 175      33.939  31.206  55.856  1.00  9.07      A
ATOM   1287  CZ  TYR A 175      34.859  31.633  56.812  1.00 11.83      A
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FIGURE 5 (continued)

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ATOM   1288  OH  TYR A 175      35.348  30.731  57.746  1.00  8.85      A
ATOM   1289  C   TYR A 175      31.424  35.365  54.761  1.00 12.71      A
ATOM   1290  O   TYR A 175      31.649  36.556  54.806  1.00  7.92      A
ATOM   1291  N   SER A 176      30.695  34.727  55.683  1.00  9.13      A
ATOM   1292  CA  SER A 176      30.104  35.431  56.828  1.00  9.94      A
ATOM   1293  CB  SER A 176      29.372  34.433  57.737  1.00 11.72      A
ATOM   1294  OG  SER A 176      30.248  33.426  58.245  1.00  9.80      A
ATOM   1295  C   SER A 176      31.092  36.247  57.659  1.00 11.68      A
ATOM   1296  O   SER A 176      30.737  37.302  58.184  1.00 12.94      A
ATOM   1297  N   LEU A 177      32.332  35.787  57.788  1.00 10.90      A
ATOM   1298  CA  LEU A 177      33.303  36.559  58.561  1.00 12.59      A
ATOM   1299  CB  LEU A 177      34.231  35.613  59.349  1.00 14.55      A
ATOM   1300  CG  LEU A 177      33.537  34.649  60.324  1.00 15.21      A
ATOM   1301  CD1 LEU A 177      34.579  33.649  60.872  1.00 18.41      A
ATOM   1302  CD2 LEU A 177      32.856  35.452  61.476  1.00 11.73      A
ATOM   1303  C   LEU A 177      34.139  37.522  57.692  1.00 13.68      A
ATOM   1304  O   LEU A 177      35.126  38.104  58.163  1.00 12.71      A
ATOM   1305  N   GLY A 178      33.754  37.680  56.434  1.00  9.18      A
ATOM   1306  CA  GLY A 178      34.475  38.585  55.541  1.00 12.34      A
ATOM   1307  C   GLY A 178      35.803  38.098  54.975  1.00 12.74      A
ATOM   1308  O   GLY A 178      36.205  36.939  55.208  1.00 13.97      A
ATOM   1309  N   LEU A 179      36.492  38.974  54.224  1.00  9.84      A
ATOM   1310  CA  LEU A 179      37.787  38.610  53.621  1.00 10.63      A
ATOM   1311  CB  LEU A 179      38.078  39.437  52.350  1.00 11.33      A
ATOM   1312  CG  LEU A 179      37.189  39.202  51.120  1.00 10.67      A
ATOM   1313  CD1 LEU A 179      37.729  40.017  49.934  1.00 12.85      A
ATOM   1314  CD2 LEU A 179      37.134  37.692  50.787  1.00 15.70      A
ATOM   1315  C   LEU A 179      38.986  38.779  54.555  1.00 12.52      A
ATOM   1316  O   LEU A 179      40.096  38.319  54.233  1.00 13.43      A
ATOM   1317  N   SER A 180      38.788  39.426  55.702  1.00 13.88      A
ATOM   1318  CA  SER A 180      39.910  39.635  56.612  1.00 17.84      A
ATOM   1319  CB  SER A 180      39.438  40.187  57.954  1.00 23.37      A
ATOM   1320  OG  SER A 180      39.006  41.521  57.770  1.00 30.75      A
ATOM   1321  C   SER A 180      40.776  38.411  56.839  1.00 18.97      A
ATOM   1322  O   SER A 180      41.990  38.527  56.856  1.00 16.57      A
ATOM   1323  N   PRO A 181      40.170  37.223  57.010  1.00 17.96      A
ATOM   1324  CD  PRO A 181      38.739  36.923  57.219  1.00 18.24      A
ATOM   1325  CA  PRO A 181      40.989  36.023  57.228  1.00 19.35      A
ATOM   1326  CB  PRO A 181      39.948  34.925  57.436  1.00 20.22      A
ATOM   1327  CG  PRO A 181      38.804  35.657  58.063  1.00 20.57      A
ATOM   1328  C   PRO A 181      41.927  35.697  56.063  1.00 24.47      A
ATOM   1329  O   PRO A 181      42.893  34.943  56.237  1.00 26.18      A
ATOM   1330  N   LEU A 182      41.646  36.251  54.880  1.00 17.84      A
ATOM   1331  CA  LEU A 182      42.470  36.002  53.688  1.00 21.43      A
ATOM   1332  CB  LEU A 182      41.615  36.019  52.410  1.00 20.15      A
ATOM   1333  CG  LEU A 182      40.748  34.780  52.178  1.00 20.14      A
ATOM   1334  CD1 LEU A 182      39.849  34.968  50.952  1.00 17.30      A
ATOM   1335  CD2 LEU A 182      41.679  33.580  52.004  1.00 15.09      A
ATOM   1336  C   LEU A 182      43.614  36.985  53.490  1.00 27.88      A
ATOM   1337  O   LEU A 182      43.499  37.909  52.682  1.00 31.51      A
ATOM   1338  N   ALA A 183      44.726  36.761  54.185  1.00 23.49      A
ATOM   1339  CA  ALA A 183      45.893  37.639  54.073  1.00 26.24      A
ATOM   1340  CB  ALA A 183      47.066  37.047  54.860  1.00 22.25      A
ATOM   1341  C   ALA A 183      46.325  37.920  52.629  1.00 20.58      A
ATOM   1342  O   ALA A 183      46.623  37.001  51.856  1.00 17.37      A
ATOM   1343  N   GLY A 184      46.354  39.202  52.278  1.00 17.97      A
ATOM   1344  CA  GLY A 184      46.762  39.603  50.949  1.00 17.46      A
ATOM   1345  C   GLY A 184      45.908  39.186  49.755  1.00 12.78      A
ATOM   1346  O   GLY A 184      46.413  39.159  48.636  1.00 15.39      A
ATOM   1347  N   ALA A 185      44.634  38.878  49.956  1.00 12.15      A
ATOM   1348  CA  ALA A 185      43.798  38.500  48.811  1.00 14.55      A
ATOM   1349  CB  ALA A 185      42.374  38.212  49.271  1.00 14.22      A
ATOM   1350  C   ALA A 185      43.812  39.649  47.795  1.00 16.74      A
ATOM   1351  O   ALA A 185      43.780  40.826  48.181  1.00 15.66      A
ATOM   1352  N   VAL A 186      43.836  39.300  46.507  1.00  9.90      A
ATOM   1353  CA  VAL A 186      43.880  40.276  45.419  1.00 11.92      A
ATOM   1354  CB  VAL A 186      45.093  39.969  44.484  1.00 14.98      A
ATOM   1355  CG1 VAL A 186      45.026  40.816  43.229  1.00 13.29      A
ATOM   1356  CG2 VAL A 186      46.398  40.226  45.244  1.00 19.64      A
ATOM   1357  C   VAL A 186      42.608  40.254  44.571  1.00 11.79      A
ATOM   1358  O   VAL A 186      42.152  39.182  44.149  1.00 11.34      A
ATOM   1359  N   ALA A 187      42.035  41.430  44.331  1.00 11.06      A
ATOM   1360  CA  ALA A 187      40.829  41.543  43.508  1.00 10.57      A
ATOM   1361  CB  ALA A 187      39.897  42.606  44.096  1.00 12.53      A
ATOM   1362  C   ALA A 187      41.211  41.923  42.079  1.00 13.16      A
ATOM   1363  O   ALA A 187      42.128  42.736  41.876  1.00 14.58      A
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FIGURE 5 (continued)

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ATOM   1364  N   ALA A 188      40.543  41.328  41.085  1.00  8.38      A
ATOM   1365  CA  ALA A 188      40.832  41.672  39.672  1.00  8.09      A
ATOM   1366  CB  ALA A 188      41.725  40.609  39.018  1.00 10.94      A
ATOM   1367  C   ALA A 188      39.515  41.759  38.913  1.00  9.75      A
ATOM   1368  O   ALA A 188      38.510  41.196  39.349  1.00 10.74      A
ATOM   1369  N   ILE A 189      39.543  42.434  37.766  1.00 10.19      A
ATOM   1370  CA  ILE A 189      38.355  42.646  36.936  1.00  9.71      A
ATOM   1371  CB  ILE A 189      38.300  44.126  36.487  1.00 14.84      A
ATOM   1372  CG2 ILE A 189      37.056  44.394  35.606  1.00 12.56      A
ATOM   1373  CG1 ILE A 189      38.247  45.007  37.720  1.00 13.85      A
ATOM   1374  CD1 ILE A 189      36.964  44.848  38.520  1.00 20.17      A
ATOM   1375  C   ILE A 189      38.307  41.760  35.705  1.00 11.18      A
ATOM   1376  O   ILE A 189      39.260  41.715  34.930  1.00 12.80      A
ATOM   1377  N   GLY A 190      37.185  41.062  35.518  1.00 12.93      A
ATOM   1378  CA  GLY A 190      37.039  40.181  34.368  1.00  9.66      A
ATOM   1379  C   GLY A 190      37.836  38.881  34.432  1.00 11.20      A
ATOM   1380  O   GLY A 190      38.763  38.745  35.238  1.00 12.00      A
ATOM   1381  N   SER A 191      37.494  37.919  33.570  1.00 12.31      A
ATOM   1382  CA  SER A 191      38.216  36.644  33.539  1.00 11.69      A
ATOM   1383  CB  SER A 191      37.530  35.671  32.568  1.00  8.59      A
ATOM   1384  OG  SER A 191      36.224  35.299  33.026  1.00 10.08      A
ATOM   1385  C   SER A 191      39.678  36.896  33.104  1.00 14.30      A
ATOM   1386  O   SER A 191      40.612  36.295  33.638  1.00 11.39      A
ATOM   1387  N   VAL A 192      39.880  37.809  32.156  1.00 11.76      A
ATOM   1388  CA  VAL A 192      41.235  38.101  31.704  1.00 14.84      A
ATOM   1389  CB  VAL A 192      41.273  39.029  30.449  1.00 13.34      A
ATOM   1390  CG1 VAL A 192      40.838  38.252  29.213  1.00 24.13      A
ATOM   1391  CG2 VAL A 192      40.396  40.246  30.678  1.00 29.05      A
ATOM   1392  C   VAL A 192      42.056  38.767  32.804  1.00 11.65      A
ATOM   1393  O   VAL A 192      43.247  38.485  32.940  1.00 14.10      A
ATOM   1394  N   GLY A 193      41.431  39.670  33.559  1.00 12.08      A
ATOM   1395  CA  GLY A 193      42.149  40.344  34.626  1.00 12.16      A
ATOM   1396  C   GLY A 193      42.575  39.354  35.700  1.00 14.30      A
ATOM   1397  O   GLY A 193      43.652  39.486  36.291  1.00  9.20      A
ATOM   1398  N   VAL A 194      41.725  38.369  35.976  1.00  9.32      A
ATOM   1399  CA  VAL A 194      42.069  37.370  36.992  1.00  9.16      A
ATOM   1400  CB  VAL A 194      40.845  36.459  37.341  1.00  7.74      A
ATOM   1401  CG1 VAL A 194      41.309  35.168  38.071  1.00  8.55      A
ATOM   1402  CG2 VAL A 194      39.873  37.247  38.259  1.00 11.33      A
ATOM   1403  C   VAL A 194      43.256  36.524  36.530  1.00 10.65      A
ATOM   1404  O   VAL A 194      44.158  36.255  37.318  1.00 10.00      A
ATOM   1405  N   MET A 195      43.261  36.090  35.265  1.00  9.82      A
ATOM   1406  CA  MET A 195      44.391  35.306  34.775  1.00 11.27      A
ATOM   1407  CB  MET A 195      44.125  34.727  33.381  1.00 13.33      A
ATOM   1408  CG  MET A 195      43.342  33.449  33.381  1.00 16.98      A
ATOM   1409  SD  MET A 195      43.794  32.237  34.698  1.00 19.79      A
ATOM   1410  CE  MET A 195      45.205  31.419  34.043  1.00 16.46      A
ATOM   1411  C   MET A 195      45.672  36.118  34.719  1.00 12.67      A
ATOM   1412  O   MET A 195      46.757  35.579  34.948  1.00 15.56      A
ATOM   1413  N   ALA A 196      45.566  37.401  34.385  1.00 11.82      A
ATOM   1414  CA  ALA A 196      46.750  38.239  34.346  1.00 15.74      A
ATOM   1415  CB  ALA A 196      46.404  39.633  33.833  1.00 14.20      A
ATOM   1416  C   ALA A 196      47.331  38.323  35.768  1.00 16.81      A
ATOM   1417  O   ALA A 196      48.544  38.245  35.945  1.00 15.03      A
ATOM   1418  N   ALA A 197      46.464  38.468  36.778  1.00 13.86      A
ATOM   1419  CA  ALA A 197      46.939  38.538  38.151  1.00 13.25      A
ATOM   1420  CB  ALA A 197      45.790  38.865  39.108  1.00 13.70      A
ATOM   1421  C   ALA A 197      47.547  37.203  38.542  1.00 13.49      A
ATOM   1422  O   ALA A 197      48.618  37.159  39.147  1.00 13.32      A
ATOM   1423  N   ASP A 198      46.853  36.119  38.202  1.00 12.41      A
ATOM   1424  CA  ASP A 198      47.326  34.777  38.547  1.00 16.61      A
ATOM   1425  CB  ASP A 198      46.311  33.719  38.074  1.00 18.96      A
ATOM   1426  CG  ASP A 198      46.605  32.327  38.629  1.00 29.19      A
ATOM   1427  OD1 ASP A 198      46.440  32.107  39.857  1.00 32.24      A
ATOM   1428  OD2 ASP A 198      47.004  31.449  37.834  1.00 34.04      A
ATOM   1429  C   ASP A 198      48.699  34.509  37.928  1.00 17.95      A
ATOM   1430  O   ASP A 198      49.570  33.942  38.585  1.00 18.27      A
ATOM   1431  N   ASN A 199      48.900  34.941  36.684  1.00 16.24      A
ATOM   1432  CA  ASN A 199      50.173  34.733  35.980  1.00 17.75      A
ATOM   1433  CB  ASN A 199      49.941  34.565  34.478  1.00 19.50      A
ATOM   1434  CG  ASN A 199      49.270  33.263  34.122  1.00 21.16      A
ATOM   1435  OD1 ASN A 199      49.454  32.254  34.786  1.00 29.31      A
ATOM   1436  ND2 ASN A 199      48.504  33.275  33.041  1.00 24.39      A
ATOM   1437  C   ASN A 199      51.227  35.832  36.144  1.00 20.64      A
ATOM   1438  O   ASN A 199      52.272  35.762  35.507  1.00 27.47      A
ATOM   1439  N   ASP A 200      50.973  36.838  36.970  1.00 19.22      A
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FIGURE 5 (continued)

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ATOM   1440  CA  ASP A 200      51.925  37.937  37.148  1.00 20.54      A
ATOM   1441  CB  ASP A 200      51.350  38.985  38.092  1.00 22.32      A
ATOM   1442  CG  ASP A 200      52.166  40.271  38.105  1.00 23.11      A
ATOM   1443  OD1 ASP A 200      53.356  40.256  37.713  1.00 21.11      A
ATOM   1444  OD2 ASP A 200      51.612  41.296  38.526  1.00 26.57      A
ATOM   1445  C   ASP A 200      53.252  37.431  37.716  1.00 21.98      A
ATOM   1446  O   ASP A 200      53.315  36.967  38.855  1.00 19.25      A
ATOM   1447  N   VAL A 201      54.315  37.511  36.922  1.00 21.71      A
ATOM   1448  CA  VAL A 201      55.611  37.033  37.390  1.00 24.01      A
ATOM   1449  CB  VAL A 201      56.519  36.597  36.216  1.00 23.59      A
ATOM   1450  CG1 VAL A 201      55.910  35.377  35.519  1.00 25.93      A
ATOM   1451  CG2 VAL A 201      56.710  37.754  35.246  1.00 26.53      A
ATOM   1452  C   VAL A 201      56.370  38.046  38.222  1.00 24.27      A
ATOM   1453  O   VAL A 201      57.451  37.744  38.715  1.00 30.90      A
ATOM   1454  N   THR A 202      55.817  39.241  38.402  1.00 23.14      A
ATOM   1455  CA  THR A 202      56.511  40.251  39.190  1.00 23.53      A
ATOM   1456  CB  THR A 202      56.216  41.664  38.696  1.00 22.33      A
ATOM   1457  OG1 THR A 202      54.846  41.999  38.979  1.00 24.30      A
ATOM   1458  CG2 THR A 202      56.489  41.759  37.210  1.00 25.94      A
ATOM   1459  C   THR A 202      56.171  40.184  40.677  1.00 24.49      A
ATOM   1460  O   THR A 202      56.543  41.073  41.444  1.00 25.68      A
ATOM   1461  N   THR A 203      55.440  39.147  41.076  1.00 19.97      A
ATOM   1462  CA  THR A 203      55.116  38.957  42.484  1.00 20.69      A
ATOM   1463  CB  THR A 203      53.608  39.167  42.768  1.00 26.13      A
ATOM   1464  OG1 THR A 203      52.825  38.196  42.047  1.00 25.13      A
ATOM   1465  CG2 THR A 203      53.202  40.581  42.363  1.00 26.59      A
ATOM   1466  C   THR A 203      55.523  37.521  42.834  1.00 17.47      A
ATOM   1467  O   THR A 203      55.771  36.703  41.947  1.00 18.21      A
ATOM   1468  N   ALA A 204      55.624  37.217  44.116  1.00 16.96      A
ATOM   1469  CA  ALA A 204      56.011  35.867  44.528  1.00 16.26      A
ATOM   1470  CB  ALA A 204      56.175  35.825  46.065  1.00 18.50      A
ATOM   1471  C   ALA A 204      54.978  34.832  44.092  1.00 14.92      A
ATOM   1472  O   ALA A 204      53.806  35.157  43.906  1.00 16.09      A
ATOM   1473  N   GLN A 205      55.409  33.582  43.921  1.00 16.21      A
ATOM   1474  CA  GLN A 205      54.483  32.501  43.560  1.00 16.27      A
ATOM   1475  CB  GLN A 205      55.232  31.191  43.316  1.00 15.65      A
ATOM   1476  CG  GLN A 205      56.103  31.148  42.097  1.00 22.41      A
ATOM   1477  CD  GLN A 205      56.469  29.716  41.717  1.00 29.28      A
ATOM   1478  OE1 GLN A 205      56.446  28.801  42.565  1.00 20.67      A
ATOM   1479  NE2 GLN A 205      56.813  29.510  40.442  1.00 25.77      A
ATOM   1480  C   GLN A 205      53.529  32.262  44.728  1.00 14.53      A
ATOM   1481  O   GLN A 205      53.783  32.717  45.846  1.00 14.81      A
ATOM   1482  N   GLY A 206      52.438  31.540  44.478  1.00 11.64      A
ATOM   1483  CA  GLY A 206      51.509  31.236  45.554  1.00 11.46      A
ATOM   1484  C   GLY A 206      50.042  31.518  45.284  1.00 11.44      A
ATOM   1485  O   GLY A 206      49.162  31.067  46.046  1.00  9.87      A
ATOM   1486  N   ARG A 207      49.764  32.236  44.199  1.00  7.71      A
ATOM   1487  CA  ARG A 207      48.383  32.606  43.878  1.00  7.50      A
ATOM   1488  CB  ARG A 207      48.364  33.763  42.863  1.00  9.66      A
ATOM   1489  CG  ARG A 207      48.719  35.114  43.493  1.00  7.35      A
ATOM   1490  CD  ARG A 207      48.774  36.286  42.497  1.00  6.76      A
ATOM   1491  NE  ARG A 207      49.079  37.532  43.221  1.00 10.86      A
ATOM   1492  CZ  ARG A 207      49.156  38.738  42.654  1.00 13.78      A
ATOM   1493  NH1 ARG A 207      48.957  38.881  41.350  1.00  9.77      A
ATOM   1494  NH2 ARG A 207      49.415  39.811  43.398  1.00 15.04      A
ATOM   1495  C   ARG A 207      47.500  31.475  43.389  1.00 11.20      A
ATOM   1496  O   ARG A 207      47.959  30.549  42.713  1.00 12.10      A
ATOM   1497  N   ILE A 208      46.214  31.572  43.721  1.00  8.65      A
ATOM   1498  CA  ILE A 208      45.245  30.557  43.331  1.00  8.62      A
ATOM   1499  CB  ILE A 208      45.073  29.491  44.476  1.00 11.42      A
ATOM   1500  CG2 ILE A 208      44.533  30.157  45.766  1.00  8.84      A
ATOM   1501  CG1 ILE A 208      44.158  28.359  43.984  1.00 12.09      A
ATOM   1502  CD1 ILE A 208      44.207  27.094  44.823  1.00 11.77      A
ATOM   1503  C   ILE A 208      43.924  31.286  43.056  1.00 10.31      A
ATOM   1504  O   ILE A 208      43.664  32.335  43.649  1.00 12.81      A
ATOM   1505  N   THR A 209      43.098  30.776  42.145  1.00  7.78      A
ATOM   1506  CA  THR A 209      41.825  31.470  41.864  1.00  9.01      A
ATOM   1507  CB  THR A 209      42.055  32.610  40.849  1.00 11.48      A
ATOM   1508  OG1 THR A 209      40.906  33.455  40.789  1.00 11.18      A
ATOM   1509  CG2 THR A 209      42.310  32.030  39.460  1.00 12.27      A
ATOM   1510  C   THR A 209      40.751  30.534  41.319  1.00 10.48      A
ATOM   1511  O   THR A 209      40.978  29.326  41.215  1.00 10.85      A
ATOM   1512  N   TYR A 210      39.577  31.087  40.997  1.00  8.58      A
ATOM   1513  CA  TYR A 210      38.476  30.303  40.422  1.00  8.34      A
ATOM   1514  CB  TYR A 210      37.244  30.304  41.350  1.00  4.35      A
ATOM   1515  CG  TYR A 210      36.685  31.664  41.695  1.00  7.98      A
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FIGURE 5 (continued)

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ATOM   1516  CD1 TYR A 210      35.656  32.240  40.927  1.00  6.11      A
ATOM   1517  CE1 TYR A 210      35.153  33.509  41.235  1.00  7.73      A
ATOM   1518  CD2 TYR A 210      37.188  32.386  42.778  1.00  6.57      A
ATOM   1519  CE2 TYR A 210      36.699  33.643  43.086  1.00  5.93      A
ATOM   1520  CZ  TYR A 210      35.687  34.203  42.313  1.00  8.47      A
ATOM   1521  OH  TYR A 210      35.242  35.475  42.598  1.00  8.24      A
ATOM   1522  C   TYR A 210      38.169  30.983  39.087  1.00  5.52      A
ATOM   1523  O   TYR A 210      38.184  32.222  39.010  1.00  9.37      A
ATOM   1524  N   ILE A 211      37.934  30.201  38.032  1.00  6.28      A
ATOM   1525  CA  ILE A 211      37.720  30.832  36.735  1.00  7.52      A
ATOM   1526  CB  ILE A 211      39.085  31.384  36.235  1.00 11.97      A
ATOM   1527  CG2 ILE A 211      39.990  30.231  35.830  1.00 10.21      A
ATOM   1528  CG1 ILE A 211      38.902  32.361  35.075  1.00 14.62      A
ATOM   1529  CD1 ILE A 211      40.159  33.203  34.806  1.00 15.71      A
ATOM   1530  C   ILE A 211      37.132  29.936  35.648  1.00  8.22      A
ATOM   1531  O   ILE A 211      37.080  28.703  35.778  1.00  8.13      A
ATOM   1532  N   SER A 212      36.634  30.590  34.602  1.00  9.06      A
ATOM   1533  CA  SER A 212      36.140  29.913  33.394  1.00  9.98      A
ATOM   1534  CB  SER A 212      35.984  30.934  32.256  1.00  8.45      A
ATOM   1535  OG  SER A 212      35.637  30.283  31.037  1.00  9.53      A
ATOM   1536  C   SER A 212      37.181  28.904  32.914  1.00 10.00      A
ATOM   1537  O   SER A 212      38.361  29.234  32.812  1.00  7.50      A
ATOM   1538  N   PRO A 213      36.761  27.668  32.585  1.00  8.50      A
ATOM   1539  CD  PRO A 213      35.436  27.030  32.686  1.00  4.78      A
ATOM   1540  CA  PRO A 213      37.781  26.728  32.117  1.00  8.39      A
ATOM   1541  CB  PRO A 213      37.035  25.392  32.059  1.00 10.29      A
ATOM   1542  CG  PRO A 213      35.578  25.849  31.743  1.00  9.33      A
ATOM   1543  C   PRO A 213      38.360  27.149  30.777  1.00 10.79      A
ATOM   1544  O   PRO A 213      39.433  26.698  30.390  1.00 10.83      A
ATOM   1545  N   ASP A 214      37.668  28.038  30.074  1.00  5.80      A
ATOM   1546  CA  ASP A 214      38.164  28.514  28.775  1.00  8.50      A
ATOM   1547  CB  ASP A 214      37.033  29.175  27.997  1.00  7.35      A
ATOM   1548  CG  ASP A 214      37.248  29.146  26.497  1.00 11.12      A
ATOM   1549  OD1 ASP A 214      36.479  29.849  25.801  1.00 11.42      A
ATOM   1550  OD2 ASP A 214      38.159  28.428  26.007  1.00 10.72      A
ATOM   1551  C   ASP A 214      39.314  29.526  28.935  1.00 12.08      A
ATOM   1552  O   ASP A 214      39.933  29.931  27.943  1.00 13.08      A
ATOM   1553  N   PHE A 215      39.572  29.958  30.170  1.00  9.47      A
ATOM   1554  CA  PHE A 215      40.662  30.901  30.459  1.00  9.63      A
ATOM   1555  CB  PHE A 215      40.121  32.106  31.233  1.00 12.63      A
ATOM   1556  CG  PHE A 215      39.375  33.081  30.402  1.00  9.86      A
ATOM   1557  CD1 PHE A 215      39.957  34.301  30.067  1.00 11.72      A
ATOM   1558  CD2 PHE A 215      38.074  32.812  29.986  1.00 11.34      A
ATOM   1559  CE1 PHE A 215      39.250  35.250  29.332  1.00 11.89      A
ATOM   1560  CE2 PHE A 215      37.357  33.759  29.245  1.00  6.37      A
ATOM   1561  CZ  PHE A 215      37.949  34.976  28.921  1.00 13.90      A
ATOM   1562  C   PHE A 215      41.748  30.286  31.356  1.00 13.88      A
ATOM   1563  O   PHE A 215      42.837  30.865  31.480  1.00 12.28      A
ATOM   1564  N   ALA A 216      41.463  29.131  31.976  1.00  9.02      A
ATOM   1565  CA  ALA A 216      42.404  28.535  32.936  1.00  9.41      A
ATOM   1566  CB  ALA A 216      41.705  27.432  33.753  1.00  9.18      A
ATOM   1567  C   ALA A 216      43.727  28.007  32.406  1.00 13.18      A
ATOM   1568  O   ALA A 216      44.679  27.844  33.178  1.00 16.82      A
ATOM   1569  N   ALA A 217      43.790  27.719  31.106  1.00 12.39      A
ATOM   1570  CA  ALA A 217      45.031  27.224  30.522  1.00 14.59      A
ATOM   1571  CB  ALA A 217      45.094  25.693  30.625  1.00 15.34      A
ATOM   1572  C   ALA A 217      45.136  27.660  29.063  1.00 16.52      A
ATOM   1573  O   ALA A 217      44.128  27.958  28.418  1.00 14.71      A
ATOM   1574  N   PRO A 218      46.358  27.690  28.517  1.00 18.85      A
ATOM   1575  CD  PRO A 218      47.657  27.532  29.194  1.00 19.53      A
ATOM   1576  CA  PRO A 218      46.533  28.101  27.111  1.00 17.17      A
ATOM   1577  CB  PRO A 218      48.053  28.171  26.952  1.00 22.03      A
ATOM   1578  CG  PRO A 218      48.553  28.433  28.357  1.00 24.10      A
ATOM   1579  C   PRO A 218      45.889  27.162  26.076  1.00 17.95      A
ATOM   1580  O   PRO A 218      45.490  27.606  24.986  1.00 20.60      A
ATOM   1581  N   SER A 219      45.804  25.872  26.395  1.00 12.39      A
ATOM   1582  CA  SER A 219      45.212  24.883  25.490  1.00 11.61      A
ATOM   1583  CB  SER A 219      46.308  24.053  24.816  1.00 17.69      A
ATOM   1584  OG  SER A 219      46.870  23.140  25.749  1.00 17.25      A
ATOM   1585  C   SER A 219      44.341  23.942  26.324  1.00 14.52      A
ATOM   1586  O   SER A 219      44.454  23.896  27.559  1.00 15.86      A
ATOM   1587  N   LEU A 220      43.479  23.180  25.664  1.00 13.85      A
ATOM   1588  CA  LEU A 220      42.614  22.250  26.389  1.00 13.63      A
ATOM   1589  CB  LEU A 220      41.705  21.491  25.401  1.00 15.59      A
ATOM   1590  CG  LEU A 220      40.632  22.337  24.707  1.00 16.07      A
ATOM   1591  CD1 LEU A 220      39.908  21.517  23.646  1.00 15.58      A
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FIGURE 5 (continued)

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ATOM   1592  CD2 LEU A 220      39.635  22.855  25.752  1.00 16.33      A
ATOM   1593  C   LEU A 220      43.401  21.251  27.245  1.00 15.71      A
ATOM   1594  O   LEU A 220      43.034  20.986  28.395  1.00 15.65      A
ATOM   1595  N   ALA A 221      44.481  20.693  26.698  1.00 15.60      A
ATOM   1596  CA  ALA A 221      45.283  19.714  27.452  1.00 18.03      A
ATOM   1597  CB  ALA A 221      46.452  19.175  26.604  1.00 17.58      A
ATOM   1598  C   ALA A 221      45.834  20.298  28.738  1.00 11.01      A
ATOM   1599  O   ALA A 221      46.085  19.573  29.687  1.00 15.45      A
ATOM   1600  N   GLY A 222      46.038  21.612  28.754  1.00 15.25      A
ATOM   1601  CA  GLY A 222      46.561  22.267  29.947  1.00 11.71      A
ATOM   1602  C   GLY A 222      45.641  22.101  31.144  1.00 10.72      A
ATOM   1603  O   GLY A 222      46.105  22.139  32.280  1.00 14.13      A
ATOM   1604  N   LEU A 223      44.340  21.938  30.914  1.00 11.19      A
ATOM   1605  CA  LEU A 223      43.406  21.751  32.033  1.00  8.14      A
ATOM   1606  CB  LEU A 223      41.946  21.728  31.525  1.00  9.90      A
ATOM   1607  CG  LEU A 223      41.481  23.046  30.874  1.00  9.91      A
ATOM   1608  CD1 LEU A 223      40.035  22.918  30.331  1.00  9.85      A
ATOM   1609  CD2 LEU A 223      41.570  24.153  31.926  1.00  9.05      A
ATOM   1610  C   LEU A 223      43.720  20.444  32.773  1.00 11.22      A
ATOM   1611  O   LEU A 223      43.369  20.297  33.939  1.00  7.21      A
ATOM   1612  N   ASN A 224      44.389  19.505  32.100  1.00  9.60      A
ATOM   1613  CA  ASN A 224      44.742  18.231  32.727  1.00 10.35      A
ATOM   1614  CB  ASN A 224      44.651  17.078  31.706  1.00 13.70      A
ATOM   1615  CG  ASN A 224      43.214  16.768  31.301  1.00 15.75      A
ATOM   1616  OD1 ASN A 224      42.347  16.610  32.146  1.00 21.72      A
ATOM   1617  ND2 ASN A 224      42.968  16.666  30.012  1.00 14.86      A
ATOM   1618  C   ASN A 224      46.138  18.239  33.359  1.00 12.93      A
ATOM   1619  O   ASN A 224      46.580  17.226  33.898  1.00 14.86      A
ATOM   1620  N   ASP A 225      46.833  19.370  33.308  1.00  8.74      A
ATOM   1621  CA  ASP A 225      48.163  19.437  33.932  1.00 12.69      A
ATOM   1622  CB  ASP A 225      49.031  20.467  33.199  1.00 11.40      A
ATOM   1623  CG  ASP A 225      50.402  20.654  33.843  1.00 15.89      A
ATOM   1624  OD1 ASP A 225      50.673  20.076  34.922  1.00 14.10      A
ATOM   1625  OD2 ASP A 225      51.211  21.401  33.261  1.00 16.19      A
ATOM   1626  C   ASP A 225      47.960  19.844  35.398  1.00 13.53      A
ATOM   1627  O   ASP A 225      47.776  21.016  35.691  1.00 10.79      A
ATOM   1628  N   ALA A 226      48.035  18.882  36.317  1.00 10.49      A
ATOM   1629  CA  ALA A 226      47.792  19.178  37.720  1.00  9.18      A
ATOM   1630  CB  ALA A 226      47.424  17.889  38.478  1.00 13.20      A
ATOM   1631  C   ALA A 226      48.881  19.939  38.461  1.00 12.23      A
ATOM   1632  O   ALA A 226      48.773  20.144  39.678  1.00 13.15      A
ATOM   1633  N   THR A 227      49.935  20.347  37.762  1.00 10.64      A
ATOM   1634  CA  THR A 227      50.955  21.148  38.426  1.00 10.50      A
ATOM   1635  CB  THR A 227      52.405  20.854  37.917  1.00 15.63      A
ATOM   1636  OG1 THR A 227      52.541  21.287  36.561  1.00 13.88      A
ATOM   1637  CG2 THR A 227      52.718  19.374  38.009  1.00 16.59      A
ATOM   1638  C   THR A 227      50.620  22.628  38.154  1.00  9.17      A
ATOM   1639  O   THR A 227      51.320  23.509  38.626  1.00 10.52      A
ATOM   1640  N   LYS A 228      49.530  22.876  37.414  1.00  9.27      A
ATOM   1641  CA  LYS A 228      49.079  24.226  37.069  1.00 12.05      A
ATOM   1642  CB  LYS A 228      49.378  24.511  35.594  1.00 15.38      A
ATOM   1643  CG  LYS A 228      50.877  24.607  35.272  1.00 22.71      A
ATOM   1644  CD  LYS A 228      51.125  24.652  33.758  1.00 20.66      A
ATOM   1645  CE  LYS A 228      52.613  24.720  33.447  1.00 26.84      A
ATOM   1646  NZ  LYS A 228      53.205  25.974  33.986  1.00 37.16      A
ATOM   1647  C   LYS A 228      47.576  24.453  37.313  1.00  8.78      A
ATOM   1648  O   LYS A 228      47.153  25.574  37.634  1.00  9.99      A
ATOM   1649  N   VAL A 229      46.777  23.407  37.100  1.00  9.98      A
ATOM   1650  CA  VAL A 229      45.327  23.465  37.282  1.00  6.71      A
ATOM   1651  CB  VAL A 229      44.611  23.300  35.939  1.00  8.87      A
ATOM   1652  CG1 VAL A 229      43.082  23.303  36.150  1.00 10.77      A
ATOM   1653  CG2 VAL A 229      45.019  24.468  34.988  1.00 10.90      A
ATOM   1654  C   VAL A 229      44.913  22.339  38.245  1.00 10.51      A
ATOM   1655  O   VAL A 229      45.107  21.154  37.967  1.00  8.04      A
ATOM   1656  N   ALA A 230      44.343  22.706  39.383  1.00 10.29      A
ATOM   1657  CA  ALA A 230      43.985  21.696  40.387  1.00  8.30      A
ATOM   1658  CB  ALA A 230      43.612  22.380  41.677  1.00 10.71      A
ATOM   1659  C   ALA A 230      42.900  20.691  40.064  1.00 12.18      A
ATOM   1660  O   ALA A 230      41.884  21.020  39.435  1.00 12.58      A
ATOM   1661  N   ARG A 231      43.120  19.452  40.501  1.00  8.23      A
ATOM   1662  CA  ARG A 231      42.080  18.436  40.382  1.00  8.98      A
ATOM   1663  CB  ARG A 231      42.656  17.021  40.495  1.00 11.67      A
ATOM   1664  CG  ARG A 231      43.433  16.581  39.265  1.00 14.58      A
ATOM   1665  CD  ARG A 231      44.130  15.244  39.487  1.00 18.76      A
ATOM   1666  NE  ARG A 231      44.972  14.941  38.336  1.00 19.63      A
ATOM   1667  CZ  ARG A 231      45.931  14.029  38.331  1.00 26.24      A
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FIGURE 5 (continued)

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ATOM   1668  NH1 ARG A 231      46.184  13.312  39.426  1.00 22.17      A
ATOM   1669  NH2 ARG A 231      46.649  13.848  37.228  1.00 31.31      A
ATOM   1670  C   ARG A 231      41.271  18.738  41.632  1.00  8.66      A
ATOM   1671  O   ARG A 231      41.801  19.332  42.582  1.00 13.24      A
ATOM   1672  N   THR A 232      39.997  18.371  41.640  1.00  9.11      A
ATOM   1673  CA  THR A 232      39.180  18.607  42.822  1.00 11.84      A
ATOM   1674  CB  THR A 232      38.236  19.820  42.623  1.00 13.64      A
ATOM   1675  OG1 THR A 232      39.017  21.004  42.384  1.00 17.60      A
ATOM   1676  CG2 THR A 232      37.382  20.025  43.883  1.00 14.43      A
ATOM   1677  C   THR A 232      38.357  17.351  43.071  1.00  9.12      A
ATOM   1678  O   THR A 232      37.869  16.747  42.118  1.00 13.13      A
ATOM   1679  N   GLY A 233      38.240  16.934  44.332  1.00  9.55      A
ATOM   1680  CA  GLY A 233      37.466  15.739  44.636  1.00 13.57      A
ATOM   1681  C   GLY A 233      38.197  14.616  45.364  1.00 14.09      A
ATOM   1682  O   GLY A 233      37.634  13.556  45.591  1.00 16.30      A
ATOM   1683  N   LYS A 234      39.460  14.831  45.706  1.00 14.67      A
ATOM   1684  CA  LYS A 234      40.226  13.834  46.438  1.00 15.04      A
ATOM   1685  CB  LYS A 234      41.577  14.442  46.830  1.00 13.37      A
ATOM   1686  CG  LYS A 234      42.483  13.576  47.688  1.00 14.40      A
ATOM   1687  CD  LYS A 234      43.807  14.314  47.968  1.00 17.84      A
ATOM   1688  CE  LYS A 234      43.594  15.567  48.839  1.00 15.78      A
ATOM   1689  NZ  LYS A 234      44.766  16.501  48.832  1.00 12.74      A
ATOM   1690  C   LYS A 234      39.450  13.411  47.697  1.00 17.96      A
ATOM   1691  O   LYS A 234      38.826  14.240  48.369  1.00 13.45      A
ATOM   1692  N   GLY A 235      39.489  12.124  48.031  1.00 15.80      A
ATOM   1693  CA  GLY A 235      38.785  11.694  49.223  1.00 15.51      A
ATOM   1694  C   GLY A 235      38.764  10.191  49.402  1.00 19.91      A
ATOM   1695  O   GLY A 235      39.586   9.472  48.825  1.00 21.77      A
ATOM   1696  N   SER A 236      37.811   9.731  50.204  1.00 21.18      A
ATOM   1697  CA  SER A 236      37.624   8.311  50.489  1.00 24.63      A
ATOM   1698  CB  SER A 236      38.018   8.004  51.929  1.00 25.33      A
ATOM   1699  OG  SER A 236      39.359   8.397  52.161  1.00 33.33      A
ATOM   1700  C   SER A 236      36.159   7.969  50.291  1.00 26.45      A
ATOM   1701  O   SER A 236      35.282   8.624  50.855  1.00 27.89      A
ATOM   1702  N   SER A 237      35.891   6.947  49.488  1.00 22.58      A
ATOM   1703  CA  SER A 237      34.522   6.520  49.238  1.00 23.79      A
ATOM   1704  CB  SER A 237      34.123   6.799  47.786  1.00 25.37      A
ATOM   1705  OG  SER A 237      34.019   8.197  47.578  1.00 38.24      A
ATOM   1706  C   SER A 237      34.429   5.036  49.514  1.00 21.92      A
ATOM   1707  O   SER A 237      35.244   4.267  49.009  1.00 20.25      A
ATOM   1708  N   SER A 238      33.423   4.640  50.295  1.00 25.14      A
ATOM   1709  CA  SER A 238      33.233   3.236  50.662  1.00 24.45      A
ATOM   1710  CB  SER A 238      32.716   2.427  49.471  1.00 27.22      A
ATOM   1711  OG  SER A 238      31.371   2.785  49.163  1.00 39.35      A
ATOM   1712  C   SER A 238      34.559   2.670  51.159  1.00 23.39      A
ATOM   1713  O   SER A 238      34.961   1.557  50.809  1.00 24.29      A
ATOM   1714  N   GLY A 239      35.249   3.468  51.966  1.00 24.50      A
ATOM   1715  CA  GLY A 239      36.519   3.040  52.524  1.00 25.11      A
ATOM   1716  C   GLY A 239      37.705   2.973  51.584  1.00 28.40      A
ATOM   1717  O   GLY A 239      38.755   2.452  51.969  1.00 28.03      A
ATOM   1718  N   GLY A 240      37.563   3.495  50.365  1.00 21.59      A
ATOM   1719  CA  GLY A 240      38.677   3.459  49.431  1.00 26.05      A
ATOM   1720  C   GLY A 240      39.082   4.858  48.984  1.00 24.32      A
ATOM   1721  O   GLY A 240      38.218   5.685  48.714  1.00 23.70      A
ATOM   1722  N   GLY A 241      40.386   5.121  48.920  1.00 21.49      A
ATOM   1723  CA  GLY A 241      40.873   6.422  48.500  1.00 27.38      A
ATOM   1724  C   GLY A 241      40.495   6.715  47.058  1.00 28.81      A
ATOM   1725  O   GLY A 241      40.585   5.840  46.200  1.00 28.58      A
ATOM   1726  N   ALA A 242      40.057   7.939  46.784  1.00 24.66      A
ATOM   1727  CA  ALA A 242      39.663   8.303  45.434  1.00 22.08      A
ATOM   1728  CB  ALA A 242      38.159   8.527  45.367  1.00 25.95      A
ATOM   1729  C   ALA A 242      40.385   9.573  45.043  1.00 22.46      A
ATOM   1730  O   ALA A 242      40.541  10.472  45.869  1.00 16.67      A
ATOM   1731  N   GLU A 243      40.813   9.647  43.785  1.00 16.24      A
ATOM   1732  CA  GLU A 243      41.502  10.830  43.289  1.00 18.78      A
ATOM   1733  CB  GLU A 243      42.444  10.473  42.132  1.00 23.30      A
ATOM   1734  CG  GLU A 243      43.643   9.624  42.499  1.00 31.37      A
ATOM   1735  CD  GLU A 243      44.658   9.584  41.368  1.00 37.64      A
ATOM   1736  OE1 GLU A 243      44.234   9.507  40.195  1.00 38.59      A
ATOM   1737  OE2 GLU A 243      45.876   9.628  41.644  1.00 41.94      A
ATOM   1738  C   GLU A 243      40.469  11.817  42.757  1.00 15.80      A
ATOM   1739  O   GLU A 243      39.417  11.406  42.285  1.00 17.65      A
ATOM   1740  N   GLY A 244      40.765  13.111  42.827  1.00 15.34      A
ATOM   1741  CA  GLY A 244      39.832  14.101  42.286  1.00 16.23      A
ATOM   1742  C   GLY A 244      39.994  14.161  40.770  1.00 16.48      A
ATOM   1743  O   GLY A 244      40.894  13.528  40.228  1.00 14.37      A
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FIGURE 5 (continued)

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ATOM   1744  N   LYS A 245      39.148  14.939  40.096  1.00 14.99      A
ATOM   1745  CA  LYS A 245      39.186  15.079  38.632  1.00 14.88      A
ATOM   1746  CB  LYS A 245      37.792  14.795  38.060  1.00 13.06      A
ATOM   1747  CG  LYS A 245      37.294  13.363  38.289  1.00 22.95      A
ATOM   1748  CD  LYS A 245      38.174  12.353  37.540  1.00 27.44      A
ATOM   1749  CE  LYS A 245      37.596  10.939  37.643  1.00 27.64      A
ATOM   1750  NZ  LYS A 245      37.298  10.599  39.063  1.00 36.34      A
ATOM   1751  C   LYS A 245      39.617  16.471  38.165  1.00 13.81      A
ATOM   1752  O   LYS A 245      39.580  17.431  38.932  1.00 10.66      A
ATOM   1753  N   SER A 246      40.022  16.572  36.902  1.00 14.72      A
ATOM   1754  CA  SER A 246      40.405  17.856  36.344  1.00 11.87      A
ATOM   1755  CB  SER A 246      41.299  17.687  35.104  1.00 12.31      A
ATOM   1756  OG  SER A 246      40.515  17.215  34.011  1.00  9.67      A
ATOM   1757  C   SER A 246      39.095  18.500  35.913  1.00 10.79      A
ATOM   1758  O   SER A 246      38.076  17.815  35.735  1.00 10.08      A
ATOM   1759  N   PRO A 247      39.114  19.825  35.698  1.00 10.98      A
ATOM   1760  CD  PRO A 247      40.243  20.747  35.947  1.00  7.03      A
ATOM   1761  CA  PRO A 247      37.909  20.545  35.275  1.00  9.29      A
ATOM   1762  CB  PRO A 247      38.210  21.988  35.692  1.00  7.19      A
ATOM   1763  CG  PRO A 247      39.737  22.094  35.385  1.00  9.12      A
ATOM   1764  C   PRO A 247      37.632  20.416  33.765  1.00  9.99      A
ATOM   1765  O   PRO A 247      36.865  21.197  33.222  1.00 11.54      A
ATOM   1766  N   ALA A 248      38.253  19.449  33.083  1.00  9.23      A
ATOM   1767  CA  ALA A 248      37.992  19.278  31.638  1.00 12.63      A
ATOM   1768  CB  ALA A 248      38.832  18.097  31.069  1.00 10.35      A
ATOM   1769  C   ALA A 248      36.487  19.021  31.431  1.00 15.07      A
ATOM   1770  O   ALA A 248      35.838  18.390  32.278  1.00 11.60      A
ATOM   1771  N   ALA A 249      35.935  19.497  30.311  1.00 12.95      A
ATOM   1772  CA  ALA A 249      34.498  19.332  30.037  1.00 11.90      A
ATOM   1773  CB  ALA A 249      34.141  19.886  28.633  1.00 12.61      A
ATOM   1774  C   ALA A 249      34.037  17.890  30.149  1.00 15.30      A
ATOM   1775  O   ALA A 249      32.953  17.617  30.666  1.00 14.63      A
ATOM   1776  N   ALA A 250      34.845  16.949  29.672  1.00 14.76      A
ATOM   1777  CA  ALA A 250      34.426  15.542  29.769  1.00 18.41      A
ATOM   1778  CB  ALA A 250      35.486  14.623  29.168  1.00 15.53      A
ATOM   1779  C   ALA A 250      34.118  15.102  31.200  1.00 15.76      A
ATOM   1780  O   ALA A 250      33.366  14.154  31.410  1.00 14.59      A
ATOM   1781  N   ASN A 251      34.677  15.785  32.190  1.00 14.82      A
ATOM   1782  CA  ASN A 251      34.433  15.380  33.575  1.00 13.85      A
ATOM   1783  CB  ASN A 251      35.665  15.696  34.441  1.00 12.26      A
ATOM   1784  CG  ASN A 251      36.880  14.885  34.022  1.00 14.85      A
ATOM   1785  OD1 ASN A 251      36.755  13.712  33.653  1.00 14.23      A
ATOM   1786  ND2 ASN A 251      38.056  15.487  34.091  1.00 13.09      A
ATOM   1787  C   ASN A 251      33.168  15.968  34.210  1.00 16.10      A
ATOM   1788  O   ASN A 251      32.877  15.686  35.357  1.00 14.41      A
ATOM   1789  N   SER A 252      32.431  16.806  33.482  1.00 13.25      A
ATOM   1790  CA  SER A 252      31.191  17.346  34.039  1.00 10.81      A
ATOM   1791  CB  SER A 252      31.262  18.868  34.209  1.00 22.32      A
ATOM   1792  OG  SER A 252      31.266  19.536  32.953  1.00 23.58      A
ATOM   1793  C   SER A 252      30.027  16.982  33.101  1.00 11.68      A
ATOM   1794  O   SER A 252      28.862  17.077  33.479  1.00 12.18      A
ATOM   1795  N   SER A 253      30.365  16.501  31.904  1.00 11.74      A
ATOM   1796  CA  SER A 253      29.367  16.138  30.918  1.00 10.64      A
ATOM   1797  CB  SER A 253      30.048  15.572  29.665  1.00 18.81      A
ATOM   1798  OG  SER A 253      29.052  15.263  28.704  1.00 27.87      A
ATOM   1799  C   SER A 253      28.294  15.139  31.382  1.00 15.51      A
ATOM   1800  O   SER A 253      27.112  15.319  31.102  1.00 11.29      A
ATOM   1801  N   ALA A 254      28.692  14.080  32.081  1.00 12.85      A
ATOM   1802  CA  ALA A 254      27.700  13.084  32.525  1.00 14.75      A
ATOM   1803  CB  ALA A 254      28.423  11.868  33.216  1.00 13.94      A
ATOM   1804  C   ALA A 254      26.656  13.667  33.472  1.00 14.13      A
ATOM   1805  O   ALA A 254      25.457  13.394  33.342  1.00 14.40      A
ATOM   1806  N   ALA A 255      27.111  14.457  34.441  1.00 11.77      A
ATOM   1807  CA  ALA A 255      26.205  15.070  35.401  1.00 13.30      A
ATOM   1808  CB  ALA A 255      27.009  15.838  36.460  1.00 12.60      A
ATOM   1809  C   ALA A 255      25.223  16.017  34.698  1.00 15.34      A
ATOM   1810  O   ALA A 255      24.068  16.162  35.113  1.00 14.03      A
ATOM   1811  N   ILE A 256      25.684  16.680  33.644  1.00 13.10      A
ATOM   1812  CA  ILE A 256      24.812  17.599  32.920  1.00 14.09      A
ATOM   1813  CB  ILE A 256      25.614  18.445  31.900  1.00 11.60      A
ATOM   1814  CG2 ILE A 256      24.655  19.233  30.987  1.00 13.12      A
ATOM   1815  CG1 ILE A 256      26.577  19.378  32.657  1.00  8.87      A
ATOM   1816  CD1 ILE A 256      25.878  20.335  33.703  1.00  6.00      A
ATOM   1817  C   ILE A 256      23.716  16.813  32.195  1.00 12.88      A
ATOM   1818  O   ILE A 256      22.569  17.268  32.118  1.00 12.14      A
ATOM   1819  N   SER A 257      24.069  15.639  31.678  1.00 12.01      A
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FIGURE 5 (continued)

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ATOM   1820  CA  SER A 257      23.105  14.793  30.960  1.00 17.17      A
ATOM   1821  CB  SER A 257      23.773  13.529  30.418  1.00 20.37      A
ATOM   1822  OG  SER A 257      24.331  13.802  29.157  1.00 27.40      A
ATOM   1823  C   SER A 257      21.886  14.359  31.750  1.00 21.46      A
ATOM   1824  O   SER A 257      20.885  13.975  31.161  1.00 25.54      A
ATOM   1825  N   VAL A 258      21.949  14.417  33.070  1.00 18.37      A
ATOM   1826  CA  VAL A 258      20.803  13.983  33.849  1.00 22.61      A
ATOM   1827  CB  VAL A 258      21.230  13.049  34.996  1.00 23.45      A
ATOM   1828  CG1 VAL A 258      22.055  11.887  34.443  1.00 28.56      A
ATOM   1829  CG2 VAL A 258      22.004  13.831  36.041  1.00 29.85      A
ATOM   1830  C   VAL A 258      20.002  15.133  34.436  1.00 20.13      A
ATOM   1831  O   VAL A 258      19.056  14.907  35.193  1.00 19.13      A
ATOM   1832  N   VAL A 259      20.367  16.365  34.092  1.00 17.82      A
ATOM   1833  CA  VAL A 259      19.628  17.503  34.621  1.00 12.10      A
ATOM   1834  CB  VAL A 259      20.345  18.816  34.305  1.00  9.61      A
ATOM   1835  CG1 VAL A 259      19.448  20.009  34.655  1.00  9.95      A
ATOM   1836  CG2 VAL A 259      21.661  18.870  35.110  1.00  9.60      A
ATOM   1837  C   VAL A 259      18.257  17.470  33.946  1.00 10.93      A
ATOM   1838  O   VAL A 259      18.154  17.543  32.719  1.00 12.34      A
ATOM   1839  N   PRO A 260      17.185  17.372  34.746  1.00 12.49      A
ATOM   1840  CD  PRO A 260      17.178  17.349  36.227  1.00 15.54      A
ATOM   1841  CA  PRO A 260      15.823  17.321  34.204  1.00 12.14      A
ATOM   1842  CB  PRO A 260      14.992  16.881  35.415  1.00 18.68      A
ATOM   1843  CG  PRO A 260      15.705  17.553  36.556  1.00 20.90      A
ATOM   1844  C   PRO A 260      15.326  18.629  33.592  1.00 13.33      A
ATOM   1845  O   PRO A 260      15.719  19.704  34.025  1.00 11.59      A
ATOM   1846  N   LEU A 261      14.462  18.517  32.583  1.00 10.89      A
ATOM   1847  CA  LEU A 261      13.906  19.697  31.899  1.00 14.89      A
ATOM   1848  CB  LEU A 261      13.190  19.272  30.612  1.00 14.36      A
ATOM   1849  CG  LEU A 261      14.033  18.724  29.470  1.00 23.33      A
ATOM   1850  CD1 LEU A 261      13.132  18.115  28.388  1.00 17.91      A
ATOM   1851  CD2 LEU A 261      14.860  19.854  28.927  1.00 21.86      A
ATOM   1852  C   LEU A 261      12.868  20.354  32.782  1.00 14.14      A
ATOM   1853  O   LEU A 261      12.313  19.715  33.667  1.00 13.00      A
ATOM   1854  N   PRO A 262      12.598  21.646  32.570  1.00 16.56      A
ATOM   1855  CD  PRO A 262      13.154  22.620  31.613  1.00 18.10      A
ATOM   1856  CA  PRO A 262      11.576  22.260  33.421  1.00 16.86      A
ATOM   1857  CB  PRO A 262      11.753  23.752  33.137  1.00 16.37      A
ATOM   1858  CG  PRO A 262      12.147  23.764  31.698  1.00 22.55      A
ATOM   1859  C   PRO A 262      10.239  21.709  32.911  1.00 14.68      A
ATOM   1860  O   PRO A 262      10.136  21.357  31.743  1.00 14.32      A
ATOM   1861  N   ALA A 263       9.234  21.605  33.776  1.00 13.42      A
ATOM   1862  CA  ALA A 263       7.943  21.085  33.344  1.00 16.60      A
ATOM   1863  CB  ALA A 263       6.994  20.952  34.539  1.00 20.02      A
ATOM   1864  C   ALA A 263       7.343  22.011  32.292  1.00 16.04      A
ATOM   1865  O   ALA A 263       7.480  23.235  32.377  1.00 14.70      A
ATOM   1866  N   ALA A 264       6.664  21.426  31.309  1.00 15.42      A
ATOM   1867  CA  ALA A 264       6.050  22.206  30.239  1.00 12.74      A
ATOM   1868  CB  ALA A 264       5.248  21.287  29.308  1.00 19.88      A
ATOM   1869  C   ALA A 264       5.149  23.329  30.747  1.00 15.82      A
ATOM   1870  O   ALA A 264       5.247  24.461  30.264  1.00 17.34      A
ATOM   1871  N   ALA A 265       4.284  23.037  31.721  1.00 13.78      A
ATOM   1872  CA  ALA A 265       3.370  24.071  32.242  1.00 15.17      A
ATOM   1873  CB  ALA A 265       2.464  23.478  33.363  1.00 15.42      A
ATOM   1874  C   ALA A 265       4.057  25.333  32.772  1.00 15.06      A
ATOM   1875  O   ALA A 265       3.437  26.398  32.838  1.00 13.78      A
ATOM   1876  N   ASN A 266       5.320  25.212  33.175  1.00 13.85      A
ATOM   1877  CA  ASN A 266       6.057  26.343  33.733  1.00 12.11      A
ATOM   1878  CB  ASN A 266       6.987  25.895  34.873  1.00 13.94      A
ATOM   1879  CG  ASN A 266       6.253  25.239  36.028  1.00 23.25      A
ATOM   1880  OD1 ASN A 266       5.175  25.676  36.425  1.00 21.92      A
ATOM   1881  ND2 ASN A 266       6.856  24.200  36.592  1.00 19.37      A
ATOM   1882  C   ASN A 266       6.969  27.039  32.730  1.00 12.06      A
ATOM   1883  O   ASN A 266       7.662  27.965  33.100  1.00 13.88      A
ATOM   1884  N   ARG A 267       6.980  26.600  31.483  1.00 10.11      A
ATOM   1885  CA  ARG A 267       7.933  27.162  30.534  1.00 12.44      A
ATOM   1886  CB  ARG A 267       8.029  26.254  29.306  1.00 10.57      A
ATOM   1887  CG  ARG A 267       8.746  24.945  29.675  1.00 12.04      A
ATOM   1888  CD  ARG A 267       8.892  23.924  28.540  1.00  9.95      A
ATOM   1889  NE  ARG A 267       9.275  22.637  29.124  1.00 14.76      A
ATOM   1890  CZ  ARG A 267       9.533  21.530  28.439  1.00 14.94      A
ATOM   1891  NH1 ARG A 267       9.477  21.543  27.118  1.00 16.59      A
ATOM   1892  NH2 ARG A 267       9.782  20.387  29.084  1.00 12.17      A
ATOM   1893  C   ARG A 267       7.785  28.629  30.168  1.00 13.15      A
ATOM   1894  O   ARG A 267       8.658  29.207  29.505  1.00 13.32      A
ATOM   1895  N   GLY A 268       6.711  29.240  30.663  1.00 11.13      A
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FIGURE 5 (continued)

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ATOM   1896  CA  GLY A 268       6.491  30.653  30.439  1.00 13.33      A
ATOM   1897  C   GLY A 268       7.212  31.457  31.507  1.00 13.92      A
ATOM   1898  O   GLY A 268       7.219  32.679  31.452  1.00 14.39      A
ATOM   1899  N   ASP A 269       7.804  30.767  32.486  1.00 11.00      A
ATOM   1900  CA  ASP A 269       8.554  31.398  33.594  1.00 14.58      A
ATOM   1901  CB  ASP A 269       8.233  30.665  34.914  1.00 13.17      A
ATOM   1902  CG  ASP A 269       8.943  31.263  36.117  1.00 16.24      A
ATOM   1903  OD1 ASP A 269       9.767  32.179  35.944  1.00 17.40      A
ATOM   1904  OD2 ASP A 269       8.667  30.804  37.244  1.00 19.44      A
ATOM   1905  C   ASP A 269      10.064  31.290  33.303  1.00 10.72      A
ATOM   1906  O   ASP A 269      10.616  30.196  33.348  1.00 11.39      A
ATOM   1907  N   PRO A 270      10.742  32.417  33.010  1.00 11.52      A
ATOM   1908  CD  PRO A 270      10.217  33.796  32.924  1.00 11.48      A
ATOM   1909  CA  PRO A 270      12.184  32.394  32.709  1.00 10.44      A
ATOM   1910  CB  PRO A 270      12.523  33.867  32.491  1.00 11.04      A
ATOM   1911  CG  PRO A 270      11.225  34.465  32.026  1.00 13.30      A
ATOM   1912  C   PRO A 270      13.042  31.786  33.793  1.00 12.77      A
ATOM   1913  O   PRO A 270      14.097  31.243  33.521  1.00 10.58      A
ATOM   1914  N   ASN A 271      12.578  31.870  35.032  1.00 11.41      A
ATOM   1915  CA  ASN A 271      13.337  31.332  36.145  1.00 11.19      A
ATOM   1916  CB  ASN A 271      12.660  31.729  37.463  1.00 14.43      A
ATOM   1917  CG  ASN A 271      13.533  31.434  38.683  1.00 22.14      A
ATOM   1918  OD1 ASN A 271      14.734  31.726  38.696  1.00 16.89      A
ATOM   1919  ND2 ASN A 271      12.934  30.854  39.703  1.00 16.43      A
ATOM   1920  C   ASN A 271      13.545  29.816  36.090  1.00 16.21      A
ATOM   1921  O   ASN A 271      14.595  29.319  36.510  1.00 15.74      A
ATOM   1922  N   VAL A 272      12.574  29.065  35.575  1.00 10.21      A
ATOM   1923  CA  VAL A 272      12.749  27.613  35.547  1.00 11.32      A
ATOM   1924  CB  VAL A 272      11.378  26.849  35.440  1.00 13.38      A
ATOM   1925  CG1 VAL A 272      10.450  27.297  36.548  1.00 14.31      A
ATOM   1926  CG2 VAL A 272      10.759  27.074  34.078  1.00 11.03      A
ATOM   1927  C   VAL A 272      13.651  27.086  34.434  1.00 12.71      A
ATOM   1928  O   VAL A 272      14.028  25.907  34.459  1.00 10.89      A
ATOM   1929  N   TRP A 273      13.991  27.930  33.461  1.00  7.57      A
ATOM   1930  CA  TRP A 273      14.862  27.465  32.366  1.00  7.83      A
ATOM   1931  CB  TRP A 273      14.741  28.403  31.150  1.00  7.08      A
ATOM   1932  CG  TRP A 273      13.496  28.126  30.364  1.00 10.87      A
ATOM   1933  CD2 TRP A 273      13.359  27.161  29.325  1.00  9.80      A
ATOM   1934  CE2 TRP A 273      12.020  27.228  28.860  1.00  9.21      A
ATOM   1935  CE3 TRP A 273      14.241  26.240  28.732  1.00 10.74      A
ATOM   1936  CD1 TRP A 273      12.271  28.728  30.500  1.00  7.74      A
ATOM   1937  NE1 TRP A 273      11.375  28.192  29.590  1.00 12.31      A
ATOM   1938  CZ2 TRP A 273      11.545  26.412  27.838  1.00 10.97      A
ATOM   1939  CZ3 TRP A 273      13.764  25.428  27.700  1.00 10.91      A
ATOM   1940  CH2 TRP A 273      12.427  25.522  27.267  1.00 14.13      A
ATOM   1941  C   TRP A 273      16.338  27.311  32.755  1.00  9.26      A
ATOM   1942  O   TRP A 273      17.119  26.663  32.042  1.00  9.73      A
ATOM   1943  N   THR A 274      16.736  27.893  33.880  1.00  8.74      A
ATOM   1944  CA  THR A 274      18.123  27.769  34.281  1.00 11.71      A
ATOM   1945  CB  THR A 274      18.759  29.147  34.542  1.00 12.87      A
ATOM   1946  OG1 THR A 274      18.701  29.940  33.334  1.00 16.61      A
ATOM   1947  CG2 THR A 274      20.240  28.973  34.959  1.00  9.96      A
ATOM   1948  C   THR A 274      18.271  26.918  35.535  1.00 10.53      A
ATOM   1949  O   THR A 274      18.020  27.378  36.645  1.00 11.96      A
ATOM   1950  N   PRO A 275      18.673  25.657  35.373  1.00 11.80      A
ATOM   1951  CD  PRO A 275      18.885  24.916  34.119  1.00 13.30      A
ATOM   1952  CA  PRO A 275      18.841  24.782  36.543  1.00 11.14      A
ATOM   1953  CB  PRO A 275      19.180  23.424  35.921  1.00 15.21      A
ATOM   1954  CG  PRO A 275      18.600  23.506  34.528  1.00 15.39      A
ATOM   1955  C   PRO A 275      20.004  25.253  37.445  1.00 12.51      A
ATOM   1956  O   PRO A 275      21.007  25.723  36.950  1.00 12.15      A
ATOM   1957  N   VAL A 276      19.869  25.148  38.764  1.00  9.91      A
ATOM   1958  CA  VAL A 276      20.999  25.502  39.615  1.00 10.08      A
ATOM   1959  CB  VAL A 276      20.738  26.762  40.478  1.00 15.02      A
ATOM   1960  CG1 VAL A 276      20.534  27.990  39.568  1.00 16.57      A
ATOM   1961  CG2 VAL A 276      19.551  26.543  41.388  1.00 17.45      A
ATOM   1962  C   VAL A 276      21.236  24.293  40.500  1.00 12.75      A
ATOM   1963  O   VAL A 276      20.315  23.498  40.743  1.00  7.21      A
ATOM   1964  N   PHE A 277      22.472  24.149  40.969  1.00 13.38      A
ATOM   1965  CA  PHE A 277      22.848  23.017  41.798  1.00 12.43      A
ATOM   1966  CB  PHE A 277      24.231  22.491  41.373  1.00  8.49      A
ATOM   1967  CG  PHE A 277      24.229  21.828  40.017  1.00  8.19      A
ATOM   1968  CD1 PHE A 277      24.404  22.568  38.858  1.00  9.76      A
ATOM   1969  CD2 PHE A 277      23.999  20.461  39.909  1.00  8.15      A
ATOM   1970  CE1 PHE A 277      24.350  21.934  37.585  1.00 13.41      A
ATOM   1971  CE2 PHE A 277      23.938  19.825  38.654  1.00 13.62      A
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FIGURE 5 (continued)

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ATOM   1972  CZ  PHE A 277      24.114  20.555  37.499  1.00  8.74      A
ATOM   1973  C   PHE A 277      22.848  23.377  43.272  1.00 12.19      A
ATOM   1974  O   PHE A 277      22.892  24.553  43.634  1.00 12.80      A
ATOM   1975  N   GLY A 278      22.781  22.356  44.116  1.00 12.01      A
ATOM   1976  CA  GLY A 278      22.767  22.601  45.547  1.00 10.29      A
ATOM   1977  C   GLY A 278      23.113  21.342  46.309  1.00  9.39      A
ATOM   1978  O   GLY A 278      23.379  20.302  45.704  1.00 12.45      A
ATOM   1979  N   ALA A 279      23.087  21.414  47.637  1.00 11.15      A
ATOM   1980  CA  ALA A 279      23.436  20.246  48.450  1.00 14.32      A
ATOM   1981  CB  ALA A 279      23.362  20.604  49.930  1.00 16.91      A
ATOM   1982  C   ALA A 279      22.542  19.029  48.157  1.00 20.18      A
ATOM   1983  O   ALA A 279      23.038  17.896  48.017  1.00 18.69      A
ATOM   1984  N   VAL A 280      21.238  19.262  48.040  1.00 14.35      A
ATOM   1985  CA  VAL A 280      20.302  18.176  47.796  1.00 19.81      A
ATOM   1986  CB  VAL A 280      19.500  17.847  49.076  1.00 23.28      A
ATOM   1987  CG1 VAL A 280      20.457  17.579  50.225  1.00 23.97      A
ATOM   1988  CG2 VAL A 280      18.603  18.992  49.436  1.00 21.87      A
ATOM   1989  C   VAL A 280      19.311  18.483  46.686  1.00 20.63      A
ATOM   1990  O   VAL A 280      19.004  19.635  46.407  1.00 21.63      A
ATOM   1991  N   THR A 281      18.812  17.436  46.055  1.00 20.03      A
ATOM   1992  CA  THR A 281      17.838  17.599  44.982  1.00 19.32      A
ATOM   1993  CB  THR A 281      17.732  16.327  44.136  1.00 20.70      A
ATOM   1994  OG1 THR A 281      18.989  16.096  43.493  1.00 24.83      A
ATOM   1995  CG2 THR A 281      16.637  16.473  43.062  1.00 20.23      A
ATOM   1996  C   THR A 281      16.500  17.882  45.618  1.00 24.45      A
ATOM   1997  O   THR A 281      16.073  17.159  46.520  1.00 22.56      A
ATOM   1998  N   GLY A 282      15.854  18.949  45.164  1.00 22.37      A
ATOM   1999  CA  GLY A 282      14.564  19.316  45.706  1.00 26.62      A
ATOM   2000  C   GLY A 282      14.183  20.735  45.343  1.00 31.11      A
ATOM   2001  O   GLY A 282      15.048  21.603  45.206  1.00 27.54      A
ATOM   2002  N   GLY A 283      12.883  20.971  45.181  1.00 32.42      A
ATOM   2003  CA  GLY A 283      12.401  22.301  44.855  1.00 30.56      A
ATOM   2004  C   GLY A 283      13.051  22.950  43.654  1.00 30.47      A
ATOM   2005  O   GLY A 283      13.307  24.154  43.666  1.00 33.57      A
ATOM   2006  N   GLY A 284      13.298  22.171  42.607  1.00 26.82      A
ATOM   2007  CA  GLY A 284      13.925  22.723  41.415  1.00 26.01      A
ATOM   2008  C   GLY A 284      15.450  22.687  41.439  1.00 26.04      A
ATOM   2009  O   GLY A 284      16.115  22.822  40.406  1.00 25.82      A
ATOM   2010  N   VAL A 285      16.022  22.521  42.622  1.00 19.46      A
ATOM   2011  CA  VAL A 285      17.467  22.461  42.722  1.00 19.85      A
ATOM   2012  CB  VAL A 285      17.903  22.894  44.135  1.00 19.90      A
ATOM   2013  CG1 VAL A 285      19.389  22.673  44.319  1.00 16.38      A
ATOM   2014  CG2 VAL A 285      17.521  24.376  44.360  1.00 20.29      A
ATOM   2015  C   VAL A 285      17.958  21.037  42.428  1.00 18.72      A
ATOM   2016  O   VAL A 285      17.298  20.055  42.794  1.00 18.51      A
ATOM   2017  N   VAL A 286      19.103  20.932  41.755  1.00 14.01      A
ATOM   2018  CA  VAL A 286      19.706  19.645  41.423  1.00 16.59      A
ATOM   2019  CB  VAL A 286      20.200  19.625  39.964  1.00 14.25      A
ATOM   2020  CG1 VAL A 286      20.729  18.254  39.623  1.00 19.16      A
ATOM   2021  CG2 VAL A 286      19.068  19.997  39.036  1.00 20.67      A
ATOM   2022  C   VAL A 286      20.917  19.416  42.325  1.00 17.27      A
ATOM   2023  O   VAL A 286      21.757  20.302  42.484  1.00 13.49      A
ATOM   2024  N   ALA A 287      21.041  18.229  42.896  1.00 15.01      A
ATOM   2025  CA  ALA A 287      22.188  18.000  43.778  1.00 17.78      A
ATOM   2026  CB  ALA A 287      22.039  16.649  44.527  1.00 16.62      A
ATOM   2027  C   ALA A 287      23.483  18.011  42.999  1.00 12.88      A
ATOM   2028  O   ALA A 287      23.520  17.533  41.854  1.00 10.29      A
ATOM   2029  N   TYR A 288      24.538  18.576  43.603  1.00 11.08      A
ATOM   2030  CA  TYR A 288      25.867  18.554  42.979  1.00  8.88      A
ATOM   2031  CB  TYR A 288      26.877  19.297  43.862  1.00 12.41      A
ATOM   2032  CG  TYR A 288      26.891  20.803  43.649  1.00  9.59      A
ATOM   2033  CD1 TYR A 288      26.329  21.677  44.589  1.00  8.82      A
ATOM   2034  CE1 TYR A 288      26.320  23.086  44.382  1.00 10.11      A
ATOM   2035  CD2 TYR A 288      27.463  21.356  42.491  1.00 10.87      A
ATOM   2036  CE2 TYR A 288      27.464  22.744  42.275  1.00  6.63      A
ATOM   2037  CZ  TYR A 288      26.883  23.601  43.223  1.00  7.60      A
ATOM   2038  OH  TYR A 288      26.842  24.960  42.960  1.00  7.46      A
ATOM   2039  C   TYR A 288      26.263  17.061  42.851  1.00 12.67      A
ATOM   2040  O   TYR A 288      25.989  16.265  43.750  1.00 10.55      A
ATOM   2041  N   PRO A 289      26.929  16.672  41.746  1.00 12.61      A
ATOM   2042  CD  PRO A 289      27.338  17.560  40.625  1.00 13.50      A
ATOM   2043  CA  PRO A 289      27.346  15.280  41.495  1.00 12.99      A
ATOM   2044  CB  PRO A 289      27.863  15.328  40.051  1.00 15.51      A
ATOM   2045  CG  PRO A 289      28.424  16.734  39.920  1.00 10.53      A
ATOM   2046  C   PRO A 289      28.366  14.644  42.439  1.00 17.46      A
ATOM   2047  O   PRO A 289      29.342  15.282  42.835  1.00 15.29      A
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FIGURE 5 (continued)

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ATOM   2048  N   ASP A 290      28.149  13.372  42.782  1.00 16.57      A
ATOM   2049  CA  ASP A 290      29.092  12.691  43.652  1.00 20.97      A
ATOM   2050  CB  ASP A 290      28.360  11.751  44.628  1.00 25.52      A
ATOM   2051  CG  ASP A 290      27.489  10.723  43.929  1.00 34.64      A
ATOM   2052  OD1 ASP A 290      26.599  10.146  44.604  1.00 38.07      A
ATOM   2053  OD2 ASP A 290      27.693  10.478  42.716  1.00 39.24      A
ATOM   2054  C   ASP A 290      30.154  11.952  42.824  1.00 21.23      A
ATOM   2055  O   ASP A 290      30.990  11.231  43.362  1.00 21.11      A
ATOM   2056  N   SER A 291      30.136  12.152  41.509  1.00 14.24      A
ATOM   2057  CA  SER A 291      31.143  11.538  40.645  1.00 16.28      A
ATOM   2058  CB  SER A 291      30.592  10.290  39.925  1.00 16.14      A
ATOM   2059  OG  SER A 291      29.549  10.625  39.031  1.00 22.17      A
ATOM   2060  C   SER A 291      31.555  12.609  39.643  1.00 14.75      A
ATOM   2061  O   SER A 291      30.842  13.605  39.493  1.00 13.50      A
ATOM   2062  N   GLY A 292      32.692  12.419  38.971  1.00 13.79      A
ATOM   2063  CA  GLY A 292      33.181  13.423  38.019  1.00 14.60      A
ATOM   2064  C   GLY A 292      33.713  14.688  38.707  1.00 11.05      A
ATOM   2065  O   GLY A 292      33.964  14.669  39.909  1.00 14.10      A
ATOM   2066  N   TYR A 293      33.904  15.779  37.955  1.00 10.56      A
ATOM   2067  CA  TYR A 293      34.380  17.049  38.529  1.00  9.23      A
ATOM   2068  CB  TYR A 293      34.838  18.014  37.443  1.00 10.30      A
ATOM   2069  CG  TYR A 293      35.535  19.229  38.012  1.00 11.13      A
ATOM   2070  CD1 TYR A 293      36.829  19.138  38.526  1.00  7.85      A
ATOM   2071  CE1 TYR A 293      37.482  20.269  39.049  1.00  8.64      A
ATOM   2072  CD2 TYR A 293      34.900  20.470  38.038  1.00 11.82      A
ATOM   2073  CE2 TYR A 293      35.547  21.601  38.554  1.00 11.43      A
ATOM   2074  CZ  TYR A 293      36.839  21.488  39.052  1.00  8.40      A
ATOM   2075  OH  TYR A 293      37.488  22.625  39.496  1.00  8.49      A
ATOM   2076  C   TYR A 293      33.183  17.645  39.252  1.00  9.71      A
ATOM   2077  O   TYR A 293      32.142  17.834  38.657  1.00 12.02      A
ATOM   2078  N   PRO A 294      33.347  18.021  40.531  1.00 12.25      A
ATOM   2079  CD  PRO A 294      34.575  17.923  41.350  1.00 12.44      A
ATOM   2080  CA  PRO A 294      32.229  18.559  41.302  1.00 14.24      A
ATOM   2081  CB  PRO A 294      32.644  18.263  42.748  1.00 12.15      A
ATOM   2082  CG  PRO A 294      34.132  18.499  42.712  1.00 15.49      A
ATOM   2083  C   PRO A 294      31.682  19.963  41.133  1.00 13.85      A
ATOM   2084  O   PRO A 294      30.511  20.171  41.429  1.00 11.37      A
ATOM   2085  N   ILE A 295      32.476  20.907  40.628  1.00 10.88      A
ATOM   2086  CA  ILE A 295      31.990  22.280  40.510  1.00  9.12      A
ATOM   2087  CB  ILE A 295      33.062  23.301  40.934  1.00 10.07      A
ATOM   2088  CG2 ILE A 295      32.375  24.666  41.232  1.00 10.52      A
ATOM   2089  CG1 ILE A 295      33.733  22.853  42.236  1.00 12.06      A
ATOM   2090  CD1 ILE A 295      34.841  23.801  42.703  1.00 12.46      A
ATOM   2091  C   ILE A 295      31.564  22.574  39.087  1.00 12.87      A
ATOM   2092  O   ILE A 295      32.397  22.660  38.182  1.00 10.57      A
ATOM   2093  N   LEU A 296      30.257  22.743  38.902  1.00 10.82      A
ATOM   2094  CA  LEU A 296      29.703  22.951  37.570  1.00  8.61      A
ATOM   2095  CB  LEU A 296      29.370  21.578  36.949  1.00  9.63      A
ATOM   2096  CG  LEU A 296      28.032  20.884  37.276  1.00  7.75      A
ATOM   2097  CD1 LEU A 296      27.971  19.517  36.572  1.00 11.60      A
ATOM   2098  CD2 LEU A 296      27.852  20.690  38.784  1.00 10.20      A
ATOM   2099  C   LEU A 296      28.461  23.828  37.612  1.00  7.00      A
ATOM   2100  O   LEU A 296      27.945  24.137  38.690  1.00 11.47      A
ATOM   2101  N   GLY A 297      27.988  24.236  36.436  1.00  8.98      A
ATOM   2102  CA  GLY A 297      26.812  25.093  36.353  1.00  8.75      A
ATOM   2103  C   GLY A 297      26.503  25.452  34.906  1.00 14.03      A
ATOM   2104  O   GLY A 297      27.128  24.917  33.979  1.00  9.23      A
ATOM   2105  N   PHE A 298      25.544  26.353  34.700  1.00  7.40      A
ATOM   2106  CA  PHE A 298      25.177  26.758  33.350  1.00  7.84      A
ATOM   2107  CB  PHE A 298      23.666  26.550  33.105  1.00  6.30      A
ATOM   2108  CG  PHE A 298      23.249  25.102  32.984  1.00 10.10      A
ATOM   2109  CD1 PHE A 298      22.775  24.398  34.094  1.00  9.62      A
ATOM   2110  CD2 PHE A 298      23.356  24.444  31.763  1.00  8.37      A
ATOM   2111  CE1 PHE A 298      22.414  23.038  33.988  1.00 13.84      A
ATOM   2112  CE2 PHE A 298      23.005  23.087  31.630  1.00  7.19      A
ATOM   2113  CZ  PHE A 298      22.533  22.379  32.747  1.00 12.00      A
ATOM   2114  C   PHE A 298      25.469  28.235  33.145  1.00 10.22      A
ATOM   2115  O   PHE A 298      25.431  29.007  34.114  1.00  9.27      A
ATOM   2116  N   THR A 299      25.811  28.615  31.910  1.00  7.04      A
ATOM   2117  CA  THR A 299      25.961  30.029  31.594  1.00  8.99      A
ATOM   2118  CB  THR A 299      27.319  30.414  30.975  1.00 12.65      A
ATOM   2119  OG1 THR A 299      27.293  31.818  30.682  1.00 10.67      A
ATOM   2120  CG2 THR A 299      27.616  29.617  29.740  1.00 12.18      A
ATOM   2121  C   THR A 299      24.798  30.220  30.616  1.00  8.12      A
ATOM   2122  O   THR A 299      24.482  29.325  29.810  1.00  9.48      A
ATOM   2123  N   ASP A 300      24.173  31.392  30.677  1.00  8.49      A
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FIGURE 5 (continued)

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ATOM   2124  CA  ASP A 300      22.930  31.636  29.950  1.00 10.66      A
ATOM   2125  CB  ASP A 300      21.849  31.816  31.023  1.00  8.23      A
ATOM   2126  CG  ASP A 300      22.055  30.877  32.193  1.00 14.11      A
ATOM   2127  OD1 ASP A 300      22.141  29.660  31.928  1.00  8.23      A
ATOM   2128  OD2 ASP A 300      22.149  31.341  33.373  1.00 15.65      A
ATOM   2129  C   ASP A 300      22.828  32.790  28.975  1.00 10.65      A
ATOM   2130  O   ASP A 300      23.690  33.669  28.931  1.00  8.49      A
ATOM   2131  N   LEU A 301      21.740  32.765  28.202  1.00  8.77      A
ATOM   2132  CA  LEU A 301      21.407  33.819  27.246  1.00 10.49      A
ATOM   2133  CB  LEU A 301      21.121  33.226  25.850  1.00 10.57      A
ATOM   2134  CG  LEU A 301      22.189  32.371  25.157  1.00 17.61      A
ATOM   2135  CD1 LEU A 301      21.699  31.951  23.775  1.00 16.46      A
ATOM   2136  CD2 LEU A 301      23.456  33.151  25.057  1.00 12.96      A
ATOM   2137  C   LEU A 301      20.128  34.533  27.689  1.00  7.85      A
ATOM   2138  O   LEU A 301      19.179  33.889  28.127  1.00  7.63      A
ATOM   2139  N   ILE A 302      20.101  35.855  27.564  1.00  8.91      A
ATOM   2140  CA  ILE A 302      18.897  36.614  27.879  1.00  7.82      A
ATOM   2141  CB  ILE A 302      19.146  37.648  29.000  1.00 10.36      A
ATOM   2142  CG2 ILE A 302      17.848  38.429  29.261  1.00 12.51      A
ATOM   2143  CG1 ILE A 302      19.588  36.918  30.287  1.00  8.81      A
ATOM   2144  CD1 ILE A 302      20.089  37.867  31.411  1.00  7.82      A
ATOM   2145  C   ILE A 302      18.517  37.368  26.602  1.00  9.48      A
ATOM   2146  O   ILE A 302      19.320  38.158  26.096  1.00  8.44      A
ATOM   2147  N   PHE A 303      17.311  37.120  26.081  1.00  8.80      A
ATOM   2148  CA  PHE A 303      16.843  37.786  24.854  1.00  8.37      A
ATOM   2149  CB  PHE A 303      16.751  36.821  23.651  1.00  7.07      A
ATOM   2150  CG  PHE A 303      18.054  36.583  22.944  1.00  8.30      A
ATOM   2151  CD1 PHE A 303      19.027  35.770  23.500  1.00  8.48      A
ATOM   2152  CD2 PHE A 303      18.316  37.205  21.725  1.00  7.08      A
ATOM   2153  CE1 PHE A 303      20.265  35.582  22.851  1.00  7.30      A
ATOM   2154  CE2 PHE A 303      19.559  37.023  21.065  1.00  9.28      A
ATOM   2155  CZ  PHE A 303      20.528  36.210  21.637  1.00 11.64      A
ATOM   2156  C   PHE A 303      15.437  38.305  25.032  1.00  9.03      A
ATOM   2157  O   PHE A 303      14.797  38.052  26.031  1.00  9.30      A
ATOM   2158  N   SER A 304      14.947  39.002  24.014  1.00  7.56      A
ATOM   2159  CA  SER A 304      13.566  39.465  24.044  1.00  9.72      A
ATOM   2160  CB  SER A 304      13.470  40.870  23.444  1.00 11.08      A
ATOM   2161  OG  SER A 304      12.117  41.291  23.498  1.00 10.08      A
ATOM   2162  C   SER A 304      12.707  38.530  23.170  1.00  6.80      A
ATOM   2163  O   SER A 304      13.198  38.018  22.162  1.00 10.90      A
ATOM   2164  N   GLU A 305      11.451  38.293  23.534  1.00  8.14      A
ATOM   2165  CA  GLU A 305      10.605  37.482  22.655  1.00 11.11      A
ATOM   2166  CB  GLU A 305       9.268  37.125  23.316  1.00 10.66      A
ATOM   2167  CG  GLU A 305       8.447  36.161  22.439  1.00 11.71      A
ATOM   2168  CD  GLU A 305       7.073  35.820  22.985  1.00 12.77      A
ATOM   2169  OE1 GLU A 305       6.767  36.154  24.147  1.00 14.12      A
ATOM   2170  OE2 GLU A 305       6.288  35.192  22.228  1.00 16.70      A
ATOM   2171  C   GLU A 305      10.305  38.329  21.399  1.00 15.34      A
ATOM   2172  O   GLU A 305      10.154  37.800  20.283  1.00 10.74      A
ATOM   2173  N   CYS A 306      10.239  39.649  21.574  1.00 11.86      A
ATOM   2174  CA  CYS A 306       9.889  40.534  20.450  1.00 12.96      A
ATOM   2175  C   CYS A 306      10.859  41.666  20.140  1.00 14.14      A
ATOM   2176  O   CYS A 306      11.434  42.270  21.046  1.00 11.98      A
ATOM   2177  CB  CYS A 306       8.531  41.185  20.726  1.00 11.40      A
ATOM   2178  SG  CYS A 306       7.188  40.111  21.313  1.00 15.63      A
ATOM   2179  N   TYR A 307      11.017  41.956  18.854  1.00 12.82      A
ATOM   2180  CA  TYR A 307      11.872  43.060  18.397  1.00 10.85      A
ATOM   2181  CB  TYR A 307      13.143  42.533  17.712  1.00  8.88      A
ATOM   2182  CG  TYR A 307      14.066  41.850  18.703  1.00 13.96      A
ATOM   2183  CD1 TYR A 307      13.902  40.499  19.020  1.00 13.44      A
ATOM   2184  CE1 TYR A 307      14.683  39.882  20.020  1.00 13.43      A
ATOM   2185  CD2 TYR A 307      15.035  42.579  19.401  1.00 11.32      A
ATOM   2186  CE2 TYR A 307      15.821  41.972  20.410  1.00 11.99      A
ATOM   2187  CZ  TYR A 307      15.637  40.625  20.712  1.00 12.10      A
ATOM   2188  OH  TYR A 307      16.379  40.019  21.724  1.00 12.32      A
ATOM   2189  C   TYR A 307      11.056  43.908  17.424  1.00 13.04      A
ATOM   2190  O   TYR A 307      10.318  43.370  16.588  1.00 11.71      A
ATOM   2191  N   ALA A 308      11.161  45.229  17.546  1.00 13.47      A
ATOM   2192  CA  ALA A 308      10.420  46.123  16.660  1.00 19.16      A
ATOM   2193  CB  ALA A 308      10.623  47.583  17.116  1.00 19.39      A
ATOM   2194  C   ALA A 308      10.827  45.960  15.176  1.00 16.58      A
ATOM   2195  O   ALA A 308       9.990  46.011  14.290  1.00 15.94      A
ATOM   2196  N   ASN A 309      12.109  45.752  14.919  1.00 16.56      A
ATOM   2197  CA  ASN A 309      12.621  45.602  13.565  1.00 15.71      A
ATOM   2198  CB  ASN A 309      14.084  46.052  13.558  1.00 11.74      A
ATOM   2199  CG  ASN A 309      14.704  46.002  12.183  1.00 20.62      A
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FIGURE 5 (continued)

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ATOM   2200  OD1 ASN A 309      15.130  44.946  11.713  1.00 17.26      A
ATOM   2201  ND2 ASN A 309      14.741  47.153  11.517  1.00 13.84      A
ATOM   2202  C   ASN A 309      12.493  44.142  13.066  1.00 16.39      A
ATOM   2203  O   ASN A 309      13.031  43.221  13.678  1.00 11.54      A
ATOM   2204  N   ALA A 310      11.806  43.942  11.941  1.00 12.69      A
ATOM   2205  CA  ALA A 310      11.583  42.584  11.430  1.00 16.06      A
ATOM   2206  CB  ALA A 310      10.564  42.618  10.281  1.00 16.44      A
ATOM   2207  C   ALA A 310      12.836  41.828  10.997  1.00 14.76      A
ATOM   2208  O   ALA A 310      12.907  40.599  11.128  1.00 15.90      A
ATOM   2209  N   THR A 311      13.827  42.546  10.485  1.00 13.61      A
ATOM   2210  CA  THR A 311      15.074  41.922  10.069  1.00 14.28      A
ATOM   2211  CB  THR A 311      15.949  42.927   9.314  1.00 15.47      A
ATOM   2212  OG1 THR A 311      15.284  43.307   8.097  1.00 18.10      A
ATOM   2213  CG2 THR A 311      17.291  42.322   8.977  1.00 16.40      A
ATOM   2214  C   THR A 311      15.813  41.407  11.324  1.00 15.00      A
ATOM   2215  O   THR A 311      16.371  40.313  11.318  1.00 12.29      A
ATOM   2216  N   GLN A 312      15.798  42.180  12.409  1.00 13.08      A
ATOM   2217  CA  GLN A 312      16.477  41.717  13.623  1.00 12.35      A
ATOM   2218  CB  GLN A 312      16.545  42.827  14.682  1.00 10.08      A
ATOM   2219  CG  GLN A 312      17.501  43.960  14.273  1.00  7.89      A
ATOM   2220  CD  GLN A 312      17.696  44.997  15.377  1.00 13.93      A
ATOM   2221  OE1 GLN A 312      16.897  45.087  16.311  1.00 14.28      A
ATOM   2222  NE2 GLN A 312      18.743  45.799  15.255  1.00 16.18      A
ATOM   2223  C   GLN A 312      15.768  40.486  14.191  1.00 11.19      A
ATOM   2224  O   GLN A 312      16.418  39.537  14.639  1.00 14.09      A
ATOM   2225  N   THR A 313      14.439  40.507  14.189  1.00  9.72      A
ATOM   2226  CA  THR A 313      13.670  39.363  14.685  1.00  8.88      A
ATOM   2227  CB  THR A 313      12.149  39.541  14.449  1.00 13.95      A
ATOM   2228  OG1 THR A 313      11.660  40.660  15.197  1.00 14.46      A
ATOM   2229  CG2 THR A 313      11.398  38.288  14.882  1.00 12.76      A
ATOM   2230  C   THR A 313      14.108  38.096  13.935  1.00 10.80      A
ATOM   2231  O   THR A 313      14.318  37.042  14.538  1.00 11.41      A
ATOM   2232  N   GLY A 314      14.218  38.204  12.615  1.00 11.55      A
ATOM   2233  CA  GLY A 314      14.628  37.067  11.810  1.00 12.96      A
ATOM   2234  C   GLY A 314      16.060  36.638  12.090  1.00 10.31      A
ATOM   2235  O   GLY A 314      16.370  35.439  12.111  1.00 11.80      A
ATOM   2236  N   GLN A 315      16.952  37.603  12.291  1.00 10.00      A
ATOM   2237  CA  GLN A 315      18.360  37.280  12.586  1.00 10.98      A
ATOM   2238  CB  GLN A 315      19.219  38.542  12.512  1.00 12.34      A
ATOM   2239  CG  GLN A 315      19.286  39.069  11.071  1.00 13.86      A
ATOM   2240  CD  GLN A 315      20.014  40.385  10.958  1.00 16.05      A
ATOM   2241  OE1 GLN A 315      19.868  41.254  11.818  1.00 15.65      A
ATOM   2242  NE2 GLN A 315      20.787  40.552   9.880  1.00 15.34      A
ATOM   2243  C   GLN A 315      18.518  36.613  13.952  1.00 11.33      A
ATOM   2244  O   GLN A 315      19.385  35.743  14.136  1.00 12.86      A
ATOM   2245  N   VAL A 316      17.677  37.006  14.909  1.00 11.99      A
ATOM   2246  CA  VAL A 316      17.719  36.389  16.238  1.00 11.29      A
ATOM   2247  CB  VAL A 316      16.803  37.131  17.251  1.00 12.97      A
ATOM   2248  CG1 VAL A 316      16.658  36.292  18.541  1.00 12.95      A
ATOM   2249  CG2 VAL A 316      17.401  38.493  17.602  1.00 11.75      A
ATOM   2250  C   VAL A 316      17.232  34.929  16.092  1.00 13.11      A
ATOM   2251  O   VAL A 316      17.813  33.996  16.667  1.00 12.64      A
ATOM   2252  N   ARG A 317      16.164  34.723  15.327  1.00  9.04      A
ATOM   2253  CA  ARG A 317      15.672  33.364  15.115  1.00 12.87      A
ATOM   2254  CB  ARG A 317      14.348  33.372  14.303  1.00 14.06      A
ATOM   2255  CG  ARG A 317      13.148  33.951  15.076  1.00 13.07      A
ATOM   2256  CD  ARG A 317      11.823  33.964  14.243  1.00 14.93      A
ATOM   2257  NE  ARG A 317      11.520  32.611  13.765  1.00 14.57      A
ATOM   2258  CZ  ARG A 317      10.894  31.677  14.480  1.00 10.03      A
ATOM   2259  NH1 ARG A 317      10.470  31.934  15.704  1.00  9.62      A
ATOM   2260  NH2 ARG A 317      10.730  30.461  13.983  1.00 13.56      A
ATOM   2261  C   ARG A 317      16.730  32.491  14.434  1.00 12.01      A
ATOM   2262  O   ARG A 317      16.879  31.320  14.783  1.00 12.09      A
ATOM   2263  N   ASN A 318      17.462  33.033  13.464  1.00 11.68      A
ATOM   2264  CA  ASN A 318      18.503  32.246  12.796  1.00 13.18      A
ATOM   2265  CB  ASN A 318      19.123  33.028  11.629  1.00 11.52      A
ATOM   2266  CG  ASN A 318      18.145  33.249  10.500  1.00 15.15      A
ATOM   2267  OD1 ASN A 318      17.140  32.557  10.402  1.00 13.70      A
ATOM   2268  ND2 ASN A 318      18.438  34.211   9.638  1.00 17.31      A
ATOM   2269  C   ASN A 318      19.613  31.841  13.771  1.00 12.19      A
ATOM   2270  O   ASN A 318      20.207  30.753  13.658  1.00  9.01      A
ATOM   2271  N   PHE A 319      19.904  32.715  14.733  1.00 10.68      A
ATOM   2272  CA  PHE A 319      20.936  32.376  15.707  1.00  9.90      A
ATOM   2273  CB  PHE A 319      21.274  33.577  16.584  1.00  7.66      A
ATOM   2274  CG  PHE A 319      22.105  33.212  17.794  1.00 10.09      A
ATOM   2275  CD1 PHE A 319      23.351  32.644  17.631  1.00  6.01      A
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FIGURE 5 (continued)

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ATOM   2276  CD2 PHE A 319      21.593  33.356  19.087  1.00 10.54      A
ATOM   2277  CE1 PHE A 319      24.102  32.203  18.738  1.00 12.72      A
ATOM   2278  CE2 PHE A 319      22.333  32.919  20.212  1.00 15.07      A
ATOM   2279  CZ  PHE A 319      23.589  32.338  20.027  1.00 12.59      A
ATOM   2280  C   PHE A 319      20.449  31.222  16.587  1.00 10.27      A
ATOM   2281  O   PHE A 319      21.203  30.282  16.868  1.00 12.47      A
ATOM   2282  N   PHE A 320      19.188  31.275  17.013  1.00 10.21      A
ATOM   2283  CA  PHE A 320      18.649  30.213  17.860  1.00 10.79      A
ATOM   2284  CB  PHE A 320      17.247  30.581  18.363  1.00  9.11      A
ATOM   2285  CG  PHE A 320      17.246  31.285  19.698  1.00  7.96      A
ATOM   2286  CD1 PHE A 320      16.762  30.642  20.833  1.00  9.52      A
ATOM   2287  CD2 PHE A 320      17.723  32.583  19.822  1.00 12.60      A
ATOM   2288  CE1 PHE A 320      16.750  31.282  22.082  1.00  6.69      A
ATOM   2289  CE2 PHE A 320      17.712  33.244  21.075  1.00  9.45      A
ATOM   2290  CZ  PHE A 320      17.220  32.579  22.209  1.00  8.89      A
ATOM   2291  C   PHE A 320      18.598  28.912  17.089  1.00  7.76      A
ATOM   2292  O   PHE A 320      18.856  27.838  17.634  1.00  9.90      A
ATOM   2293  N   THR A 321      18.274  29.013  15.801  1.00  8.04      A
ATOM   2294  CA  THR A 321      18.199  27.829  14.950  1.00  6.79      A
ATOM   2295  CB  THR A 321      17.687  28.224  13.551  1.00  7.01      A
ATOM   2296  OG1 THR A 321      16.334  28.695  13.691  1.00 11.25      A
ATOM   2297  CG2 THR A 321      17.731  27.032  12.573  1.00  9.32      A
ATOM   2298  C   THR A 321      19.535  27.128  14.872  1.00 11.09      A
ATOM   2299  O   THR A 321      19.594  25.896  14.823  1.00 10.46      A
ATOM   2300  N   LYS A 322      20.617  27.904  14.873  1.00  8.41      A
ATOM   2301  CA  LYS A 322      21.950  27.319  14.849  1.00  8.00      A
ATOM   2302  CB  LYS A 322      22.970  28.329  14.299  1.00  6.38      A
ATOM   2303  CG  LYS A 322      24.410  27.805  14.359  1.00 10.15      A
ATOM   2304  CD  LYS A 322      25.396  28.712  13.615  1.00  8.08      A
ATOM   2305  CE  LYS A 322      26.665  27.922  13.317  1.00 11.78      A
ATOM   2306  NZ  LYS A 322      27.577  28.702  12.437  1.00 18.79      A
ATOM   2307  C   LYS A 322      22.415  26.857  16.242  1.00  9.52      A
ATOM   2308  O   LYS A 322      22.864  25.711  16.425  1.00  9.02      A
ATOM   2309  N   HIS A 323      22.289  27.735  17.231  1.00 10.06      A
ATOM   2310  CA  HIS A 323      22.793  27.420  18.569  1.00  9.00      A
ATOM   2311  CB  HIS A 323      22.710  28.677  19.469  1.00  7.78      A
ATOM   2312  CG  HIS A 323      23.655  28.657  20.637  1.00  9.56      A
ATOM   2313  CD2 HIS A 323      23.426  28.762  21.970  1.00  9.53      A
ATOM   2314  ND1 HIS A 323      25.028  28.560  20.494  1.00  7.88      A
ATOM   2315  CE1 HIS A 323      25.602  28.615  21.683  1.00  9.47      A
ATOM   2316  NE2 HIS A 323      24.653  28.736  22.598  1.00 12.97      A
ATOM   2317  C   HIS A 323      22.082  26.230  19.222  1.00  9.52      A
ATOM   2318  O   HIS A 323      22.687  25.507  20.019  1.00  8.65      A
ATOM   2319  N   TYR A 324      20.808  26.034  18.877  1.00  9.61      A
ATOM   2320  CA  TYR A 324      20.024  24.911  19.427  1.00 10.38      A
ATOM   2321  CB  TYR A 324      18.767  25.434  20.149  1.00  6.95      A
ATOM   2322  CG  TYR A 324      19.137  26.376  21.277  1.00  7.33      A
ATOM   2323  CD1 TYR A 324      19.195  27.752  21.072  1.00  5.99      A
ATOM   2324  CE1 TYR A 324      19.656  28.618  22.097  1.00  8.99      A
ATOM   2325  CD2 TYR A 324      19.533  25.882  22.513  1.00  7.61      A
ATOM   2326  CE2 TYR A 324      19.994  26.731  23.525  1.00  5.98      A
ATOM   2327  CZ  TYR A 324      20.052  28.094  23.303  1.00  7.54      A
ATOM   2328  OH  TYR A 324      20.547  28.926  24.294  1.00  7.56      A
ATOM   2329  C   TYR A 324      19.627  23.893  18.338  1.00  7.02      A
ATOM   2330  O   TYR A 324      18.677  23.118  18.498  1.00 10.94      A
ATOM   2331  N   GLY A 325      20.387  23.868  17.254  1.00  7.94      A
ATOM   2332  CA  GLY A 325      20.064  22.938  16.181  1.00  7.51      A
ATOM   2333  C   GLY A 325      20.514  21.493  16.386  1.00 12.01      A
ATOM   2334  O   GLY A 325      21.492  21.227  17.097  1.00 10.59      A
ATOM   2335  N   THR A 326      19.788  20.564  15.752  1.00  8.75      A
ATOM   2336  CA  THR A 326      20.113  19.132  15.790  1.00 10.25      A
ATOM   2337  CB  THR A 326      19.005  18.311  15.135  1.00  9.46      A
ATOM   2338  OG1 THR A 326      17.759  18.707  15.708  1.00 10.73      A
ATOM   2339  CG2 THR A 326      19.212  16.788  15.369  1.00  7.67      A
ATOM   2340  C   THR A 326      21.432  18.937  15.038  1.00  9.78      A
ATOM   2341  O   THR A 326      22.278  18.131  15.452  1.00 10.90      A
ATOM   2342  N   SER A 327      21.614  19.688  13.953  1.00 12.37      A
ATOM   2343  CA  SER A 327      22.858  19.666  13.176  1.00 11.58      A
ATOM   2344  CB  SER A 327      22.743  18.752  11.935  1.00 14.65      A
ATOM   2345  OG  SER A 327      21.725  19.192  11.051  1.00 10.13      A
ATOM   2346  C   SER A 327      23.158  21.118  12.764  1.00 10.87      A
ATOM   2347  O   SER A 327      22.419  22.031  13.149  1.00  9.05      A
ATOM   2348  N   ALA A 328      24.228  21.331  12.000  1.00 11.22      A
ATOM   2349  CA  ALA A 328      24.637  22.690  11.567  1.00 10.30      A
ATOM   2350  CB  ALA A 328      23.682  23.234  10.518  1.00 12.01      A
ATOM   2351  C   ALA A 328      24.602  23.592  12.790  1.00 11.88      A
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FIGURE 5 (continued)

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ATOM   2352  O   ALA A 328      24.046  24.674  12.742  1.00 13.69      A
ATOM   2353  N   ASN A 329      25.197  23.140  13.887  1.00 11.26      A
ATOM   2354  CA  ASN A 329      25.150  23.910  15.123  1.00 10.51      A
ATOM   2355  CB  ASN A 329      24.422  23.083  16.205  1.00  8.81      A
ATOM   2356  CG  ASN A 329      25.132  21.771  16.536  1.00  9.32      A
ATOM   2357  OD1 ASN A 329      26.352  21.717  16.573  1.00 11.49      A
ATOM   2358  ND2 ASN A 329      24.360  20.714  16.792  1.00 10.75      A
ATOM   2359  C   ASN A 329      26.526  24.402  15.604  1.00 12.21      A
ATOM   2360  O   ASN A 329      27.515  24.381  14.849  1.00  9.35      A
ATOM   2361  N   ASP A 330      26.586  24.863  16.851  1.00 10.38      A
ATOM   2362  CA  ASP A 330      27.837  25.386  17.412  1.00  9.41      A
ATOM   2363  CB  ASP A 330      27.575  26.677  18.208  1.00 10.91      A
ATOM   2364  CG  ASP A 330      27.239  27.852  17.331  1.00 13.71      A
ATOM   2365  OD1 ASP A 330      26.333  28.653  17.720  1.00 14.93      A
ATOM   2366  OD2 ASP A 330      27.880  27.981  16.261  1.00 10.16      A
ATOM   2367  C   ASP A 330      28.536  24.416  18.346  1.00 10.31      A
ATOM   2368  O   ASP A 330      29.484  24.809  19.029  1.00  8.29      A
ATOM   2369  N   ASN A 331      28.111  23.153  18.363  1.00  8.79      A
ATOM   2370  CA  ASN A 331      28.698  22.217  19.311  1.00 10.91      A
ATOM   2371  CB  ASN A 331      27.942  20.869  19.267  1.00 11.40      A
ATOM   2372  CG  ASN A 331      26.579  20.924  19.989  1.00 15.36      A
ATOM   2373  OD1 ASN A 331      25.926  19.893  20.194  1.00 12.09      A
ATOM   2374  ND2 ASN A 331      26.156  22.115  20.372  1.00  9.71      A
ATOM   2375  C   ASN A 331      30.220  22.012  19.218  1.00 12.28      A
ATOM   2376  O   ASN A 331      30.877  21.866  20.255  1.00 12.57      A
ATOM   2377  N   ALA A 332      30.795  22.001  18.012  1.00 10.00      A
ATOM   2378  CA  ALA A 332      32.252  21.842  17.903  1.00 12.41      A
ATOM   2379  CB  ALA A 332      32.677  21.733  16.445  1.00 12.06      A
ATOM   2380  C   ALA A 332      32.964  23.028  18.548  1.00  8.53      A
ATOM   2381  O   ALA A 332      33.973  22.872  19.247  1.00 11.75      A
ATOM   2382  N   ALA A 333      32.447  24.216  18.297  1.00  9.64      A
ATOM   2383  CA  ALA A 333      33.057  25.422  18.858  1.00 10.83      A
ATOM   2384  CB  ALA A 333      32.424  26.655  18.223  1.00  9.42      A
ATOM   2385  C   ALA A 333      32.910  25.473  20.379  1.00 10.44      A
ATOM   2386  O   ALA A 333      33.787  25.982  21.096  1.00  9.81      A
ATOM   2387  N   ILE A 334      31.787  24.963  20.869  1.00  9.49      A
ATOM   2388  CA  ILE A 334      31.536  24.919  22.305  1.00 10.34      A
ATOM   2389  CB  ILE A 334      30.099  24.404  22.567  1.00  7.35      A
ATOM   2390  CG2 ILE A 334      29.902  24.030  24.056  1.00  4.48      A
ATOM   2391  CG1 ILE A 334      29.093  25.467  22.091  1.00  8.68      A
ATOM   2392  CD1 ILE A 334      27.628  24.953  22.043  1.00  8.29      A
ATOM   2393  C   ILE A 334      32.593  24.003  22.946  1.00  9.03      A
ATOM   2394  O   ILE A 334      33.239  24.352  23.954  1.00  6.82      A
ATOM   2395  N   GLN A 335      32.805  22.847  22.333  1.00  6.99      A
ATOM   2396  CA  GLN A 335      33.800  21.903  22.831  1.00  8.99      A
ATOM   2397  CB  GLN A 335      33.695  20.589  22.053  1.00 11.58      A
ATOM   2398  CG  GLN A 335      32.448  19.784  22.446  1.00 21.44      A
ATOM   2399  CD  GLN A 335      32.279  18.518  21.598  1.00 30.71      A
ATOM   2400  OE1 GLN A 335      33.212  18.083  20.927  1.00 34.68      A
ATOM   2401  NE2 GLN A 335      31.089  17.926  21.638  1.00 37.34      A
ATOM   2402  C   GLN A 335      35.223  22.438  22.774  1.00 12.27      A
ATOM   2403  O   GLN A 335      36.014  22.219  23.704  1.00 10.25      A
ATOM   2404  N   ALA A 336      35.547  23.143  21.690  1.00 10.75      A
ATOM   2405  CA  ALA A 336      36.868  23.726  21.514  1.00 12.71      A
ATOM   2406  CB  ALA A 336      36.989  24.375  20.091  1.00  9.35      A
ATOM   2407  C   ALA A 336      37.109  24.794  22.591  1.00 11.11      A
ATOM   2408  O   ALA A 336      38.247  25.134  22.894  1.00 11.00      A
ATOM   2409  N   ASN A 337      36.025  25.310  23.164  1.00  8.06      A
ATOM   2410  CA  ASN A 337      36.125  26.342  24.185  1.00  9.10      A
ATOM   2411  CB  ASN A 337      35.098  27.440  23.887  1.00  8.86      A
ATOM   2412  CG  ASN A 337      35.621  28.457  22.874  1.00 12.21      A
ATOM   2413  OD1 ASN A 337      36.333  29.417  23.230  1.00 12.38      A
ATOM   2414  ND2 ASN A 337      35.301  28.237  21.605  1.00 13.95      A
ATOM   2415  C   ASN A 337      35.979  25.816  25.622  1.00  9.52      A
ATOM   2416  O   ASN A 337      35.647  26.565  26.534  1.00  7.92      A
ATOM   2417  N   ALA A 338      36.242  24.523  25.806  1.00  8.29      A
ATOM   2418  CA  ALA A 338      36.194  23.863  27.117  1.00  8.92      A
ATOM   2419  CB  ALA A 338      37.188  24.526  28.069  1.00 10.50      A
ATOM   2420  C   ALA A 338      34.825  23.786  27.785  1.00  8.55      A
ATOM   2421  O   ALA A 338      34.732  23.671  29.000  1.00 10.41      A
ATOM   2422  N   PHE A 339      33.765  23.844  27.002  1.00  7.84      A
ATOM   2423  CA  PHE A 339      32.410  23.781  27.553  1.00  8.93      A
ATOM   2424  CB  PHE A 339      31.624  25.034  27.120  1.00  7.76      A
ATOM   2425  CG  PHE A 339      32.258  26.345  27.576  1.00 10.23      A
ATOM   2426  CD1 PHE A 339      32.566  26.557  28.923  1.00 11.28      A
ATOM   2427  CD2 PHE A 339      32.497  27.369  26.664  1.00  9.75      A
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FIGURE 5 (continued)

ATOM	2428	CE1	PHE	A	339	33.108	27.795	29.360	1.00	11.58	A
ATOM	2429	CE2	PHE	A	339	33.033	28.613	27.077	1.00	8.17	A
ATOM	2430	CZ	PHE	A	339	33.339	28.820	28.437	1.00	8.56	A
ATOM	2431	C	PHE	A	339	31.647	22.514	27.151	1.00	9.93	A
ATOM	2432	O	PHE	A	339	32.084	21.742	26.279	1.00	9.23	A
ATOM	2433	N	VAL	A	340	30.508	22.304	27.797	1.00	8.19	A
ATOM	2434	CA	VAL	A	340	29.669	21.139	27.531	1.00	10.26	A
ATOM	2435	CB	VAL	A	340	29.169	20.468	28.851	1.00	11.72	A
ATOM	2436	CG1	VAL	A	340	28.219	19.269	28.538	1.00	8.46	A
ATOM	2437	CG2	VAL	A	340	30.346	19.998	29.679	1.00	8.91	A
ATOM	2438	C	VAL	A	340	28.439	21.577	26.742	1.00	6.33	A
ATOM	2439	O	VAL	A	340	27.675	22.433	27.186	1.00	6.81	A
ATOM	2440	N	PRO	A	341	28.255	21.021	25.547	1.00	6.85	A
ATOM	2441	CD	PRO	A	341	29.193	20.162	24.797	1.00	10.26	A
ATOM	2442	CA	PRO	A	341	27.082	21.373	24.736	1.00	9.67	A
ATOM	2443	CB	PRO	A	341	27.275	20.537	23.468	1.00	11.39	A
ATOM	2444	CG	PRO	A	341	28.752	20.386	23.363	1.00	14.97	A
ATOM	2445	C	PRO	A	341	25.807	20.931	25.497	1.00	10.96	A
ATOM	2446	O	PRO	A	341	25.851	20.024	26.342	1.00	10.96	A
ATOM	2447	N	LEU	A	342	24.673	21.558	25.211	1.00	8.13	A
ATOM	2448	CA	LEU	A	342	23.435	21.157	25.870	1.00	10.08	A
ATOM	2449	CB	LEU	A	342	22.326	22.194	25.646	1.00	12.81	A
ATOM	2450	CG	LEU	A	342	22.558	23.605	26.207	1.00	16.13	A
ATOM	2451	CD1	LEU	A	342	21.280	24.428	26.007	1.00	10.84	A
ATOM	2452	CD2	LEU	A	342	22.908	23.542	27.715	1.00	14.00	A
ATOM	2453	C	LEU	A	342	22.981	19.821	25.288	1.00	11.91	A
ATOM	2454	O	LEU	A	342	23.142	19.565	24.072	1.00	10.04	A
ATOM	2455	N	PRO	A	343	22.437	18.937	26.147	1.00	10.12	A
ATOM	2456	CD	PRO	A	343	22.407	19.074	27.618	1.00	8.23	A
ATOM	2457	CA	PRO	A	343	21.947	17.622	25.721	1.00	11.60	A
ATOM	2458	CB	PRO	A	343	21.407	17.006	27.021	1.00	11.29	A
ATOM	2459	CG	PRO	A	343	22.287	17.643	28.083	1.00	12.10	A
ATOM	2460	C	PRO	A	343	20.850	17.839	24.688	1.00	11.38	A
ATOM	2461	O	PRO	A	343	20.229	18.896	24.648	1.00	10.75	A
ATOM	2462	N	SER	A	344	20.590	16.836	23.861	1.00	9.55	A
ATOM	2463	CA	SER	A	344	19.592	16.995	22.801	1.00	8.34	A
ATOM	2464	CB	SER	A	344	19.547	15.741	21.940	1.00	15.39	A
ATOM	2465	OG	SER	A	344	19.245	14.625	22.760	1.00	23.25	A
ATOM	2466	C	SER	A	344	18.185	17.315	23.281	1.00	8.79	A
ATOM	2467	O	SER	A	344	17.474	18.051	22.615	1.00	11.06	A
ATOM	2468	N	ASN	A	345	17.751	16.744	24.410	1.00	11.97	A
ATOM	2469	CA	ASN	A	345	16.403	17.061	24.874	1.00	13.51	A
ATOM	2470	CB	ASN	A	345	15.962	16.128	26.015	1.00	11.25	A
ATOM	2471	CG	ASN	A	345	16.896	16.145	27.206	1.00	19.63	A
ATOM	2472	OD1	ASN	A	345	18.105	16.399	27.083	1.00	15.65	A
ATOM	2473	ND2	ASN	A	345	16.343	15.822	28.379	1.00	15.03	A
ATOM	2474	C	ASN	A	345	16.296	18.532	25.277	1.00	12.03	A
ATOM	2475	O	ASN	A	345	15.236	19.131	25.167	1.00	11.72	A
ATOM	2476	N	TRP	A	346	17.397	19.115	25.739	1.00	10.97	A
ATOM	2477	CA	TRP	A	346	17.397	20.533	26.097	1.00	9.55	A
ATOM	2478	CB	TRP	A	346	18.663	20.890	26.881	1.00	8.50	A
ATOM	2479	CG	TRP	A	346	18.475	20.695	28.372	1.00	9.10	A
ATOM	2480	CD2	TRP	A	346	17.927	21.660	29.285	1.00	10.08	A
ATOM	2481	CE2	TRP	A	346	17.831	21.036	30.549	1.00	12.11	A
ATOM	2482	CE3	TRP	A	346	17.502	22.994	29.149	1.00	9.60	A
ATOM	2483	CD1	TRP	A	346	18.694	19.553	29.099	1.00	9.06	A
ATOM	2484	NE1	TRP	A	346	18.304	19.752	30.411	1.00	9.93	A
ATOM	2485	CZ2	TRP	A	346	17.323	21.705	31.682	1.00	9.30	A
ATOM	2486	CZ3	TRP	A	346	17.004	23.662	30.261	1.00	10.14	A
ATOM	2487	CH2	TRP	A	346	16.917	23.012	31.522	1.00	12.99	A
ATOM	2488	C	TRP	A	346	17.298	21.390	24.824	1.00	10.69	A
ATOM	2489	O	TRP	A	346	16.509	22.333	24.769	1.00	13.16	A
ATOM	2490	N	LYS	A	347	18.087	21.074	23.804	1.00	9.34	A
ATOM	2491	CA	LYS	A	347	17.984	21.852	22.557	1.00	8.27	A
ATOM	2492	CB	LYS	A	347	18.902	21.287	21.466	1.00	12.86	A
ATOM	2493	CG	LYS	A	347	20.416	21.357	21.748	1.00	11.51	A
ATOM	2494	CD	LYS	A	347	21.221	21.071	20.440	1.00	14.73	A
ATOM	2495	CE	LYS	A	347	22.733	21.317	20.590	1.00	14.12	A
ATOM	2496	NZ	LYS	A	347	23.467	20.312	21.462	1.00	10.37	A
ATOM	2497	C	LYS	A	347	16.549	21.789	22.030	1.00	10.83	A
ATOM	2498	O	LYS	A	347	15.956	22.814	21.631	1.00	8.78	A
ATOM	2499	N	ALA	A	348	15.987	20.583	21.997	1.00	9.70	A
ATOM	2500	CA	ALA	A	348	14.627	20.418	21.472	1.00	9.41	A
ATOM	2501	CB	ALA	A	348	14.238	18.928	21.448	1.00	12.04	A
ATOM	2502	C	ALA	A	348	13.589	21.224	22.251	1.00	10.82	A
ATOM	2503	O	ALA	A	348	12.678	21.830	21.657	1.00	9.58	A

FIGURE 5 (continued)

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ATOM   2504  N   ALA A 349      13.735  21.261  23.569  1.00  9.39      A
ATOM   2505  CA  ALA A 349      12.791  22.018  24.392  1.00  8.51      A
ATOM   2506  CB  ALA A 349      13.045  21.750  25.891  1.00  8.51      A
ATOM   2507  C   ALA A 349      12.909  23.518  24.095  1.00 10.22      A
ATOM   2508  O   ALA A 349      11.888  24.224  24.012  1.00  8.91      A
ATOM   2509  N   VAL A 350      14.140  24.002  23.930  1.00 12.16      A
ATOM   2510  CA  VAL A 350      14.347  25.423  23.649  1.00  8.94      A
ATOM   2511  CB  VAL A 350      15.863  25.794  23.629  1.00  8.30      A
ATOM   2512  CG1 VAL A 350      16.075  27.221  23.071  1.00  8.00      A
ATOM   2513  CG2 VAL A 350      16.439  25.729  25.075  1.00  8.81      A
ATOM   2514  C   VAL A 350      13.709  25.763  22.305  1.00 10.89      A
ATOM   2515  O   VAL A 350      13.046  26.787  22.177  1.00 11.46      A
ATOM   2516  N   ARG A 351      13.890  24.895  21.313  1.00 10.91      A
ATOM   2517  CA  ARG A 351      13.289  25.144  20.002  1.00 11.54      A
ATOM   2518  CB  ARG A 351      13.765  24.106  18.988  1.00 10.07      A
ATOM   2519  CG  ARG A 351      15.237  24.167  18.647  1.00 10.05      A
ATOM   2520  CD  ARG A 351      15.527  23.433  17.312  1.00 14.16      A
ATOM   2521  NE  ARG A 351      14.971  22.067  17.282  1.00 17.52      A
ATOM   2522  CZ  ARG A 351      15.577  20.991  17.780  1.00 14.15      A
ATOM   2523  NH1 ARG A 351      14.993  19.802  17.708  1.00 14.19      A
ATOM   2524  NH2 ARG A 351      16.775  21.097  18.338  1.00 15.54      A
ATOM   2525  C   ARG A 351      11.750  25.097  20.069  1.00 13.24      A
ATOM   2526  O   ARG A 351      11.061  25.925  19.477  1.00 10.64      A
ATOM   2527  N   ALA A 352      11.221  24.112  20.786  1.00 10.94      A
ATOM   2528  CA  ALA A 352       9.772  23.942  20.890  1.00 13.45      A
ATOM   2529  CB  ALA A 352       9.447  22.656  21.636  1.00 14.54      A
ATOM   2530  C   ALA A 352       9.028  25.112  21.527  1.00 14.05      A
ATOM   2531  O   ALA A 352       7.875  25.385  21.193  1.00  9.92      A
ATOM   2532  N   SER A 353       9.669  25.802  22.454  1.00  9.51      A
ATOM   2533  CA  SER A 353       9.024  26.932  23.094  1.00 10.39      A
ATOM   2534  CB  SER A 353       9.503  27.088  24.548  1.00 11.56      A
ATOM   2535  OG  SER A 353       8.802  26.220  25.436  1.00 14.83      A
ATOM   2536  C   SER A 353       9.308  28.245  22.386  1.00 12.07      A
ATOM   2537  O   SER A 353       8.403  29.033  22.178  1.00 12.33      A
ATOM   2538  N   TYR A 354      10.568  28.459  22.015  1.00 10.56      A
ATOM   2539  CA  TYR A 354      10.955  29.733  21.455  1.00  8.65      A
ATOM   2540  CB  TYR A 354      12.240  30.188  22.159  1.00 11.42      A
ATOM   2541  CG  TYR A 354      12.077  30.164  23.670  1.00 11.26      A
ATOM   2542  CD1 TYR A 354      11.168  31.007  24.296  1.00 11.16      A
ATOM   2543  CE1 TYR A 354      10.962  30.955  25.673  1.00 13.86      A
ATOM   2544  CD2 TYR A 354      12.795  29.265  24.455  1.00 12.94      A
ATOM   2545  CE2 TYR A 354      12.608  29.204  25.846  1.00 13.83      A
ATOM   2546  CZ  TYR A 354      11.692  30.048  26.437  1.00 15.93      A
ATOM   2547  OH  TYR A 354      11.496  29.985  27.784  1.00 31.84      A
ATOM   2548  C   TYR A 354      11.069  29.882  19.951  1.00 11.12      A
ATOM   2549  O   TYR A 354      11.137  31.011  19.456  1.00 11.00      A
ATOM   2550  N   LEU A 355      11.097  28.778  19.218  1.00  9.87      A
ATOM   2551  CA  LEU A 355      11.156  28.896  17.757  1.00 11.35      A
ATOM   2552  CB  LEU A 355      12.292  28.069  17.185  1.00 12.01      A
ATOM   2553  CG  LEU A 355      13.697  28.633  17.424  1.00 18.77      A
ATOM   2554  CD1 LEU A 355      14.731  27.617  16.930  1.00 13.44      A
ATOM   2555  CD2 LEU A 355      13.856  29.963  16.666  1.00 19.42      A
ATOM   2556  C   LEU A 355       9.848  28.484  17.086  1.00 12.49      A
ATOM   2557  O   LEU A 355       9.337  29.208  16.231  1.00 13.91      A
ATOM   2558  N   THR A 356       9.300  27.331  17.458  1.00 13.88      A
ATOM   2559  CA  THR A 356       8.036  26.866  16.849  1.00 16.44      A
ATOM   2560  CB  THR A 356       7.414  25.759  17.704  1.00 19.06      A
ATOM   2561  OG1 THR A 356       8.352  24.678  17.794  1.00 22.02      A
ATOM   2562  CG2 THR A 356       6.108  25.265  17.077  1.00 20.44      A
ATOM   2563  C   THR A 356       7.058  28.040  16.684  1.00 15.88      A
ATOM   2564  O   THR A 356       6.609  28.642  17.658  1.00 14.53      A
ATOM   2565  N   ALA A 357       6.720  28.362  15.441  1.00 16.53      A
ATOM   2566  CA  ALA A 357       5.892  29.536  15.175  1.00 15.13      A
ATOM   2567  CB  ALA A 357       5.654  29.669  13.662  1.00 17.87      A
ATOM   2568  C   ALA A 357       4.569  29.630  15.918  1.00 18.27      A
ATOM   2569  O   ALA A 357       4.141  30.714  16.295  1.00 19.17      A
ATOM   2570  N   SER A 358       3.930  28.492  16.127  1.00 18.84      A
ATOM   2571  CA  SER A 358       2.643  28.444  16.800  1.00 22.62      A
ATOM   2572  CB  SER A 358       1.953  27.125  16.459  1.00 18.79      A
ATOM   2573  OG  SER A 358       2.853  26.049  16.654  1.00 21.93      A
ATOM   2574  C   SER A 358       2.716  28.607  18.318  1.00 22.54      A
ATOM   2575  O   SER A 358       1.719  28.918  18.949  1.00 19.82      A
ATOM   2576  N   ASN A 359       3.886  28.410  18.916  1.00 20.48      A
ATOM   2577  CA  ASN A 359       3.950  28.550  20.358  1.00 16.65      A
ATOM   2578  CB  ASN A 359       5.249  27.956  20.909  1.00 12.27      A
ATOM   2579  CG  ASN A 359       5.180  27.718  22.387  1.00 11.80      A
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FIGURE 5 (continued)

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ATOM   2580  OD1 ASN A 359       4.992  28.652  23.170  1.00 16.11      A
ATOM   2581  ND2 ASN A 359       5.329  26.451  22.793  1.00 14.58      A
ATOM   2582  C   ASN A 359       3.844  30.019  20.745  1.00 16.93      A
ATOM   2583  O   ASN A 359       4.550  30.861  20.194  1.00 15.08      A
ATOM   2584  N   ALA A 360       2.972  30.306  21.712  1.00 15.71      A
ATOM   2585  CA  ALA A 360       2.759  31.664  22.208  1.00 18.67      A
ATOM   2586  CB  ALA A 360       1.688  31.651  23.320  1.00 22.67      A
ATOM   2587  C   ALA A 360       4.041  32.309  22.744  1.00 18.59      A
ATOM   2588  O   ALA A 360       4.138  33.532  22.825  1.00 16.11      A
ATOM   2589  N   LEU A 361       5.010  31.488  23.144  1.00 14.62      A
ATOM   2590  CA  LEU A 361       6.276  32.021  23.653  1.00 11.27      A
ATOM   2591  CB  LEU A 361       6.863  31.060  24.685  1.00 15.51      A
ATOM   2592  CG  LEU A 361       6.087  30.788  25.971  1.00 15.37      A
ATOM   2593  CD1 LEU A 361       6.713  29.586  26.688  1.00 15.50      A
ATOM   2594  CD2 LEU A 361       6.086  32.030  26.849  1.00 14.07      A
ATOM   2595  C   LEU A 361       7.334  32.219  22.545  1.00 12.87      A
ATOM   2596  O   LEU A 361       8.430  32.716  22.818  1.00 12.41      A
ATOM   2597  N   SER A 362       7.036  31.821  21.314  1.00  9.97      A
ATOM   2598  CA  SER A 362       8.044  31.936  20.257  1.00 10.76      A
ATOM   2599  CB  SER A 362       7.627  31.145  19.011  1.00 15.72      A
ATOM   2600  OG  SER A 362       6.470  31.707  18.416  1.00 18.79      A
ATOM   2601  C   SER A 362       8.454  33.338  19.822  1.00 12.29      A
ATOM   2602  O   SER A 362       7.637  34.258  19.742  1.00 12.85      A
ATOM   2603  N   ILE A 363       9.741  33.457  19.512  1.00 10.84      A
ATOM   2604  CA  ILE A 363      10.353  34.698  19.072  1.00 14.99      A
ATOM   2605  CB  ILE A 363      11.850  34.461  18.777  1.00 13.05      A
ATOM   2606  CG2 ILE A 363      12.483  35.713  18.198  1.00 12.46      A
ATOM   2607  CG1 ILE A 363      12.578  34.071  20.064  1.00 15.60      A
ATOM   2608  CD1 ILE A 363      13.960  33.442  19.815  1.00 11.48      A
ATOM   2609  C   ILE A 363       9.639  35.206  17.807  1.00 14.29      A
ATOM   2610  O   ILE A 363       9.509  34.481  16.830  1.00 12.01      A
ATOM   2611  N   GLY A 364       9.176  36.451  17.848  1.00 15.53      A
ATOM   2612  CA  GLY A 364       8.477  37.034  16.717  1.00 14.88      A
ATOM   2613  C   GLY A 364       7.040  36.567  16.514  1.00 19.34      A
ATOM   2614  O   GLY A 364       6.436  36.872  15.487  1.00 19.36      A
ATOM   2615  N   ASP A 365       6.471  35.842  17.474  1.00 15.42      A
ATOM   2616  CA  ASP A 365       5.094  35.360  17.323  1.00 16.08      A
ATOM   2617  CB  ASP A 365       4.625  34.691  18.613  1.00 17.24      A
ATOM   2618  CG  ASP A 365       3.195  34.201  18.516  1.00 22.13      A
ATOM   2619  OD1 ASP A 365       2.992  33.003  18.238  1.00 24.97      A
ATOM   2620  OD2 ASP A 365       2.272  35.025  18.698  1.00 22.46      A
ATOM   2621  C   ASP A 365       4.100  36.490  16.954  1.00 20.12      A
ATOM   2622  O   ASP A 365       3.979  37.482  17.668  1.00 17.92      A
ATOM   2623  N   SER A 366       3.379  36.317  15.848  1.00 21.25      A
ATOM   2624  CA  SER A 366       2.419  37.319  15.360  1.00 19.32      A
ATOM   2625  CB  SER A 366       1.704  36.787  14.108  1.00 21.13      A
ATOM   2626  OG  SER A 366       2.640  36.400  13.125  1.00 29.92      A
ATOM   2627  C   SER A 366       1.359  37.814  16.342  1.00 15.84      A
ATOM   2628  O   SER A 366       1.155  39.010  16.461  1.00 22.39      A
ATOM   2629  N   ALA A 367       0.655  36.920  17.024  1.00 18.40      A
ATOM   2630  CA  ALA A 367      -0.384  37.363  17.965  1.00 22.33      A
ATOM   2631  CB  ALA A 367      -1.220  36.175  18.431  1.00 19.13      A
ATOM   2632  C   ALA A 367       0.182  38.093  19.187  1.00 25.24      A
ATOM   2633  O   ALA A 367      -0.402  39.066  19.682  1.00 26.45      A
ATOM   2634  N   VAL A 368       1.311  37.612  19.692  1.00 24.39      A
ATOM   2635  CA  VAL A 368       1.903  38.229  20.864  1.00 21.43      A
ATOM   2636  CB  VAL A 368       2.729  37.182  21.657  1.00 23.84      A
ATOM   2637  CG1 VAL A 368       3.447  37.838  22.850  1.00 19.42      A
ATOM   2638  CG2 VAL A 368       1.810  36.094  22.148  1.00 25.28      A
ATOM   2639  C   VAL A 368       2.770  39.447  20.558  1.00 19.50      A
ATOM   2640  O   VAL A 368       2.713  40.440  21.277  1.00 22.77      A
ATOM   2641  N   CYS A 369       3.557  39.396  19.491  1.00 17.47      A
ATOM   2642  CA  CYS A 369       4.448  40.505  19.195  1.00 20.32      A
ATOM   2643  C   CYS A 369       3.919  41.648  18.322  1.00 23.64      A
ATOM   2644  O   CYS A 369       4.617  42.639  18.120  1.00 26.98      A
ATOM   2645  CB  CYS A 369       5.746  39.977  18.581  1.00 22.42      A
ATOM   2646  SG  CYS A 369       6.819  38.961  19.671  1.00 19.53      A
ATOM   2647  N   GLY A 370       2.698  41.521  17.812  1.00 25.38      A
ATOM   2648  CA  GLY A 370       2.154  42.575  16.966  1.00 27.80      A
ATOM   2649  C   GLY A 370       2.190  43.938  17.627  1.00 21.46      A
ATOM   2650  O   GLY A 370       1.631  44.112  18.705  1.00 25.76      A
ATOM   2651  N   GLY A 371       2.872  44.885  16.988  1.00 20.44      A
ATOM   2652  CA  GLY A 371       2.970  46.237  17.516  1.00 23.12      A
ATOM   2653  C   GLY A 371       3.913  46.463  18.695  1.00 26.63      A
ATOM   2654  O   GLY A 371       3.946  47.561  19.263  1.00 23.97      A
ATOM   2655  N   LYS A 372       4.689  45.443  19.057  1.00 23.24      A
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FIGURE 5 (continued)

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ATOM   2656  CA  LYS A 372       5.612  45.537  20.197  1.00 21.66      A
ATOM   2657  CB  LYS A 372       5.141  44.605  21.296  1.00 19.20      A
ATOM   2658  CG  LYS A 372       3.715  44.856  21.675  1.00 25.31      A
ATOM   2659  CD  LYS A 372       3.278  43.936  22.769  1.00 24.34      A
ATOM   2660  CE  LYS A 372       1.884  44.315  23.208  1.00 29.63      A
ATOM   2661  NZ  LYS A 372       1.426  43.423  24.285  1.00 25.95      A
ATOM   2662  C   LYS A 372       7.037  45.167  19.855  1.00 18.74      A
ATOM   2663  O   LYS A 372       7.337  44.799  18.721  1.00 17.43      A
ATOM   2664  N   GLY A 373       7.917  45.247  20.852  1.00 15.44      A
ATOM   2665  CA  GLY A 373       9.297  44.876  20.616  1.00 12.87      A
ATOM   2666  C   GLY A 373      10.366  45.876  21.015  1.00 17.42      A
ATOM   2667  O   GLY A 373      10.168  47.106  20.965  1.00 13.70      A
ATOM   2668  N   ARG A 374      11.517  45.342  21.419  1.00 14.49      A
ATOM   2669  CA  ARG A 374      12.639  46.187  21.792  1.00 13.29      A
ATOM   2670  CB  ARG A 374      13.786  45.339  22.333  1.00 15.72      A
ATOM   2671  CG  ARG A 374      13.456  44.710  23.692  1.00 18.10      A
ATOM   2672  CD  ARG A 374      14.668  44.080  24.332  1.00 20.11      A
ATOM   2673  NE  ARG A 374      15.729  45.034  24.665  1.00 13.47      A
ATOM   2674  CZ  ARG A 374      16.143  45.296  25.899  1.00 13.50      A
ATOM   2675  NH1 ARG A 374      15.564  44.694  26.928  1.00 11.14      A
ATOM   2676  NH2 ARG A 374      17.206  46.082  26.100  1.00  9.65      A
ATOM   2677  C   ARG A 374      13.097  46.989  20.563  1.00 14.09      A
ATOM   2678  O   ARG A 374      13.008  46.517  19.411  1.00 13.90      A
ATOM   2679  N   PRO A 375      13.575  48.225  20.797  1.00 13.52      A
ATOM   2680  CD  PRO A 375      13.680  48.834  22.133  1.00 12.37      A
ATOM   2681  CA  PRO A 375      14.051  49.137  19.753  1.00 15.51      A
ATOM   2682  CB  PRO A 375      14.304  50.445  20.516  1.00 18.56      A
ATOM   2683  CG  PRO A 375      14.669  49.958  21.903  1.00 16.56      A
ATOM   2684  C   PRO A 375      15.282  48.622  19.017  1.00 16.94      A
ATOM   2685  O   PRO A 375      16.130  47.953  19.605  1.00 16.29      A
ATOM   2686  N   GLU A 376      15.384  48.956  17.733  1.00 14.83      A
ATOM   2687  CA  GLU A 376      16.501  48.480  16.928  1.00 14.54      A
ATOM   2688  CB  GLU A 376      16.191  48.638  15.429  1.00 20.94      A
ATOM   2689  CG  GLU A 376      15.989  50.054  14.930  1.00 25.93      A
ATOM   2690  CD  GLU A 376      15.840  50.093  13.408  1.00 28.12      A
ATOM   2691  OE1 GLU A 376      16.852  50.265  12.693  1.00 27.73      A
ATOM   2692  OE2 GLU A 376      14.706  49.921  12.926  1.00 22.85      A
ATOM   2693  C   GLU A 376      17.818  49.144  17.258  1.00 15.46      A
ATOM   2694  O   GLU A 376      17.779  50.308  17.715  1.00 20.34      A
ATOM   2695  OXT GLU A 376      18.870  48.501  17.040  1.00 17.16      A
ATOM   2696  OH2 WAT S1500      35.620  33.372  34.950  1.00  7.74      S
ATOM   2697  OH2 WAT S1501      26.719  26.585  54.115  1.00 13.35      S
ATOM   2698  OH2 WAT S1502      32.910  38.720  42.612  1.00 11.02      S
ATOM   2699  OH2 WAT S1503      25.842  40.990  19.393  1.00 10.30      S
ATOM   2700  OH2 WAT S1504      47.855  24.508  32.439  1.00 11.64      S
ATOM   2701  OH2 WAT S1505      37.575  38.877  30.460  1.00 13.25      S
ATOM   2702  OH2 WAT S1506      43.970  19.166  36.360  1.00 11.89      S
ATOM   2703  OH2 WAT S1507      51.431  26.280  38.870  1.00 11.08      S
ATOM   2704  OH2 WAT S1508      21.180  34.238  33.496  1.00 10.94      S
ATOM   2705  OH2 WAT S1509      34.016  23.145  55.150  1.00  7.21      S
ATOM   2706  OH2 WAT S1510      34.137  35.767  50.996  1.00 14.32      S
ATOM   2707  OH2 WAT S1511      29.833  31.064  61.815  1.00 12.62      S
ATOM   2708  OH2 WAT S1512      36.421  34.348  51.750  1.00  8.81      S
ATOM   2709  OH2 WAT S1513      24.593  22.841  22.601  1.00 14.49      S
ATOM   2710  OH2 WAT S1514      33.875  20.919  53.336  1.00 15.73      S
ATOM   2711  OH2 WAT S1515      55.590  18.894  44.228  1.00 20.22      S
ATOM   2712  OH2 WAT S1516      25.163  24.507  19.298  1.00  7.32      S
ATOM   2713  OH2 WAT S1517      29.287  27.565  53.584  1.00 10.43      S
ATOM   2714  OH2 WAT S1518      27.630  35.157  54.573  1.00 11.84      S
ATOM   2715  OH2 WAT S1519      34.308  40.814  45.314  1.00  9.91      S
ATOM   2716  OH2 WAT S1520      24.097  26.340  47.444  1.00 12.35      S
ATOM   2717  OH2 WAT S1521      26.289  17.353  26.191  1.00 14.15      S
ATOM   2718  OH2 WAT S1522      31.025  26.248  57.309  1.00  9.97      S
ATOM   2719  OH2 WAT S1523      16.012  33.323  36.822  1.00 10.61      S
ATOM   2720  OH2 WAT S1524      35.079  31.981  26.882  1.00  7.27      S
ATOM   2721  OH2 WAT S1525      48.948  16.302  35.666  1.00 22.32      S
ATOM   2722  OH2 WAT S1526      23.036  32.247  50.228  1.00 12.80      S
ATOM   2723  OH2 WAT S1527      41.445  42.204  48.819  1.00 16.71      S
ATOM   2724  OH2 WAT S1528      30.777  34.835  16.827  1.00 12.96      S
ATOM   2725  OH2 WAT S1529       9.482  33.895  27.983  1.00 10.22      S
ATOM   2726  OH2 WAT S1530      10.107  31.646  29.601  1.00 12.12      S
ATOM   2727  OH2 WAT S1531      37.836  31.446  58.127  1.00 18.63      S
ATOM   2728  OH2 WAT S1532      23.419  29.528  35.937  1.00 10.10      S
ATOM   2729  OH2 WAT S1533      36.234  16.727  51.505  1.00  9.28      S
ATOM   2730  OH2 WAT S1534       5.728  38.503  24.985  1.00 13.33      S
ATOM   2731  OH2 WAT S1535      29.914  14.295  35.432  1.00 16.41      S
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FIGURE 5 (continued)

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ATOM   2732  OH2 WAT S1536      31.310  38.281  18.695  1.00  9.93      S
ATOM   2733  OH2 WAT S1537      44.863  16.606  36.022  1.00 15.09      S
ATOM   2734  OH2 WAT S1538      40.186  22.869  38.700  1.00  9.90      S
ATOM   2735  OH2 WAT S1539      37.549  20.501  28.090  1.00 13.36      S
ATOM   2736  OH2 WAT S1540      12.913  31.829  29.436  1.00  9.36      S
ATOM   2737  OH2 WAT S1541      30.589  15.671  37.530  1.00 12.47      S
ATOM   2738  OH2 WAT S1542      23.885  35.406  43.402  1.00 18.37      S
ATOM   2739  OH2 WAT S1543       8.663  34.010  25.289  1.00 13.37      S
ATOM   2740  OH2 WAT S1544      13.484  46.444  33.757  1.00 12.24      S
ATOM   2741  OH2 WAT S1545      27.923  19.477  57.944  1.00 11.68      S
ATOM   2742  OH2 WAT S1546      17.540  33.345   7.715  1.00 19.22      S
ATOM   2743  OH2 WAT S1547      51.552  13.602  41.885  1.00 25.84      S
ATOM   2744  OH2 WAT S1548      27.270  26.074  40.675  1.00 10.51      S
ATOM   2745  OH2 WAT S1549      27.760  43.771  20.816  1.00 13.46      S
ATOM   2746  OH2 WAT S1550      37.046  17.292  27.914  1.00 14.34      S
ATOM   2747  OH2 WAT S1551      37.573  33.819  20.741  1.00 23.07      S
ATOM   2748  OH2 WAT S1552      40.930  14.067  35.565  1.00 17.08      S
ATOM   2749  OH2 WAT S1553       4.472  29.061  32.567  1.00 18.41      S
ATOM   2750  OH2 WAT S1554      26.302  32.912  28.375  1.00 10.00      S
ATOM   2751  OH2 WAT S1555      14.165  45.737  16.934  1.00 13.06      S
ATOM   2752  OH2 WAT S1556      29.555  43.029  36.030  1.00  7.32      S
ATOM   2753  OH2 WAT S1557      36.451  34.819  37.298  1.00 11.33      S
ATOM   2754  OH2 WAT S1558      31.931  17.255  49.603  1.00 39.16      S
ATOM   2755  OH2 WAT S1559      23.622  26.926  37.001  1.00 11.87      S
ATOM   2756  OH2 WAT S1560      31.327  13.311  33.059  1.00 12.47      S
ATOM   2757  OH2 WAT S1561      44.899  41.787  36.741  1.00 23.25      S
ATOM   2758  OH2 WAT S1562      44.879  35.365  50.334  1.00  9.60      S
ATOM   2759  OH2 WAT S1563      20.827  50.011  18.100  1.00 15.06      S
ATOM   2760  OH2 WAT S1564      24.374  31.041  38.304  1.00 12.38      S
ATOM   2761  OH2 WAT S1565      11.411  42.003  26.114  1.00 14.55      S
ATOM   2762  OH2 WAT S1566      21.341  35.751  40.722  1.00 12.16      S
ATOM   2763  OH2 WAT S1567      10.175  31.393  39.888  1.00 37.76      S
ATOM   2764  OH2 WAT S1568      47.181  26.945  33.704  1.00 12.30      S
ATOM   2765  OH2 WAT S1569      42.028  43.488  36.919  1.00 25.46      S
ATOM   2766  OH2 WAT S1570      31.053  24.724  15.706  1.00 12.46      S
ATOM   2767  OH2 WAT S1571      10.314  39.156  33.480  1.00 10.32      S
ATOM   2768  OH2 WAT S1572      51.433  20.485  50.130  1.00 15.09      S
ATOM   2769  OH2 WAT S1573      43.925  30.656  51.790  1.00 17.28      S
ATOM   2770  OH2 WAT S1574      23.091  53.758  28.375  1.00 12.50      S
ATOM   2771  OH2 WAT S1575      34.977  41.183  53.019  1.00 15.31      S
ATOM   2772  OH2 WAT S1576      29.766  26.781  12.309  1.00 18.82      S
ATOM   2773  OH2 WAT S1577       9.190  36.561  30.593  1.00 11.25      S
ATOM   2774  OH2 WAT S1578      36.599  15.728  48.666  1.00 21.18      S
ATOM   2775  OH2 WAT S1579      37.724  34.865  54.143  1.00 11.62      S
ATOM   2776  OH2 WAT S1580      21.457  35.713  12.303  1.00 13.24      S
ATOM   2777  OH2 WAT S1581      27.734  31.073  59.797  1.00 14.78      S
ATOM   2778  OH2 WAT S1582      51.536  35.554  40.163  1.00 14.52      S
ATOM   2779  OH2 WAT S1583      29.933  42.651  53.057  1.00 14.55      S
ATOM   2780  OH2 WAT S1584       9.469  23.677  25.125  1.00 12.14      S
ATOM   2781  OH2 WAT S1585      20.704  29.372  11.334  1.00 17.80      S
ATOM   2782  OH2 WAT S1586      56.481  22.975  38.435  1.00 29.16      S
ATOM   2783  OH2 WAT S1587       9.572  40.421  17.037  1.00 14.99      S
ATOM   2784  OH2 WAT S1588      20.542  42.224  40.862  1.00 13.90      S
ATOM   2785  OH2 WAT S1589       9.567  37.848  39.841  1.00 15.10      S
ATOM   2786  OH2 WAT S1590       6.391  48.835  28.636  1.00 19.52      S
ATOM   2787  OH2 WAT S1591      41.492  20.894  55.469  1.00 16.40      S
ATOM   2788  OH2 WAT S1592      22.505  28.556  52.952  1.00 24.23      S
ATOM   2789  OH2 WAT S1593      27.720  46.441  20.204  1.00 15.40      S
ATOM   2790  OH2 WAT S1594      37.216  41.499  30.864  1.00 19.68      S
ATOM   2791  OH2 WAT S1595      30.199  27.159  15.034  1.00 11.19      S
ATOM   2792  OH2 WAT S1596      25.139  30.964  53.858  1.00 21.47      S
ATOM   2793  OH2 WAT S1597      35.730  20.698  18.767  1.00 15.15      S
ATOM   2794  OH2 WAT S1598      44.994  20.666  23.797  1.00 17.67      S
ATOM   2795  OH2 WAT S1599      28.802  58.069  26.514  1.00 17.28      S
ATOM   2796  OH2 WAT S1600      16.767  47.104  22.319  1.00 11.98      S
ATOM   2797  OH2 WAT S1601      30.159  33.756  60.797  1.00  9.19      S
ATOM   2798  OH2 WAT S1602      48.106  27.997  36.005  1.00 14.93      S
ATOM   2799  OH2 WAT S1603      40.650  24.407  21.552  1.00 17.12      S
ATOM   2800  OH2 WAT S1604      22.968  17.449  18.008  1.00 17.85      S
ATOM   2801  OH2 WAT S1605      16.621  15.788  18.605  1.00 25.68      S
ATOM   2802  OH2 WAT S1606       7.206  32.992  16.005  1.00 14.53      S
ATOM   2803  OH2 WAT S1607      57.149  24.564  47.629  1.00 18.35      S
ATOM   2804  OH2 WAT S1608      24.205  26.840  10.350  1.00 23.21      S
ATOM   2805  OH2 WAT S1609      33.745  22.604  31.364  1.00 14.24      S
ATOM   2806  OH2 WAT S1610      21.687  28.608  49.750  1.00 41.13      S
ATOM   2807  OH2 WAT S1611      25.572  18.289  18.085  1.00 18.47      S
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FIGURE 5 (continued)

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ATOM   2808  OH2 WAT S1612      29.378  22.049  15.378  1.00 18.53      S
ATOM   2809  OH2 WAT S1613      47.580  17.180  46.156  1.00 18.00      S
ATOM   2810  OH2 WAT S1614      23.216  43.309  37.644  1.00 13.17      S
ATOM   2811  OH2 WAT S1615      22.669  24.274  48.564  1.00 24.15      S
ATOM   2812  OH2 WAT S1616       0.336  31.433  18.582  1.00 27.87      S
ATOM   2813  OH2 WAT S1617      45.294  33.053  51.773  1.00 13.88      S
ATOM   2814  OH2 WAT S1618      44.363  26.868  22.624  1.00 23.01      S
ATOM   2815  OH2 WAT S1619      24.023  16.291  14.532  1.00 14.28      S
ATOM   2816  OH2 WAT S1620      25.803  16.259  28.626  1.00 18.77      S
ATOM   2817  OH2 WAT S1621      10.423  51.944  32.078  1.00 36.29      S
ATOM   2818  OH2 WAT S1622      26.115  58.809  27.014  1.00 15.64      S
ATOM   2819  OH2 WAT S1623       1.344  28.356  22.672  1.00 26.37      S
ATOM   2820  OH2 WAT S1624      26.639  58.198  21.115  1.00 25.02      S
ATOM   2821  OH2 WAT S1625      26.622  32.997  55.284  1.00 16.24      S
ATOM   2822  OH2 WAT S1626      15.027  52.473  26.183  1.00 21.76      S
ATOM   2823  OH2 WAT S1627      57.187  25.783  44.900  1.00 20.20      S
ATOM   2824  OH2 WAT S1628      44.922  43.322  47.514  1.00 18.96      S
ATOM   2825  OH2 WAT S1629      32.001  38.779  53.199  1.00 17.42      S
ATOM   2826  OH2 WAT S1630      30.741  52.390  22.108  1.00 18.11      S
ATOM   2827  OH2 WAT S1631      14.999  39.258  44.162  1.00 19.15      S
ATOM   2828  OH2 WAT S1632      44.210  20.606  55.552  1.00 17.79      S
ATOM   2829  OH2 WAT S1633      21.471  43.377  12.416  1.00 19.05      S
ATOM   2830  OH2 WAT S1634      13.869  15.823  31.777  1.00 25.21      S
ATOM   2831  OH2 WAT S1635      52.620  30.612  55.173  1.00 30.08      S
ATOM   2832  OH2 WAT S1636      26.556  19.486  52.050  1.00 29.07      S
ATOM   2833  OH2 WAT S1637      21.965  25.980  45.841  1.00 19.07      S
ATOM   2834  OH2 WAT S1638      51.617  33.897  42.473  1.00  9.81      S
ATOM   2835  OH2 WAT S1639      11.552  20.655  19.351  1.00 16.68      S
ATOM   2836  OH2 WAT S1640      30.899  45.201  19.222  1.00 26.19      S
ATOM   2837  OH2 WAT S1641      31.709  48.342  31.000  1.00 18.10      S
ATOM   2838  OH2 WAT S1642      23.676  25.327  22.818  1.00 14.28      S
ATOM   2839  OH2 WAT S1643      25.577  17.219  46.479  1.00 20.91      S
ATOM   2840  OH2 WAT S1644      18.005  18.283  19.152  1.00 24.14      S
ATOM   2841  OH2 WAT S1645      52.881  16.705  50.095  1.00 20.16      S
ATOM   2842  OH2 WAT S1646       5.848  42.562  37.856  1.00 19.01      S
ATOM   2843  OH2 WAT S1647      43.582  14.659  34.565  1.00 28.17      S
ATOM   2844  OH2 WAT S1648      22.374  17.743  20.886  1.00 18.81      S
ATOM   2845  OH2 WAT S1649       8.712  48.989  27.030  1.00 23.87      S
ATOM   2846  OH2 WAT S1650       2.521  47.157  34.228  1.00 30.10      S
ATOM   2847  OH2 WAT S1651      44.220  43.064  40.109  1.00 29.97      S
ATOM   2848  OH2 WAT S1652      27.919  24.353  12.179  1.00 16.62      S
ATOM   2849  OH2 WAT S1653       3.523  42.077  26.249  1.00 22.83      S
ATOM   2850  OH2 WAT S1654      20.380  44.291  37.672  1.00 17.30      S
ATOM   2851  OH2 WAT S1655      57.034  28.423  45.056  1.00 27.44      S
ATOM   2852  OH2 WAT S1656      49.668  24.467  30.455  1.00 22.73      S
ATOM   2853  OH2 WAT S1657      51.259  13.409  45.586  1.00 34.23      S
ATOM   2854  OH2 WAT S1658       9.456  23.136  36.163  1.00 24.71      S
ATOM   2855  OH2 WAT S1659      52.331  23.665  57.905  1.00 18.92      S
ATOM   2856  OH2 WAT S1660      43.381  40.535  56.268  1.00 30.03      S
ATOM   2857  OH2 WAT S1661      13.806  46.776  43.159  1.00 30.72      S
ATOM   2858  OH2 WAT S1662      53.981  30.491  48.223  1.00 13.32      S
ATOM   2859  OH2 WAT S1663      41.765  26.570  28.744  1.00 27.76      S
ATOM   2860  OH2 WAT S1664      40.737  17.318  53.732  1.00 24.67      S
ATOM   2861  OH2 WAT S1665      13.225  44.990   8.674  1.00 28.84      S
ATOM   2862  OH2 WAT S1666      49.013  41.254  39.651  1.00 28.00      S
ATOM   2863  OH2 WAT S1667      44.805  37.426  30.933  1.00 16.56      S
ATOM   2864  OH2 WAT S1668      43.625  18.020  54.500  1.00 24.62      S
ATOM   2865  OH2 WAT S1669      14.317  25.699  46.118  1.00 34.64      S
ATOM   2866  OH2 WAT S1670       3.256  42.913  32.109  1.00 29.06      S
ATOM   2867  OH2 WAT S1671      10.555  49.763  20.725  1.00 28.19      S
ATOM   2868  OH2 WAT S1672      10.096  51.223  27.611  1.00 23.49      S
ATOM   2869  OH2 WAT S1673      14.363  23.946  36.209  1.00 40.49      S
ATOM   2870  OH2 WAT S1674      25.126  59.432  22.831  1.00 22.37      S
ATOM   2871  OH2 WAT S1675      36.093   4.004  46.425  1.00 41.05      S
ATOM   2872  OH2 WAT S1676      58.346  33.177  43.906  1.00 32.25      S
ATOM   2873  OH2 WAT S1677      48.932  35.192  51.801  1.00 26.68      S
ATOM   2874  OH2 WAT S1678      58.902  19.301  43.107  1.00 25.48      S
ATOM   2875  OH2 WAT S1679      44.340  42.085  50.822  1.00 28.00      S
ATOM   2876  OH2 WAT S1680      50.480  38.266  34.016  1.00 31.92      S
ATOM   2877  OH2 WAT S1681      32.259  20.178  55.706  1.00 22.68      S
ATOM   2878  OH2 WAT S1682       5.907  48.823  21.778  1.00 41.37      S
ATOM   2879  OH2 WAT S1683      50.286  29.738  36.205  1.00 41.24      S
ATOM   2880  OH2 WAT S1684      48.359  24.392  27.682  1.00 21.59      S
ATOM   2881  OH2 WAT S1685      28.819  16.491  25.944  1.00 22.91      S
ATOM   2882  OH2 WAT S1686      27.814  39.366  53.598  1.00 22.13      S
ATOM   2883  OH2 WAT S1687      23.282  56.182  29.647  1.00 21.73      S
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FIGURE 5 (continued)

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ATOM   2884  OH2 WAT S1688      11.176  51.488  23.245  1.00 39.40      S
ATOM   2885  OH2 WAT S1689      19.333  13.893  25.470  1.00 16.29      S
ATOM   2886  OH2 WAT S1690      15.528  35.966  43.442  1.00 24.55      S
ATOM   2887  OH2 WAT S1691      28.485  18.098  54.189  1.00 38.82      S
ATOM   2888  OH2 WAT S1692      49.461  42.346  42.415  1.00 29.71      S
ATOM   2889  OH2 WAT S1693       6.986  51.318  31.491  1.00 38.19      S
ATOM   2890  OH2 WAT S1694      45.805  30.330  30.352  1.00 31.74      S
ATOM   2891  OH2 WAT S1695      12.688  17.949  24.810  1.00 24.29      S
ATOM   2892  OH2 WAT S1696      10.481  44.192  41.405  1.00 30.36      S
ATOM   2893  OH2 WAT S1697      36.497  25.163  61.042  1.00 22.75      S
ATOM   2894  OH2 WAT S1698      38.997   8.895  40.582  1.00 35.83      S
ATOM   2895  OH2 WAT S1699      34.429  41.271  24.603  1.00 25.66      S
ATOM   2896  OH2 WAT S1700       9.264  39.356  31.031  1.00 12.79      S
ATOM   2897  OH2 WAT S1701      10.070  23.977  42.971  1.00 38.68      S
ATOM   2898  OH2 WAT S1702      18.383  29.372   9.706  1.00 36.59      S
ATOM   2899  OH2 WAT S1703      49.044  14.511  44.663  1.00 29.13      S
ATOM   2900  OH2 WAT S1704      24.559  26.271  39.612  1.00  9.57      S
ATOM   2901  OH2 WAT S1705      20.114  45.757  12.779  1.00 24.18      S
ATOM   2902  OH2 WAT S1706      40.248  22.113  20.074  1.00 29.44      S
ATOM   2903  OH2 WAT S1707      18.194  41.869  42.229  1.00 17.46      S
ATOM   2904  OH2 WAT S1708      37.847  20.546  20.498  1.00 18.73      S
ATOM   2905  OH2 WAT S1709      16.821  29.280  41.001  1.00 24.06      S
ATOM   2906  OH2 WAT S1710      27.294  42.193  52.815  1.00 19.46      S
ATOM   2907  OH2 WAT S1711      40.821  42.347  51.556  1.00 22.66      S
ATOM   2908  OH2 WAT S1712      26.156  40.106  48.095  1.00 24.85      S
ATOM   2909  OH2 WAT S1713      20.103  24.718  47.608  1.00 30.63      S
ATOM   2910  OH2 WAT S1714      24.148  33.741  56.397  1.00 19.34      S
ATOM   2911  OH2 WAT S1715      18.973  45.993  36.285  1.00 18.68      S
ATOM   2912  OH2 WAT S1716      14.529  44.714  35.623  1.00 11.98      S
ATOM   2913  OH2 WAT S1717      38.781  35.753  22.003  1.00 28.14      S
ATOM   2914  OH2 WAT S1718       9.031  37.190  34.220  1.00 30.97      S
ATOM   2915  OH2 WAT S1719      35.994  16.311  25.745  1.00 28.93      S
ATOM   2916  OH2 WAT S1720      13.544  49.140  34.673  1.00 19.62      S
ATOM   2917  OH2 WAT S1721      22.265  37.832  42.637  1.00 21.65      S
ATOM   2918  OH2 WAT S1722       9.246  42.739  13.991  1.00 23.76      S
ATOM   2919  OH2 WAT S1723      46.901  14.013  46.528  1.00 24.08      S
ATOM   2920  OH2 WAT S1724      27.124  17.124  56.373  1.00 20.76      S
ATOM   2921  OH2 WAT S1725       5.808  39.927  37.880  1.00 30.10      S
ATOM   2922  OH2 WAT S1726      42.361  20.811  20.431  1.00 24.61      S
ATOM   2923  OH2 WAT S1727      26.665  17.537  21.374  1.00 22.27      S
ATOM   2924  OH2 WAT S1728      57.473  29.684  48.797  1.00 33.94      S
ATOM   2925  OH2 WAT S1729       0.205  29.580  11.300  1.00 28.38      S
ATOM   2926  OH2 WAT S1730      28.982  12.144  36.663  1.00 22.16      S
ATOM   2927  OH2 WAT S1731      -2.247  31.885  18.386  1.00 37.56      S
ATOM   2928  OH2 WAT S1732      19.593  14.821  28.910  1.00 29.82      S
ATOM   2929  OH2 WAT S1733       1.174  27.052  34.363  1.00 22.10      S
ATOM   2930  OH2 WAT S1734      35.909  11.924  47.248  1.00 27.93      S
ATOM   2931  OH2 WAT S1735      41.887  40.436  52.838  1.00 28.22      S
ATOM   2932  OH2 WAT S1736      26.213  19.454  10.997  1.00 22.64      S
ATOM   2933  OH2 WAT S1737      34.114  42.884  34.175  1.00 28.42      S
ATOM   2934  OH2 WAT S1738      22.945  32.302  53.065  1.00 25.85      S
ATOM   2935  OH2 WAT S1739      39.089  15.172  28.466  1.00 31.20      S
ATOM   2936  OH2 WAT S1740      47.610  43.601  46.621  1.00 36.15      S
ATOM   2937  OH2 WAT S1741      16.327  45.853  37.179  1.00 17.39      S
ATOM   2938  OH2 WAT S1742      55.363  25.260  59.367  1.00 29.21      S
ATOM   2939  OH2 WAT S1743      30.641  36.731  14.630  1.00 26.83      S
ATOM   2940  OH2 WAT S1744      10.864  46.250  10.531  1.00 23.96      S
ATOM   2941  OH2 WAT S1745      33.170  48.399  28.312  1.00 27.45      S
ATOM   2942  OH2 WAT S1746      32.054  14.892  42.067  1.00 24.32      S
ATOM   2943  OH2 WAT S1747      42.724  28.782  21.018  1.00 34.32      S
ATOM   2944  OH2 WAT S1748      51.123  15.697  52.194  1.00 27.97      S
ATOM   2945  OH2 WAT S1749      42.354  43.166  56.140  1.00 29.49      S
ATOM   2946  OH2 WAT S1750      28.037  37.891  13.736  1.00 33.67      S
ATOM   2947  OH2 WAT S1751      51.086  26.646  30.768  1.00 30.84      S
ATOM   2948  OH2 WAT S1752      10.931  38.592  10.467  1.00 25.71      S
ATOM   2949  OH2 WAT S1753      25.655  29.886  60.929  1.00 19.64      S
ATOM   2950  OH2 WAT S1754      17.145  13.376  23.383  1.00 34.23      S
ATOM   2951  OH2 WAT S1755      44.748  12.372  45.391  1.00 18.99      S
ATOM   2952  OH2 WAT S1756      24.658  10.868  33.101  1.00 39.56      S
ATOM   2953  OH2 WAT S1757      10.322  35.265  39.792  1.00 31.55      S
ATOM   2954  OH2 WAT S1758      57.341  22.537  45.377  1.00 16.36      S
ATOM   2955  OH2 WAT S1759       9.420  34.820  36.963  1.00 32.92      S
ATOM   2956  OH2 WAT S1760      32.502  28.596  14.854  1.00 21.37      S
ATOM   2957  OH2 WAT S1761      39.205  22.929  17.441  1.00 35.60      S
ATOM   2958  OH2 WAT S1762      20.840  52.812  17.278  1.00 31.30      S
ATOM   2959  OH2 WAT S1763      34.711  11.735  35.138  1.00 32.11      S
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FIGURE 5 (continued)

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ATOM   2960  OH2 WAT S1764      51.666  34.131  47.365  1.00 35.34      S
ATOM   2961  OH2 WAT S1765      -2.014  36.180  15.830  1.00 28.16      S
ATOM   2962  OH2 WAT S1766      15.482  48.721  37.060  1.00 29.26      S
ATOM   2963  OH2 WAT S1767      40.630  14.716  31.062  1.00 40.40      S
ATOM   2964  OH2 WAT S1768      23.698  61.256  21.533  1.00 16.86      S
ATOM   2965  OH2 WAT S1769      24.781  28.532  54.977  1.00 16.20      S
ATOM   2966  OH2 WAT S1770      26.852  25.257  10.061  1.00 30.41      S
ATOM   2967  OH2 WAT S1771      43.726  10.405  46.878  1.00 29.13      S
ATOM   2968  OH2 WAT S1772      25.837  37.362  54.027  1.00 21.97      S
ATOM   2969  OH2 WAT S1773      33.373  46.686  32.566  1.00 26.20      S
ATOM   2970  OH2 WAT S1774      27.264  20.817  13.545  1.00 22.02      S
ATOM   2971  OH2 WAT S1775      47.925  30.806  31.477  1.00 33.49      S
ATOM   2972  OH2 WAT S1776       8.238  38.202  37.592  1.00 26.28      S
ATOM   2973  OH2 WAT S1777      21.090  51.641  25.222  1.00 18.54      S
ATOM   2974  OH2 WAT S1778       6.267  38.069  32.873  1.00 22.17      S
ATOM   2975  OH2 WAT S1779      23.234  49.347  16.745  1.00 24.08      S
ATOM   2976  OH2 WAT S1780      22.134  39.856  40.656  1.00 21.00      S
ATOM   2977  OH2 WAT S1781      20.856  35.405   9.637  1.00 23.13      S
ATOM   2978  OH2 WAT S1782      21.475  53.999  26.047  1.00 27.01      S
ATOM   2979  OH2 WAT S1783      34.915  27.212  15.190  1.00 31.71      S
ATOM   2980  OH2 WAT S1784      45.211  12.993  42.137  1.00 21.38      S
ATOM   2981  OH2 WAT S1785      38.126  34.805  40.034  1.00 17.57      S
ATOM   2982  OH2 WAT S1786      30.962  49.798  21.332  1.00 32.31      S
ATOM   2983  OH2 WAT S1787      33.222  19.319  25.705  1.00 29.22      S
ATOM   2984  OH2 WAT S1788      40.144  19.662  28.253  1.00 33.93      S
ATOM   2985  OH2 WAT S1789       6.555  28.590  37.281  1.00 28.90      S
ATOM   2986  OH2 WAT S1790      43.426  43.935  45.155  1.00 34.35      S
ATOM   2987  OH2 WAT S1791       3.263  33.201  14.705  1.00 33.11      S
ATOM   2988  OH2 WAT S1792      20.149  16.998  31.047  1.00 26.99      S
ATOM   2989  OH2 WAT S1793      34.123  42.842  21.180  1.00 24.49      S
ATOM   2990  OH2 WAT S1794      49.929  18.274  53.829  1.00 39.26      S
ATOM   2991  OH2 WAT S1795      14.815  31.617   9.739  1.00 35.94      S
ATOM   2992  OH2 WAT S1796      45.588  41.539  53.753  1.00 35.01      S
ATOM   2993  OH2 WAT S1797      33.245  52.433  24.002  1.00 34.85      S
ATOM   2994  OH2 WAT S1798      43.010  24.276  22.909  1.00 21.38      S
ATOM   2995  OH2 WAT S1799      19.769  14.826  46.718  1.00 30.67      S
ATOM   2996  OH2 WAT S1800      29.812  17.873  43.458  1.00 28.85      S
ATOM   2997  OH2 WAT S1801       7.028  22.438  24.718  1.00 30.13      S
ATOM   2998  OH2 WAT S1802       7.451  42.723  16.836  1.00 34.86      S
ATOM   2999  OH2 WAT S1803      13.062  50.532  16.899  1.00 27.23      S
ATOM   3000  OH2 WAT S1804      31.535  17.528  46.115  1.00 21.48      S
ATOM   3001  OH2 WAT S1805       1.214  41.199  23.409  1.00 33.03      S
ATOM   3002  OH2 WAT S1806      12.350  33.958  40.836  1.00 34.82      S
ATOM   3003  OH2 WAT S1807      33.164  41.928  54.755  1.00 33.81      S
ATOM   3004  OH2 WAT S1808       4.467  50.285  27.482  1.00 36.79      S
ATOM   3005  OH2 WAT S1809      60.702  26.732  42.684  1.00 35.13      S
ATOM   3006  OH2 WAT S1810      22.799  31.560  57.795  1.00 32.80      S
ATOM   3007  OH2 WAT S1811      16.630  35.862   8.507  1.00 29.92      S
ATOM   3008  OH2 WAT S1812      58.212  35.487  40.540  1.00 33.76      S
ATOM   3009  OH2 WAT S1813      31.566  17.525  26.426  1.00 39.01      S
ATOM   3010  OH2 WAT S1814      38.884  37.614  20.120  1.00 33.89      S
ATOM   3011  OH2 WAT S1815      58.154  24.777  37.822  1.00 35.73      S
ATOM   3012  OH2 WAT S1816      34.384  14.783  47.649  1.00 37.28      S
ATOM   3013  OH2 WAT S1817       3.439  43.153  36.372  1.00 30.78      S
ATOM   3014  OH2 WAT S1818      47.394  12.444  43.290  1.00 30.32      S
ATOM   3015  OH2 WAT S1819      24.644  13.829  44.044  1.00 32.65      S
ATOM   3016  OH2 WAT S1820      35.990  42.985  32.322  1.00 29.66      S
ATOM   3017  OH2 WAT S1821      26.914  40.212   9.947  1.00 33.58      S
ATOM   3018  OH2 WAT S1822      40.296  29.386  23.361  1.00 44.10      S
ATOM   3019  OH2 WAT S1823      42.915  30.163  27.417  1.00 33.23      S
ATOM   3020  OH2 WAT S1824      14.322  38.428   8.032  1.00 35.73      S
ATOM   3021  OH2 WAT S1825      33.329  16.000  45.385  1.00 29.78      S
ATOM   3022  OH2 WAT S1826      55.683  28.168  38.449  1.00 30.81      S
ATOM   3023  OH2 WAT S1827      18.514  45.706   9.695  1.00 34.33      S
ATOM   3024  OH2 WAT S1828      19.453  54.788  22.809  1.00 42.02      S
ATOM   3025  OH2 WAT S1829      46.686  27.005  20.816  1.00 31.17      S
ATOM   3026  OH2 WAT S1830      50.779  32.327  54.666  1.00 44.04      S
ATOM   3027  OH2 WAT S1831       5.243  43.614  40.262  1.00 40.69      S
ATOM   3028  OH2 WAT S1832      45.151  43.041  33.919  1.00 28.47      S
ATOM   3029  OH2 WAT S1833      26.385  11.949  41.104  1.00 33.70      S
ATOM   3030  OH2 WAT S1834      36.104  26.756  17.653  1.00 32.43      S
ATOM   3031  OH2 WAT S1835      40.585   7.298  41.894  1.00 32.97      S
ATOM   3032  OH2 WAT S1836      22.940  54.196  16.985  1.00 39.88      S
ATOM   3033  OH2 WAT S1837      53.968  24.450  37.442  1.00 39.29      S
ATOM   3034  OH2 WAT S1838      16.318  26.973  42.179  1.00 32.94      S
ATOM   3035  OH2 WAT S1839      14.513  48.940  39.307  1.00 29.97      S
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FIGURE 5 (continued)

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ATOM   3036  OH2 WAT S1840      31.652   6.945  51.493  1.00 27.66      S
ATOM   3037  OH2 WAT S1841      41.996  11.677  38.039  1.00 37.88      S
ATOM   3038  OH2 WAT S1842       7.510  48.642  19.668  1.00 35.11      S
ATOM   3039  OH2 WAT S1843      42.467   3.493  49.912  1.00 33.41      S
ATOM   3040  OH2 WAT S1844      59.776  22.501  42.412  1.00 44.37      S
ATOM   3041  OH2 WAT S1845       7.867  44.473  12.687  1.00 34.20      S
ATOM   3042  OH2 WAT S1846      15.405  45.353  39.658  1.00 38.08      S
ATOM   3043  OH2 WAT S1847      13.585  15.183  28.501  1.00 36.58      S
ATOM   3044  OH2 WAT S1848      48.442  41.492  47.985  1.00 26.95      S
ATOM   3045  OH2 WAT S1849      50.374  40.886  46.017  1.00 34.93      S
ATOM   3046  OH2 WAT S1850      44.568   8.030  45.822  1.00 42.34      S
ATOM   3047  OH2 WAT S1851      48.705  28.443  22.632  1.00 34.87      S
ATOM   3048  OH2 WAT S1852      38.217  33.408  18.268  1.00 40.91      S
ATOM   3049  OH2 WAT S1853      26.698  47.866  16.749  1.00 26.87      S
ATOM   3050  OH2 WAT S1854      36.624  40.405  57.361  1.00 30.57      S
ATOM   3051  OH2 WAT S1855      44.243  22.209  21.682  1.00 25.97      S
ATOM   3052  OH2 WAT S1856      50.807  22.291  30.826  1.00 30.01      S
ATOM   3053  OH2 WAT S1857       2.113  19.175  16.420  1.00 39.64      S
ATOM   3054  OH2 WAT S1858      35.799  20.261  25.717  1.00 29.95      S
ATOM   3055  OH2 WAT S1859      10.845  51.013  18.474  1.00 29.30      S
ATOM   3056  OH2 WAT S1860      13.036  16.982  18.603  1.00 35.56      S
ATOM   3057  OH2 WAT S1861      48.755  33.466  53.529  1.00 32.19      S
ATOM   3058  OH2 WAT S1862      28.542  12.640  28.777  1.00 32.37      S
ATOM   3059  OH2 WAT S1863      15.582  33.781  40.294  1.00 31.38      S
ATOM   3060  OH2 WAT S1864      15.389  51.736  31.264  1.00 35.97      S
ATOM   3061  OH2 WAT S1865      59.586  24.576  44.154  1.00 38.45      S
ATOM   3062  OH2 WAT S1866      33.931  18.197  52.470  1.00 31.45      S
ATOM   3063  OH2 WAT S1867      33.400  24.810  14.487  1.00 31.43      S
ATOM   3064  OH2 WAT S1868       2.939  39.474  28.464  1.00 42.13      S
ATOM   3065  OH2 WAT S1869      52.149  36.661  45.439  1.00 34.90      S
ATOM   3066  OH2 WAT S1870      45.901  34.119  54.146  1.00 28.55      S
ATOM   3067  OH2 WAT S1871      21.485  29.372  44.666  1.00 37.03      S
ATOM   3068  OH2 WAT S1872      10.455  19.175  23.705  1.00 36.18      S
ATOM   3069  OH2 WAT S1873      29.820  54.141  17.625  1.00 37.56      S
ATOM   3070  OH2 WAT S1874      36.824  12.036  41.616  1.00 36.62      S
ATOM   3071  OH2 WAT S1875      35.575  29.695  13.582  1.00 31.58      S
ATOM   3072  OH2 WAT S1876      47.689  26.645  56.483  1.00 29.75      S
ATOM   3073  OH2 WAT S1877      25.923  24.021   7.877  1.00 35.32      S
ATOM   3074  OH2 WAT S1878      35.914  42.663  19.444  1.00 38.13      S
ATOM   3075  OH2 WAT S1879      53.553  27.199  37.462  1.00 34.02      S
ATOM   3076  OH2 WAT S1880      31.012  18.989  51.960  1.00 32.14      S
ATOM   3077  OH2 WAT S1881       5.543  24.207  39.126  1.00 33.92      S
ATOM   3078  OH2 WAT S1882      12.515  49.450  14.280  1.00 38.32      S
ATOM   3079  OH2 WAT S1883      19.621  34.441  42.264  1.00 32.10      S
ATOM   3080  OH2 WAT S1884       0.567  34.443  15.606  1.00 41.76      S
ATOM   3081  OH2 WAT S1885      19.842  21.597  48.228  1.00 38.20      S
ATOM   3082  OH2 WAT S1886      17.245  44.489  41.443  1.00 36.34      S
ATOM   3083  OH2 WAT S1887      31.241  17.703  18.315  1.00 43.85      S
ATOM   3084  OH2 WAT S1888      47.120  35.974  31.511  1.00 44.95      S
ATOM   3085  OH2 WAT S1889      16.721  12.447  25.646  1.00 42.81      S
ATOM   3086  OH2 WAT S1890      17.002  21.309  47.530  1.00 35.74      S
ATOM   3087  OH2 WAT S1891      11.124  36.224  11.415  1.00 28.23      S
ATOM   3088  OH2 WAT S1892      31.476  35.439  12.666  1.00 29.98      S
ATOM   3089  OH2 WAT S1893      20.313  44.798   8.239  1.00 38.49      S
ATOM   3090  OH2 WAT S1894      49.492  37.692  31.490  1.00 34.21      S
ATOM   3091  OH2 WAT S1895      11.168  48.631  11.775  1.00 35.00      S
ATOM   3092  OH2 WAT S1896       8.149  35.174  12.830  1.00 43.18      S
ATOM   3093  OH2 WAT S1897      42.985  36.028  29.277  1.00 37.84      S
ATOM   3094  OH2 WAT S1898      15.722  26.088  38.269  1.00 40.56      S
ATOM   3095  OH2 WAT S1899       9.466  42.584  43.325  1.00 38.58      S
ATOM   3096  OH2 WAT S1900      55.683  27.859  55.011  1.00 40.16      S
ATOM   3097  OH2 WAT S1901      16.412  44.824   6.088  1.00 35.00      S
ATOM   3098  OH2 WAT S1902      30.819  20.863  13.376  1.00 36.12      S
ATOM   3099  OH2 WAT S1903      20.083  45.050  40.249  1.00 46.55      S
ATOM   3100  OH2 WAT S1904      55.216  16.767  37.256  1.00 32.34      S
ATOM   3101  OH2 WAT S1905      17.194  15.633  31.289  1.00 41.92      S
ATOM   3102  OH2 WAT S1906      55.468  39.305  45.956  1.00 33.48      S
ATOM   3103  OH2 WAT S1907      34.073  59.171  22.880  1.00 29.68      S
ATOM   3104  OH2 WAT S1908      11.696  23.487  37.533  1.00 44.83      S
ATOM   3105  OH2 WAT S1909      37.193  57.700  24.645  1.00 29.20      S
ATOM   3106  OH2 WAT S1910       4.958  20.071  12.971  1.00 38.75      S
ATOM   3107  OH2 WAT S1911      28.212  15.651  46.090  1.00 44.28      S
ATOM   3108  OH2 WAT S1912      25.791  17.881  50.101  1.00 44.07      S
ATOM   3109  OH2 WAT S1913      44.830  16.225  28.015  1.00 37.34      S
ATOM   3110  OH2 WAT S1914      45.538  25.603  58.524  1.00 31.60      S
ATOM   3111  OH2 WAT S1915      31.849  53.832  20.135  1.00 44.08      S
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FIGURE 5 (continued)

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ATOM   3112  OH2 WAT S1916      55.981  32.376  47.108  1.00 41.65      S
ATOM   3113  OH2 WAT S1917      35.699  24.353  16.736  1.00 43.04      S
ATOM   3114  OH2 WAT S1918       3.252  25.157  38.490  1.00 42.38      S
ATOM   3115  OH2 WAT S1919      34.711  10.496  39.861  1.00 36.97      S
ATOM   3116  OS4 PLA P1001       8.781  29.613  10.689  1.00 35.34      P
ATOM   3117  S2  PLA P1001       9.783  28.546  11.256  1.00 33.57      P
ATOM   3118  OS5 PLA P1001      10.409  27.663   9.867  1.00 40.37      P
ATOM   3119  OS6 PLA P1001      11.159  29.189  12.135  1.00 41.03      P
ATOM   3120  C15 PLA P1001       9.058  27.351  12.199  1.00 30.49      P
ATOM   3121  C14 PLA P1001       7.662  27.126  12.015  1.00 23.35      P
ATOM   3122  C16 PLA P1001       9.978  26.532  12.898  1.00 28.94      P
ATOM   3123  C10 PLA P1001       9.499  25.436  13.634  1.00 30.90      P
ATOM   3124  C11 PLA P1001       8.025  25.127  13.485  1.00 25.22      P
ATOM   3125  C13 PLA P1001       7.134  25.968  12.614  1.00 21.41      P
ATOM   3126  O3  PLA P1001       5.837  25.588  12.437  1.00 24.00      P
ATOM   3127  C12 PLA P1001       7.519  23.932  14.212  1.00 27.53      P
ATOM   3128  O2  PLA P1001       6.235  23.585  13.967  1.00 21.97      P
ATOM   3129  C9  PLA P1001      10.366  24.618  14.415  1.00 32.13      P
ATOM   3130  C8  PLA P1001       9.876  23.541  15.205  1.00 31.56      P
ATOM   3131  S1  PLA P1001      10.846  22.324  15.981  1.00 31.16      P
ATOM   3132  OS3 PLA P1001      12.358  22.881  16.679  1.00 39.44      P
ATOM   3133  OS2 PLA P1001      11.138  21.153  14.733  1.00 28.72      P
ATOM   3134  OS1 PLA P1001      10.061  21.436  17.011  1.00 39.17      P
ATOM   3135  C7  PLA P1001       8.424  23.154  15.086  1.00 20.93      P
ATOM   3136  N2  PLA P1001       7.947  21.974  15.652  1.00 27.49      P
ATOM   3137  N1  PLA P1001       6.731  21.270  15.708  1.00 26.74      P
ATOM   3138  C2  PLA P1001       6.780  19.948  16.206  1.00 29.90      P
ATOM   3139  C1  PLA P1001       7.938  19.230  16.659  1.00 26.11      P
ATOM   3140  C3  PLA P1001       5.455  19.218  16.215  1.00 29.97      P
ATOM   3141  O1  PLA P1001       4.329  19.881  15.839  1.00 27.77      P
ATOM   3142  C4  PLA P1001       5.419  17.867  16.622  1.00 27.79      P
ATOM   3143  C5  PLA P1001       6.617  17.226  17.060  1.00 24.04      P
ATOM   3144  C6  PLA P1001       7.890  17.875  17.105  1.00 28.93      P
ATOM   3145  CL1 PLA P1001       8.958  17.179  17.619  1.00 13.83      P
ATOM   3146  OS4 PLA P1002      -1.265  32.010  14.293  1.00 40.73      P
ATOM   3147  S2  PLA P1002      -2.593  31.401  14.907  1.00 34.43      P
ATOM   3148  OS5 PLA P1002      -3.293  32.318  16.225  1.00 36.70      P
ATOM   3149  OS6 PLA P1002      -3.702  31.417  13.545  1.00 38.28      P
ATOM   3150  C15 PLA P1002      -2.360  29.762  15.366  1.00 37.51      P
ATOM   3151  C14 PLA P1002      -1.339  29.023  14.693  1.00 32.35      P
ATOM   3152  C16 PLA P1002      -3.324  29.136  16.198  1.00 32.13      P
ATOM   3153  C10 PLA P1002      -3.227  27.770  16.534  1.00 32.57      P
ATOM   3154  C11 PLA P1002      -2.159  26.968  15.824  1.00 27.55      P
ATOM   3155  C13 PLA P1002      -1.219  27.623  14.849  1.00 32.76      P
ATOM   3156  O3  PLA P1002      -0.300  26.897  14.135  1.00 26.73      P
ATOM   3157  C12 PLA P1002      -2.103  25.533  16.170  1.00 29.76      P
ATOM   3158  O2  PLA P1002      -1.093  24.861  15.620  1.00 19.01      P
ATOM   3159  C9  PLA P1002      -4.076  27.177  17.503  1.00 28.28      P
ATOM   3160  C8  PLA P1002      -4.072  25.777  17.756  1.00 30.57      P
ATOM   3161  S1  PLA P1002      -4.937  25.049  19.065  1.00 30.09      P
ATOM   3162  OS3 PLA P1002      -6.417  25.925  19.382  1.00 26.32      P
ATOM   3163  OS2 PLA P1002      -3.886  25.328  20.444  1.00 39.20      P
ATOM   3164  OS1 PLA P1002      -5.060  23.483  18.960  1.00 35.43      P
ATOM   3165  C7  PLA P1002      -3.056  24.884  17.116  1.00 30.01      P
ATOM   3166  N2  PLA P1002      -2.942  23.547  17.510  1.00 30.83      P
ATOM   3167  N1  PLA P1002      -1.994  22.600  17.132  1.00 26.11      P
ATOM   3168  C2  PLA P1002      -2.109  21.347  17.777  1.00 33.57      P
ATOM   3169  C1  PLA P1002      -3.069  20.979  18.767  1.00 28.55      P
ATOM   3170  C3  PLA P1002      -1.126  20.289  17.352  1.00 32.70      P
ATOM   3171  O1  PLA P1002      -0.254  20.633  16.366  1.00 26.71      P
ATOM   3172  C4  PLA P1002      -1.181  19.011  17.978  1.00 35.63      P
ATOM   3173  C5  PLA P1002      -2.175  18.727  18.965  1.00 32.99      P
ATOM   3174  C6  PLA P1002      -3.137  19.696  19.364  1.00 34.82      P
ATOM   3175  CL1 PLA P1002      -4.110  19.418  20.286  1.00 26.50      P
ATOM   3176  P   PO4 I1000      31.378  36.578  34.442  1.00  7.30      I
ATOM   3177  O1  PO4 I1000      30.121  37.237  34.900  1.00  8.97      I
ATOM   3178  O2  PO4 I1000      32.276  37.583  33.795  1.00  6.24      I
ATOM   3179  O3  PO4 I1000      31.043  35.497  33.462  1.00  6.45      I
ATOM   3180  O4  PO4 I1000      32.089  35.965  35.624  1.00  7.79      I
ATOM   3181  U   U   I1100       0.273  22.910  15.547  1.00 30.28      I
ATOM   3182  U   U   I1101       4.450  22.112  14.520  1.00 29.14      I
ATOM   3183  U   U   I1102       2.292  24.635  12.979  0.50 39.41      I
ATOM   3184  NA  NA  I1200      37.019  13.768  54.963  1.00 21.53      I
END
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FIGURE 5 (continued)

NOVEL PHOSPHATE-BINDING PROTEIN, PHARMACEUTICAL COMPOSITIONS CONTAINING SAME AND USE THEREOF

[0001] A subject of the present invention is a novel phosphate-binding protein, obtained from human serum, pharmaceutical compositions containing it as well as uses thereof, in particular within the framework of the treatment of hyperphosphataemia and cardiovascular diseases or arthritis.

[0002] Phosphate is a very important molecule involved in numerous biological mechanisms. Phosphate is found in particular in the phospholipids, in the energy-production mechanism (ATP, ADP), in the cell signalling processes and in the composition of the genetic material in the bones (in the form of calcium phosphate).

[0003] Hyperphosphataemia is a pathology linked to an excess of phosphate in the organism and causes in particular an increase in the risks of cardiovascular diseases, by promoting the processes of atherosclerosis and calcification of the arteries (Dorozhkin and Epple, 2002; Amann et al., 2003; Blazheevich et al., 1975). As calcification takes place in the joints, hyperphosphataemia can also cause arthritis (pseudogout).

[0004] The calcium phosphate salts produced in the serum during hyperphosphataemia precipitate in the soft tissues with ectopic calcification in different tissues: vessels (cerebral or cardio vascular accidents), joints (pseudogout), lens, renal interstitium (nephrocalcinosis), sub-cutaneous (pruritis), pulmonary, and pancreatic.

[0005] Thus, half the deaths of individuals suffering from renal insufficiency is due to cardiovascular diseases linked to hyperphosphataemia. In this regard, certain phosphate chelating agents which complex the phosphate in the intestinal lumen are currently used as medicaments. However, not all these chelating agents are physiological. This results in certain complications or restrictions as to their use.

[0006] Preparations containing magnesium are limited by the appearance of digestive disorders (diarrhoea) and are to be proscribed because of the risk of hypermagnesaemia. Similarly, the prescription of aluminium hydroxide, long used because of its effectiveness, must be avoided, or at least limited to very short periods, because of the risk of aluminium intoxication (microcytic hypochromic anaemia, osteomalacia, myopathy, dementia).

[0007] The prescription of calcium salts is the best means for correcting both hypocalcaemia and hyperphosphoraemia, making it possible on the one hand to increase the quantity of calcium absorbed by the small intestine in spite of the calcitriol deficiency, and on the other hand to complex the phosphorus in the intestinal lumen in the form of calcium phosphate which is eliminated in the faeces. However, the major drawback of the chelating agents containing calcium is that of inducing hypercalcaemia, which, in certain series, has been noted in 20% of patients. This risk has lead to the development of other products capable of limiting hyperphosphoraemia.

[0008] The medicament most used at present is Renagel® (Ramsdell; 1999). This is a non-absorbable cationic polymer, capable of chelating phosphate.

[0009] The purpose of the present invention is to provide a novel physiological protein chelating agent binding to phosphate, not requiring the use of other ions which can lead to complications and offering wider use perspectives than current chelating agents.

[0010] The present invention relates to a protein characterized in that it comprises or is constituted by:

[0011] the sequence SEQ ID NO: 1,

[0012] or any sequence derived from the sequence SEQ ID NO: 1, in particular by substitution, suppression or addition of one or more amino acids, providing that said derived sequence binds to phosphate,

[0013] or any sequence homologous to the sequence SEQ ID NO: 1, preferably having a homology of at least approximately 80% with the sequence SEQ ID NO: 1, providing that said homologous sequence binds to phosphate,

[0014] or any fragment of one of the sequences defined above, providing that said fragment binds to phosphate, in particular any fragment being constituted by at least approximately 20 contiguous amino acids in the sequence SEQ ID NO: 1.

[0015] The present invention relates to a protein as defined above, characterized in that it comprises or is constituted by:

[0016] the sequence SEQ ID NO: 2 or the sequence SEQ ID NO: 3,

[0017] or any sequence derived from the sequence SEQ ID NO: 2 or SEQ ID NO: 3, in particular by substitution, suppression or addition of one or more amino acids, providing that said derived sequence binds to phosphate,

[0018] or any sequence homologous to the sequence SEQ ID NO: 2 or SEQ ID NO: 3, preferably having a homology of at least approximately 80% with the sequence SEQ ID NO: 2 or SEQ ID NO: 3, providing that said homologous sequence binds to phosphate,

[0019] or any fragment of one of the sequences defined above, providing that said fragment binds to phosphate, in particular any fragment being constituted by at least approximately 20 contiguous amino acids in the sequence SEQ ID NO: 2 or SEQ ID NO: 3.

[0020] The sequence SEQ ID NO: 2 corresponds to the human phosphate-binding protein. This novel protein has been isolated in human plasma and its three-dimensional structure shows that it belongs to the "phosphate binding protein" (PBP) class. It is also called hereafter HPBP (human phosphate binding protein).

[0021] The sequence SEQ ID NO: 3 corresponds to a protein homologous to the protein sequence SEQ ID NO: 2, having a percentage of identity of approximately 90% with the sequence SEQ ID NO: 2, and having the same phosphate-binding properties as the sequence SEQ ID NO: 2.

[0022] The phosphate-binding property of the sequences of the invention can be verified by the following phosphate-binding test by radioactive labelling:

[0023] The protein is bound to a nitrocellulose membrane (dot blot by aspiration). The membrane is left to incubate in

a radioactive buffer (^{32}P (10 mCi/ml, Amersham-Biosciences) 2M; Tris 50 mM; pH 8.0)

[0024] The membrane is rapidly rinsed 2×1 min in a Tris 50 mM buffer, pH 8.0. By exposing a photographic film with the membrane (approximately 45 min) it is possible to detect the zones which bind the radioactive phosphate (see FIG. 3 hereafter).

[0025] The present invention also relates to a nucleotide sequence encoding a protein as defined above.

[0026] The present invention also relates to a recombinant vector, in particular plasmid, cosmid, phage or virus DNA, containing a nucleotide sequence as defined above.

[0027] According to an advantageous embodiment, the present invention relates to a recombinant vector as defined above, containing the elements necessary for the expression in a host cell of the polypeptides encoded by the nucleotide sequence as defined above, inserted into said vector.

[0028] The present invention also relates to a host cell, chosen in particular from bacteria, viruses, yeasts, fungi, plants or mammal cells, said host cell being transformed, in particular using a recombinant vector as defined above.

[0029] The present invention also relates to a pharmaceutical composition comprising as active ingredient a protein as defined above, in particular SEQ ID NO: 2 or SEQ ID NO: 3, in combination with a pharmaceutically acceptable vehicle.

[0030] The present invention also relates to a pharmaceutical composition as defined above, in which the protein of the invention, in particular SEQ ID NO: 2 or SEQ ID NO: 3, is in combination with a variant of the paraoxonase protein, having a paraoxon hydrolysis activity.

[0031] Among the variants of paraoxonase, there can be mentioned the variants PON1, PON2, PON3, of human or non-human origin, such as SEQ ID NO: 4 (human PON1; Hassett et al. 1991), SEQ ID NO: 5 (human PON2; Primo-Parmo et al., 1996), SEQ ID NO: 6 (human PON3; Reddy et al., 2001), SEQ ID NO: 7 (rabbit PON1; Hassett et al., 1991), SEQ ID NO: 8 (rat PON1; Rodrigo et al., 1997), SEQ ID NO: 9 (mouse PON1; Sorenson et al., 1995), SEQ ID NO: 10 (mouse PON2; Primo-Parmo et al., 1996) and SEQ ID NO: 11 (mouse PON3; Primo-Parmo et al., 1996).

[0032] The present invention also relates to the use of a protein as defined above, in particular SEQ ID NO: 2 or SEQ ID NO: 3, for the preparation of a medicament intended for the prevention or treatment of diseases linked to hyperphosphataemia, such as cardiovascular diseases and arthritis (pseudogout).

[0033] The term "hyperphosphataemia" designates an excess of phosphate in the organism. More precisely, hyperphosphataemia is defined by an increase in the phosphate concentration in the plasma above 1.44 mmol/l (45 mg/l), said quantity being obtained by assay of the total phosphate (assay by colorimetric method is carried out after a mineralization process).

[0034] According to an advantageous embodiment, the protein of the invention can be administered in intravenous form in order to be able to bind a maximum quantity of phosphate over a long period, of the order of a week. By subsequently eliminating the protein, a large quantity of phosphate is thus rapidly eliminated. This makes it possible to space out and reduce the periods of dialysis.

[0035] The present invention relates more particularly to the use of a protein as defined above, in particular SEQ ID NO: 2 or SEQ ID NO: 3, within the framework of the prevention or treatment of cardiovascular diseases.

[0036] The present invention also relates to the use of a protein according to the invention, in particular of the protein represented by the sequence SEQ ID NO: 2 or SEQ ID NO: 3, in combination with a protein such as a variant of the paraoxonase protein, within the framework of the prophylaxis or treatment of intoxications caused by insecticides or nerve agents, such as soman, VX, tabun or sarin, or within the framework of the treatment of atherosclerosis.

[0037] The present invention also relates to a combination product comprising at least one protein as defined above, in particular SEQ ID NO: 2 or SEQ ID NO: 3, and at least one variant of the paraoxonase protein, for simultaneous or separate use or use spread over time intended for the prophylaxis or treatment of intoxications caused by insecticides or nerve agents, such as soman, VX, tabun or sarin.

[0038] The combined use of the protein of the invention, in particular SEQ ID NO: 2, with a variant of the paraoxonase protein, makes it possible to increase the stability of the paraoxonase, in particular within the framework of the prophylaxis or treatment of the intoxications caused by insecticides or nerve agents.

[0039] The present invention also relates to a protein assay method as defined above, characterized in that it comprises the following stages:

[0040] rabbit monoclonal antibodies directed against different epitopes of the protein of the invention (anti-HPB) are fixed on a plate and the human serum to be analyzed containing said protein (HPB) is applied to the above-mentioned plate,

[0041] the plate is rinsed and washed,

[0042] antibodies directed against rabbit antibodies (anti-IGrabbit-per) marked with peroxidase are applied to the plate over 30 minutes, in order to form a ternary complex between a rabbit monoclonal antibody, the protein according to the invention and an above-mentioned antibody directed against a rabbit antibody (anti-HPB-HPB-anti-IGrabbit-per),

[0043] the plate is rinsed and washed,

[0044] the peroxidase fixed to the plate is reacted with its substrate (commercially available kit, Chemiluminescent Peroxidase Substrate (Sigma)) and the reaction is stopped at the end of 30 minutes with 3,3',5,5'-tetramethylbenzidine (TMB, Sigma),

[0045] the optical density of the product formed in the preceding stage is measured at 450 nm using a spectrophotometer, and comparison of this measurement with a standard curve makes it possible to determine the concentration of the protein according to the invention (HPB) present in the serum.

[0046] Thus, the above-mentioned assay method uses an ELISA-type immunoassay method (Engvall et al., 1971).

[0047] Other methods can be used to assay the concentration of the protein of the invention in the plasma such as:

[0048] electrophoretic methods, or

[0049] the quantification of its activity.

[0050] The present invention also relates to the application of the assay method as defined above

[0051] to the in vitro diagnosis of diseases linked to hyperphosphataemia in particular when the quantity of protein as defined above, in particular SEQ ID NO: 2 or SEQ ID NO: 3, assayed according to the method as defined above, is less than the quantity of this protein normally present in the blood of a healthy individual, or

[0052] to the in vitro diagnosis of diseases linked to hypophosphataemia in particular when the quantity of protein as defined above, in particular SEQ ID NO: 2 or SEQ ID NO: 3, assayed according to the method as defined above, is greater than the quantity of this protein normally present in the blood of a healthy individual, or to the in vitro diagnosis of an individual's predisposition to such pathologies.

[0053] The level of the protein according to the invention is an indicator of predisposition to a risk of cardiovascular disease. Thus, individuals having a low level of said protein will have a higher level of free phosphate which will precipitate with the calcium in the plasma to form calcium phosphate plates, which is a factor aggravating in particular the risks of cardiovascular diseases or arthritis.

[0054] An abnormal level of this protein is also the sign of an existing pathology. For example hyperphosphataemia can trigger an increased production of protein in order to limit the phosphate level. A low level can also reveal a dysfunction.

[0055] The present invention also relates to the application as defined above to the in vitro diagnosis of diseases linked to hyperphosphataemia such as cardiovascular diseases, in particular cardiovascular diseases linked to the formation of atheroma plaques, or to the in vitro diagnosis of an individual's predisposition to develop one of the above-mentioned diseases.

[0056] The present invention also relates to the application as defined above to the in vitro diagnosis of diseases linked to hypophosphataemia, or to the in vitro diagnosis of an individual's predisposition to develop these diseases.

[0057] Among the clinical or physiological signs characterizing diseases linked to hypophosphataemia, there can be mentioned:

[0058] a demineralization of the bones,

[0059] the muscular manifestations of hypophosphataemia which comprise a proximal myopathy affecting the skeletal muscle and dysphagia and an ileus affecting the smooth muscles,

[0060] cardiopulmonary deficiencies due to the lack of ATP, and

[0061] metabolic encephalopathy.

LEGENDS TO THE FIGURES

[0062] FIG. **1** represents an SDS-PAGE gel of the final fractions within the framework of the purification of human paraoxonase and the protein of the invention SEQ ID NO: 2.

[0063] Column A corresponds to the molecular weight marker and columns B, C and D to three different purifications originating from different bags of human plasma. They all three contain human paraoxonase and the phosphate-binding protein.

[0064] FIG. **2** represents the diagrammatic structure of the protein of the invention SEQ ID NO: 2 to which a phosphate molecule is bound.

[0065] FIG. **3** corresponds to a test of phosphate binding by the protein of the invention SEQ ID NO: 2.

[0066] Columns A to F correspond to different batches of purification of the protein of the invention originating from different bags of human plasma; column G to lysozyme 1 mg/ml and column H to β-lactoglobulin.

[0067] FIG. **4** represents a two-dimensional electrophoresis gel of a mixture of the protein of the invention SEQ ID NO: 2 and paraoxonase.

[0068] FIG. **5** represents the molecular coordinates of the crystallized protein of the invention SEQ ID NO: 2.

EXPERIMENTAL PART

[0069] Isolation of the Protein

[0070] The protein SEQ ID NO: 2 is obtained from human plasma according to the following method of Gan et al. (1991):

[0071] The protein SEQ ID NO: 2 is purified from bags of frozen plasma (~200 ml) supplied by the Etablissement de Transfusion Sanguine of Lyon-Beynost. The fibrin clot, formed by the addition of 1 M (1% v/v) of $CaCl_2$ to the plasma is separated from the serum by filtration. The serum is then mixed with 400 ml of affinity gel (Cibacron 3GA-Agarose, C-1535, Sigma) equilibrated with a buffer A (Tris/HCl 50 mM, $CaCl_2$ 1 mM, NaCl 4M, pH 8). Under these conditions, mainly the HDLs ("high density lipoproteins") are adsorbed. After incubation for 6 to 8 hours, the proteins not adsorbed on the gel are eliminated by filtration on a fritted disc of porosity No. 2. This washing is carried out until no more protein is detected in the eluate (UV absorption at 280 nm). The gel is then equilibrated with a buffer B (Tris/HCl 50 mM, $CaCl_2$ 1 mM, pH 8) then placed in an XK 50/30 column (Pharmacia). The elution is carried out by adding 1 g/l of sodium deoxycholate and 0.1% of triton X-100 to buffer B. The fractions showing an arylesterase activity are injected onto 50 ml of an anion-exchange gel (DEAE Sepharose Fast Flow, Phamiacia) arranged in an XK 26/70 column (Pharmacia) and equilibrated with buffer B and 0.05% triton X-100. The elution is carried out by NaCl gradient. A first plateau is reached at 87.5 mM of NaCl in order to eliminate the apo A-I, a protein linked to paraoxonase, and the majority of the contaminating proteins. Human paraoxonase (PON1) is approximately eluted at a concentration of 140 mM of NaCl. All the fractions retained show a paraoxonase and arylesterase activity, these activities being verified according to the tests mentioned below. The eluted fractions are not brought back together. The SDS-PAGE gels of the fractions obtained show bands comprised between 38 kDa and 45 kDa (see FIG. **1**). Each purification does not always result in the same apparent mass distribution. This slight heterogeneity can be explained by the presence of 2 glycosylated chains on the PON1.

[0072] In addition to the PON1 in these batches another protein has been isolated by crystallization, by substituting C12-maltoside for triton and using ammonium sulphate as precipitating agent. The crystals obtained are those of an unknown protein characterized by radiocrystallography and corresponding to the sequence SEQ ID NO: 2 of the invention. Crystallization is at present the only existing method for purifying this protein.

[0073] The paraoxonase activity is measured in a glycine 50 mM/NaOH, $CaCl_2$ 1 mM buffer, in the presence of 1 M NaCl, pH 10.5 and is determined by means of a double beam spectrophotometer (Shimadzu UV 160A) thermostatically controlled at 25° C. The speed of hydrolysis is determined according to the variation of absorbance at 412 nm, corresponding to the formation of p-nitrophenol released by the hydrolysis of paraoxon, as a function of time, ϵ=18290 $M^{-1}cm^{-1}$ (Smolen, 1991).

[0074] The arylesterase activity is measured in a tris 50 mM/HCl, $CaCl_2$ 1 mM buffer, pH 8 and is determined by means of a double beam spectrophotometer (Shimadzu UV 160A) thermostatically controlled at 25° C. The speed of hydrolysis is determined according to the variation in absorbance at 270 nm, corresponding to the formation of phenol released by the hydrolysis of phenyl acetate, as a function of time, ϵ=1310 $M^{-1}cm^{-1}$ (Smolen, 1991).

[0075] Structure

[0076] The structure of the crystallized protein SEQ ID NO: 2 was obtained by X-ray crystallography. The structure at 1.9 Å resolution was obtained by the SIRAS (Single Isomorphous Replacement and Anomalous Scattering) method (FIG. **2**).

[0077] The X-ray diffraction data were collected on the BM30 line of the ESRF (Grenoble).

[0078] A heavy atom salt derivative was obtained by soaking a crystal in a solution containing uranium salts.

[0079] The images were integrated, scaled and combined with the XDS2000 programs (Kabsch, 1993) and the CCP4 suite (COLLABORATIVE COMPUTATIONAL PROJECT, NUMBER 4. 1994. "The CCP4 Suite: Programs for Protein Crystallography". Acta Cryst. D50, 760-763).

[0080] The CNS (BRUNGER, 1998) and SnB (Weeks, 1999) programs were used in order to locate the uranium atoms. The SHARP program (Copyright © 2001-2002 the Buster Development Group) was used in order to obtain the phases by the SIRAS technique.

[0081] 372 amino acids were constructed automatically in the electronic density map by the ARP/wARP (Perrakis, 1997) program. This first model was then refined by the CNS program.

[0082] Because of the very good quality of the electronic density map, it was possible to assign 80% reliability to the primary sequence of the protein. It was also possible to locate a phosphate molecule.

[0083] The structure obtained does not at all correspond to human paraoxonase. The sequencing obtained by identifying the amino acids from the electronic density indicates that neither this human protein nor its gene have been described previously. It is therefore a novel protein.

[0084] The structure of the protein of the invention exhibits a very strong homology with the phosphate-binding protein of *Escherichia coli*. This protein in this bacterium serves to transport the phosphate across the periplasm. It is found in many prokaryotes but in no eukaryote.

[0085] The electronic density also showed that a phosphate molecule was bound to the novel protein of the invention, in the same manner as in that of *Escherichia coli*.

[0086] Thus, it can be concluded that the protein of the invention characterized from human plasma has a very strong homology with the bacterial protein and that it is capable of binding phosphate and transporting it.

[0087] Sequencing

[0088] Digestion in the Gel

[0089] The paraoxonase-HPBP mixture was separated by electrophoretic gel with SDS-PAGE (without heating). Several bands corresponding to HPBP in the region of 70 kDa were cut out.

[0090] The digestion of the protein contained in these bands was carried out by means of the automatic digestion system, MassPrep Station (Waters Manchester, UK). The gel bands were washed twice with 50 µl of a solution of 25 mM of ammonium bicarbonate (NH_4HCO_3) and 50 µl of acetonitrile. The cysteines were reduced with 501 µl of a 10 mM dithiothreitol solution at 57° C. and acylated with 50 µl of 55 mM iodoacetamide. After dehydration with acetonitrile, the protein was digested enzymatically with 10 µl of modified porcine trypsin at 12.5 ng/µl (Promega, Madisson, Wis., U.S.A) or with lys-C of Lysobacter enzymogenes (Roche Applied Science, Penzberg, Germany) in 25 mM of NH_4HCO_3. The digestion is carried out overnight at ambient temperature. The cleaved peptides were extracted with a 60% acetonitrile solution and 5% formic acid.

[0091] Mass Spectrometry Analysis

[0092] MALDI-MS and MALDI-MS/MS

[0093] MALDI-TOF mass measurements were carried out on an Ultraflex™ TOF/TOF (Bruker, Daltonik GmbH, Bremen, Germany). This instrument was used with a maximum acceleration voltage of 25 KV in reflectron mode. The sample was prepared with the standard drop preparation dried over the stainless steel target using α-cyano-4-hydroxycinnamic acid as matrix.

[0094] The external calibration of the MALDI-MS spectrum was carried out using only the peaks of the monoisotopic charges of a known solution of peptides (bradykinin 1-7 (m/z=757.400), human angiotensin II (m/z=1046.542), human angiotensin I (m/z=1296.685), substance P (m/z=1347.735), bombesin (m/z=1619.822), renin (m/z=1758.933), ACTH 1-17 (m/z=2093.087) and ACTH 18-39 (m/z=2465.199)). The masses of the monoisotopic peptides were automatically annotated using the Flexanalysis 2.0 program.

[0095] The MS/MS spectra were obtained by analysis of the metastable ions obtained by "Laser-Induced Decomposition" (LID) of a sectioned ion precursor, without additional collision in the gas phase. The ion precursor was accelerated

to 8 kV and was selected by means of a timed ion gate. The fragments were further accelerated by 19 kV in the LIFT cell and their masses measured after passing the ion reflector.

[0096] The de novo sequencing of each of these MS/MS spectra was carried out with the Full DeNovo Sequencing program (Biotools, Bruker Daltonik GmbH, Bremen, Germany).

[0097] Nano LC-MS/MS

[0098] Nano LC-MS/MS analysis was carried out using a CapLC (Waters, Manchester, UK) coupled to a time-of-flight mass spectrometer accelerated by an Q-TOF II orthogonal hybrid quadrupole (Micromass, Manchester, UK). Separation by reversed-phase chromatography was carried out with capillaries (Pepmap C18, 75 μm i.d., 15 cm long, LC Packings) under a flow of 200 nL/min, kept constant by means of a partition pre-column. The calibration was carried out using 2 μmol/μl of GFP.

[0099] The mass data acquisition was controlled by the MassLynx program (Micromass, Manchester, UK) which automatically switches between the MS mode and the MS/MS mode.

[0100] The MS/MS spectra generated were individually sequenced de novo in order to obtain the partial or complete sequence. These interpretations were made using the PepSeq program (MassLynx, Micromass) and the PEAKS Studio program (Bioinformatics Solutions. Waterloo, Canada) which are capable of completely processing a .pkl file with a de novo automatic sequencing on each MS/MS spectrum.

[0101] Phosphate Binding

[0102] Phosphate binding by the protein of the invention SEQ ID NO: 2 was demonstrated according to the following test:

[0103] 200 μl of the protein of the invention SEQ ID NO: 2 (columns A-F of FIG. **3**), or 1 mg/ml lysozyme (column G) or of β-lactoglobulin was applied to nitrocellulose (dot blot by aspiration).

[0104] The mixture is incubated for 2 hours 30 minutes in a mixture comprising: tris 50 mM; pH 8.0; ^{32}P (10 mCi/ml) 2 mM.

[0105] Rinsing was then carried out twice for 1 minute with tris 50 mM at pH 8.0, then the mixture is exposed at ambient temperature for 45 minutes.

[0106] It is then noted (see FIG. **3**) that the protein of the invention has bound the radioactive phosphate (columns A to F), whereas the test controls have not bound it (columns G and H).

[0107] Role and Use of the Protein SEQ ID NO: 2

[0108] For assaying the concentration of this protein in the plasma the methods which can be used are:

[0109] the electrophoretic methods,

[0110] the purification of the protein,

[0111] the quantification of its activity,

[0112] the immunoassay of the protein using polyclonal/monoclonal antibodies directed against the protein.

[0113] Combination with Paraoxonase

[0114] Two-Dimensional Electrophoresis

[0115] The purified proteins (40 μg) as described previously in the protocol are mixed with 100 μL of a solution containing 9.8 M of urea, 4% (v/v) triton X100, 2 mM tributyl phosphine, 0.2% (v/v) ampholine 3-10 (Bio-Lytes 3-10; Bio-Rad), and 0.001% (m/v) bromophenol blue. Ready-to-use polyacrylamide gel strips (IPG-Strips; Bio-Rad) (T: 4%; C: 3%) are used. Ampholines were bound to the polyacrylamide in a covalent manner so as to have a pre-established linear pH gradient. The pH gradient used is between 3.0 and 10.0.

[0116] 1. Isoelectric Focusing (IEF)

[0117] The strips are placed in contact with the protein samples in the Protean IEF Cell device (Bio-Rad) and actively rehydrated (50 V constant) for 15 hours at 20° C. Isoelectric focusing is then carried out in 3 stages at 20° C. Firstly, a low voltage of 250 V is applied for 15 minutes; secondly, a rise in gradient from 250 to 4000 V (amperage limited by 50 μA strip) is programmed over 2 hours. Thirdly, the voltage is held constant at 4000 V for 4 hours. After migration, the strips are stored at −20° C.

[0118] According to the preceding purification protocol, the HPBP protein of the invention is co-purified with human paraoxonase (PON) (Fokine et al., 2003). By making a two-dimensional gel with the above protocol, 2 spots were identified by N-terminal sequencing as being respectively the protein of the invention HPBP and human paraoxonase (see FIG. **4**). The two proteins have approximately the same molecular mass (approximately 40 kDa) and distinct isoelectric points, 6.9-8.5 for HPBP and 4-5 for PON1. Taking account of the fact that it has been necessary to use drastic conditions in order to succeed in separating the 2 proteins (9M of urea and 4% triton) on gel and that the 2 proteins which have very different isoelectric points remain co-purified after passage through an anion exchange column (DEAE sepharose), it is concluded that they are combined by forming a complex.

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Gly Lys Gly Lys Ile Ala Phe Leu Glu Asn Xaa Tyr Asn Gln Phe Gly
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Gly Lys Leu Ile Xaa Val Pro Ser Val Ala Thr Ser Val Ala Ile Pro
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Phe Arg Lys Ala Gly Xaa Asn Ala Val Asp Leu Ser Val Lys Glu Leu
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Cys Gly Val Phe Ser Gly Arg Ile Ala Xaa Trp Ser Gly Ile Thr Gly
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Ala Gly Arg Ser Gly Pro Ile Gln Val Val Tyr Arg Ala Glu Xaa Ser
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Gly Thr Thr Glu Leu Phe Thr Arg Phe Leu Asn Ala Lys Cys Thr Thr
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Gln Pro Gly Thr Phe Ala Val Thr Thr Val Phe Ala Asn Ser Tyr Ser
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Leu Gly Leu Ser Pro Leu Ala Gly Ala Val Ala Ala Ile Gly Ser Val
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Gly Val Met Ala Ala Asp Asn Asp Val Thr Thr Ala Gln Gly Arg Ile
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Trp Thr Pro Val Phe Gly Ala Val Thr Gly Gly Gly Val Val Ala Tyr
        275                 280                 285

Pro Asp Ser Gly Tyr Pro Ile Leu Gly Phe Thr Asp Leu Ile Phe Ser
    290                 295                 300

Glu Cys Tyr Ala Asn Ala Thr Gln Thr Gly Gln Val Arg Asn Phe Phe
305                 310                 315                 320

Thr Lys His Tyr Gly Thr Ser Ala Asn Asp Asn Ala Ala Ile Gln Ala
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Asn Ala Phe Val Pro Leu Pro Ser Asn Trp Lys Ala Ala Val Arg Ala
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Gly Lys Gly Lys Ile Ala Phe Leu Glu Asn Lys Tyr Asn Gln Phe Gly
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Thr Asp Thr Thr Lys Asn Val His Trp Ala Gly Ser Asp Ser Lys Leu
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Thr Ala Thr Glu Leu Ala Thr Tyr Ala Ala Asp Lys Glu Pro Gly Trp
65                  70                  75                  80

Gly Lys Leu Ile Gln Val Pro Ser Val Ala Thr Ser Val Ala Ile Pro
                85                  90                  95

Phe Arg Lys Ala Gly Ala Asn Ala Val Asp Leu Ser Val Lys Glu Leu
            100                 105                 110

Cys Gly Val Phe Ser Gly Arg Ile Ala Asp Trp Ser Gly Ile Thr Gly
        115                 120                 125

Ala Gly Arg Ser Gly Pro Ile Gln Val Val Tyr Arg Ala Glu Ser Ser
    130                 135                 140

Gly Thr Thr Glu Leu Phe Thr Arg Phe Leu Asn Ala Lys Cys Thr Thr
145                 150                 155                 160

Gln Pro Gly Thr Phe Ala Val Thr Thr Val Phe Ala Asn Ser Tyr Ser
                165                 170                 175

Leu Gly Leu Ser Pro Leu Ala Gly Ala Val Ala Ala Ile Gly Ser Val
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Gly Val Met Ala Ala Asp Asn Asp Val Thr Thr Ala Gln Gly Arg Ile
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                245                 250                 255

Ser Val Val Pro Leu Pro Ala Ala Ala Asp Arg Gly Asp Pro Asn Val
            260                 265                 270

Trp Thr Pro Val Phe Gly Ala Val Thr Gly Gly Gly Val Val Ala Tyr
        275                 280                 285

Pro Asp Ser Gly Tyr Pro Ile Leu Gly Phe Thr Asp Leu Ile Phe Ser
    290                 295                 300

Glu Cys Tyr Ala Asn Ala Thr Gln Thr Gly Gln Val Arg Asn Phe Phe
305                 310                 315                 320

Thr Lys His Tyr Gly Thr Ser Ala Asn Asp Asn Ala Ala Ile Gln Ala
                325                 330                 335

Asn Ala Phe Val Pro Leu Pro Ser Asn Trp Lys Ala Ala Val Arg Ala
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Ser Tyr Leu Thr Ala Ser Asn Ala Leu Ser Ile Gly Asp Ser Ala Val
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Cys Gly Gly Lys Gly Arg Pro Glu
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Gly Lys Gly Lys Ile Ala Phe Leu Glu Asn Ser Tyr Asn Gln Phe Gly
        35                  40                  45

Thr Asn Thr Thr Lys Asp Val His Trp Ala Gly Ser Asp Ser Lys Leu
    50                  55                  60

Thr Ala Ser Gln Leu Ala Thr Tyr Ala Ala Asn Lys Gln Pro Gly Trp
65                  70                  75                  80

Gly Lys Leu Ile Glu Val Pro Ser Val Ala Thr Ser Val Ala Ile Pro
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Phe Arg Lys Ala Gly Gly Asn Ala Val Asp Leu Ser Val Lys Glu Leu
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Cys Gly Val Phe Ser Gly Arg Ile Ala Asn Trp Ser Gly Ile Thr Gly
        115                 120                 125

Ala Gly Arg Ser Gly Pro Ile Gln Val Val Tyr Arg Ala Glu Val Ser
    130                 135                 140

Gly Thr Thr Glu Leu Phe Thr Arg Phe Leu Asn Ala Lys Cys Thr Thr
145                 150                 155                 160

Gln Pro Gly Thr Phe Ala Val Thr Thr Val Phe Ala Asn Ser Tyr Ser
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Leu Gly Leu Ser Pro Leu Ala Gly Ala Val Ala Ala Ile Gly Ser Val
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Gly Ala Glu Gly Lys Ser Pro Ala Ala Ala Asn Ser Ser Ala Ala Ile
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Ser Val Val Pro Leu Pro Ala Ala Ala Asn Arg Gly Asp Pro Asn Val
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Trp Thr Pro Val Phe Gly Ala Val Thr Gly Gly Gly Val Val Ala Tyr
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Pro Asp Ser Gly Tyr Pro Ile Leu Gly Phe Thr Asp Leu Ile Phe Ser
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Glu Cys Tyr Ala Asn Ala Thr Gln Thr Gly Gln Val Arg Asn Phe Phe
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Thr Lys His Tyr Gly Thr Ser Ala Asn Asp Asn Ala Ala Ile Gln Ala
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Asn Ala Phe Val Pro Leu Pro Ser Asn Trp Lys Ala Ala Val Arg Ala
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Cys Gly Gly Lys Gly Arg Pro Glu
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            20                  25                  30

Glu Val Gln Pro Val Glu Leu Pro Asn Cys Asn Leu Val Lys Gly Ile
        35                  40                  45

Glu Thr Gly Ser Glu Asp Met Glu Ile Leu Pro Asn Gly Leu Ala Phe
    50                  55                  60

Ile Ser Ser Gly Leu Lys Tyr Pro Gly Ile Lys Ser Phe Asn Pro Asn
65                  70                  75                  80

Ser Pro Gly Lys Ile Leu Leu Met Asp Leu Asn Glu Glu Asp Pro Thr
                85                  90                  95

Val Leu Glu Leu Gly Ile Thr Gly Ser Lys Phe Asp Val Ser Ser Phe
            100                 105                 110

Asn Pro His Gly Ile Ser Thr Phe Thr Asp Glu Asp Asn Ala Met Tyr
        115                 120                 125

Leu Leu Val Val Asn His Pro Asp Ala Lys Ser Thr Val Glu Leu Phe
    130                 135                 140

Lys Phe Gln Glu Glu Glu Lys Ser Leu Leu His Leu Lys Thr Ile Arg
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His Phe Tyr Gly Thr Asn Asp His Tyr Phe Leu Asp Pro Tyr Leu Gln
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Ser Trp Glu Met Tyr Leu Gly Leu Ala Trp Ser Tyr Val Val Tyr Tyr
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Ser Pro Ser Glu Val Arg Val Val Ala Glu Gly Phe Asp Phe Ala Asn
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Gly Ile Asn Ile Ser Pro Asp Gly Lys Tyr Val Tyr Ile Ala Glu Leu
225                 230                 235                 240

Leu Ala His Lys Ile His Val Tyr Glu Lys His Ala Asn Trp Thr Leu
                245                 250                 255

Thr Pro Leu Lys Ser Leu Asp Phe Asn Thr Leu Val Asp Asn Ile Ser
            260                 265                 270

Val Asp Pro Glu Thr Gly Asp Leu Trp Val Gly Cys His Pro Asn Gly
        275                 280                 285

Met Lys Ile Phe Phe Tyr Asp Ser Glu Asn Pro Pro Ala Ser Glu Val
    290                 295                 300

Leu Arg Ile Gln Asn Ile Leu Thr Glu Glu Pro Lys Val Thr Gln Val
305                 310                 315                 320

Tyr Ala Glu Asn Gly Thr Val Leu Gln Gly Ser Thr Val Ala Ser Val
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Cys Glu Leu
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Glu Val Glu Ser Val Asp Leu Pro His Cys His Leu Ile Lys Gly Ile
        35                  40                  45

Glu Ala Gly Ser Glu Asp Ile Asp Ile Leu Pro Asn Gly Leu Ala Phe
    50                  55                  60

Phe Ser Val Gly Leu Lys Phe Pro Gly Leu His Ser Phe Ala Pro Asp
65                  70                  75                  80

Lys Pro Gly Gly Ile Leu Met Met Asp Leu Lys Glu Glu Lys Pro Arg
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Ala Arg Glu Leu Arg Ile Ser Arg Gly Phe Asp Leu Ala Ser Phe Asn
            100                 105                 110

Pro His Gly Ile Ser Thr Phe Ile Asp Asn Asp Asp Thr Val Tyr Leu
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Phe Val Val Asn His Pro Glu Phe Lys Asn Thr Val Glu Ile Phe Lys
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Phe Tyr Ala Thr Asn Asp His Tyr Phe Ser Asp Pro Phe Leu Lys Tyr
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Leu Glu Thr Tyr Leu Asn Leu His Trp Ala Asn Val Val Tyr Tyr Ser
        195                 200                 205

Pro Asn Glu Val Lys Val Val Ala Glu Gly Phe Asp Ser Ala Asn Gly
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Ile Asn Ile Ser Pro Asp Asp Lys Tyr Ile Tyr Val Ala Asp Ile Leu
225                 230                 235                 240

Ala His Glu Ile His Val Leu Glu Lys His Thr Asn Met Asn Leu Thr
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Gln Leu Lys Val Leu Glu Leu Asp Thr Leu Val Asp Asn Leu Ser Ile
            260                 265                 270

Asp Pro Ser Ser Gly Asp Ile Trp Val Gly Cys His Pro Asn Gly Gln
        275                 280                 285

Lys Leu Phe Val Tyr Asp Pro Asn Asn Pro Pro Ser Ser Glu Val Leu
    290                 295                 300

Arg Ile Gln Asn Ile Leu Cys Glu Lys Pro Thr Val Thr Thr Val Tyr
305                 310                 315                 320

Ala Asn Asn Gly Ser Val Leu Gln Gly Ser Ser Val Ala Ser Val Tyr
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Glu Val Glu Pro Val Glu Pro Glu Asn Cys His Leu Ile Glu Glu Leu
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Glu Ser Gly Ser Glu Asp Ile Asp Ile Leu Pro Ser Gly Leu Ala Phe
    50                  55                  60

Ile Ser Ser Gly Leu Lys Tyr Pro Gly Met Pro Asn Phe Ala Pro Asp
65                  70                  75                  80

Glu Pro Gly Lys Ile Phe Leu Met Asp Leu Asn Glu Gln Asn Pro Arg
                85                  90                  95

Ala Gln Ala Leu Glu Ile Ser Gly Gly Phe Asp Lys Glu Leu Phe Asn
            100                 105                 110

Pro His Gly Ile Ser Ile Phe Ile Asp Lys Asp Asn Thr Val Tyr Leu
        115                 120                 125

Tyr Val Val Asn His Pro His Met Lys Ser Thr Val Glu Ile Phe Lys
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Phe Glu Glu Gln Gln Arg Ser Leu Val Tyr Leu Lys Thr Ile Lys His
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Phe Glu Met Ile Leu Asp Leu Arg Trp Thr Tyr Val Leu Phe Tyr Ser
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Pro Arg Glu Val Lys Val Val Ala Lys Gly Phe Cys Ser Ala Asn Gly
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Ile Thr Val Ser Ala Asp Gln Lys Tyr Val Tyr Val Ala Asp Val Ala
225                 230                 235                 240

Ala Lys Asn Ile His Ile Met Glu Lys His Asp Asn Trp Asp Leu Thr
                245                 250                 255

Gln Leu Lys Val Ile Gln Leu Gly Thr Leu Val Asp Asn Leu Thr Val
            260                 265                 270

Asp Pro Ala Thr Gly Asp Ile Leu Ala Gly Cys His Pro Asn Pro Met
        275                 280                 285

Lys Leu Leu Asn Tyr Asn Pro Glu Asp Pro Pro Gly Ser Glu Val Leu
    290                 295                 300

Arg Ile Gln Asn Val Leu Ser Glu Lys Pro Arg Val Ser Thr Val Tyr
305                 310                 315                 320

Ala Asn Asn Gly Ser Val Leu Gln Gly Thr Ser Val Ala Ser Val Tyr
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Glu Val Thr Pro Val Glu Leu Pro Asn Cys Asn Leu Val Lys Gly Ile
        35                  40                  45

Asp Asn Gly Ser Glu Asp Leu Glu Ile Leu Pro Asn Gly Leu Ala Phe
    50                  55                  60

Ile Ser Ala Gly Leu Lys Tyr Pro Gly Ile Met Ser Phe Asp Pro Asp
65                  70                  75                  80

Lys Pro Gly Lys Ile Leu Leu Met Asp Leu Asn Glu Lys Asp Pro Val
                85                  90                  95

Val Leu Glu Leu Ser Ile Thr Gly Ser Thr Phe Asp Leu Ser Ser Phe
            100                 105                 110

Asn Pro His Gly Ile Ser Thr Phe Thr Asp Glu Asp Asn Ile Val Tyr
        115                 120                 125

Leu Met Val Val Asn His Pro Asp Ser Lys Ser Thr Val Glu Leu Phe
    130                 135                 140

Lys Phe Gln Glu Lys Glu Lys Ser Leu Leu His Leu Lys Thr Ile Arg
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His Phe Tyr Ala Thr Asn Asp His Tyr Phe Ile Asp Pro Tyr Leu Lys
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Ser Trp Glu Met His Leu Gly Leu Ala Trp Ser Phe Val Thr Tyr Tyr
        195                 200                 205

Ser Pro Asn Asp Val Arg Val Val Ala Glu Gly Phe Asp Phe Ala Asn
    210                 215                 220

Gly Ile Asn Ile Ser Pro Asp Gly Lys Tyr Val Tyr Ile Ala Glu Leu
225                 230                 235                 240

Leu Ala His Lys Ile His Val Tyr Glu Lys His Ala Asn Trp Thr Leu
                245                 250                 255

Thr Pro Leu Lys Ser Leu Asp Phe Asn Thr Leu Val Asp Asn Ile Ser
            260                 265                 270

Val Asp Pro Val Thr Gly Asp Leu Trp Val Gly Cys His Pro Asn Gly
        275                 280                 285

Met Arg Ile Phe Tyr Tyr Asp Pro Lys Asn Pro Pro Ala Ser Glu Val
    290                 295                 300

Leu Arg Ile Gln Asp Ile Leu Ser Lys Glu Pro Lys Val Thr Val Ala
305                 310                 315                 320

Tyr Ala Glu Asn Gly Thr Val Leu Gln Gly Ser Thr Val Ala Ala Val
                325                 330                 335

Tyr Lys Gly Lys Met Leu Val Gly Thr Val Phe His Lys Ala Leu Tyr
            340                 345                 350

Cys Glu Leu Ser Gln Ala Asn
        355


<210> SEQ ID NO 8
<211> LENGTH: 355
<212> TYPE: PRT
<213> ORGANISM: Rattus rattus

<400> SEQUENCE: 8

Met Ala Lys Leu Leu Gly Leu Thr Leu Val Gly Leu Val Leu Ala Leu
1               5                   10                  15

Tyr Lys Asn His Arg Ser Ser Tyr Gln Thr Arg Leu Asn Ala Phe Arg
            20                  25                  30

Glu Val Thr Pro Val Asp Leu Pro Asn Cys Thr Leu Val Lys Gly Ile
        35                  40                  45

Glu Ala Gly Ala Glu Asp Leu Glu Ile Leu Pro Asn Gly Leu Thr Phe
    50                  55                  60

Phe Ser Thr Phe Leu Lys Tyr Pro Gly Ile Lys Ser Phe Asp Pro Ser
65                  70                  75                  80

Lys Pro Gly Lys Ile Leu Leu Met Asp Leu Asn Glu Lys Glu Pro Ala
                85                  90                  95

Val Ser Glu Leu Ala Ile Met Gly Asn Thr Leu Asp Met Ser Ser Phe
            100                 105                 110

Asn Pro His Gly Ile Ser Thr Phe Ile Asp Glu Asp Asn Thr Val Tyr
        115                 120                 125

Leu Leu Val Val Ser His Pro Asp Ser Ser Ser Thr Val Glu Val Phe
    130                 135                 140

Lys Phe Gln Glu Glu Glu Arg Ser Leu Leu His Leu Lys Thr Ile Thr
145                 150                 155                 160
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His Glu Leu Leu Pro Ser Ile Asn Asp Ile Ala Ala Val Gly Pro Glu
                165                 170                 175

Ser Phe Tyr Ala Thr Asn Asp His Tyr Phe Ala Asp Pro Tyr Leu Arg
            180                 185                 190

Ser Trp Glu Met Tyr Leu Gly Leu Ser Trp Ser Asn Val Val Tyr Tyr
        195                 200                 205

Ser Pro Asp Lys Val Arg Val Val Ala Asp Gly Phe Asp Phe Ala Asn
    210                 215                 220

Gly Ile Gly Ile Ser Leu Asp Gly Lys Tyr Val Tyr Ile Ala Glu Leu
225                 230                 235                 240

Leu Ala His Lys Ile His Val Tyr Glu Lys His Ala Asn Trp Thr Leu
                245                 250                 255

Thr Pro Leu Lys Val Leu Ser Phe Asp Thr Leu Val Asp Asn Ile Ser
            260                 265                 270

Val Asp Pro Val Thr Gly Asp Leu Trp Val Gly Cys His Pro Asn Gly
        275                 280                 285

Met Arg Ile Phe Phe Tyr Asp Ser Glu Asn Pro Pro Gly Ser Glu Val
    290                 295                 300

Leu Arg Ile Gln Ser Ile Leu Ser Glu Asp Pro Lys Val Thr Val Val
305                 310                 315                 320

Tyr Ala Glu Asn Gly Thr Val Leu Gln Gly Thr Thr Val Ala Ala Val
                325                 330                 335

Tyr Lys Gly Lys Leu Leu Ile Gly Thr Val Phe His Arg Ala Leu Cys
            340                 345                 350

Cys Tyr Leu
        355


<210> SEQ ID NO 9
<211> LENGTH: 355
<212> TYPE: PRT
<213> ORGANISM: Mus musculus

<400> SEQUENCE: 9

Met Ala Lys Leu Leu Ala Leu Thr Leu Val Gly Leu Val Leu Ala Leu
1               5                   10                  15

Tyr Lys Asn His Arg Ser Ser Tyr Gln Thr Arg Leu Asn Ala Phe Arg
            20                  25                  30

Glu Val Thr Pro Val Glu Leu Pro Asn Cys Asn Leu Val Lys Gly Ile
        35                  40                  45

Glu Thr Gly Ala Glu Asp Leu Glu Ile Leu Pro Asn Gly Leu Thr Phe
    50                  55                  60

Phe Ser Thr Gly Leu Lys Tyr Pro Gly Ile Lys Ser Phe Asp Pro Ser
65                  70                  75                  80

Lys Pro Gly Lys Ile Leu Leu Met Asp Leu Asn Lys Lys Glu Pro Ala
                85                  90                  95

Val Ser Glu Leu Glu Ile Ile Gly Asn Thr Leu Asp Ile Ser Ser Phe
            100                 105                 110

Asn Pro His Gly Ile Ser Thr Phe Thr Asp Glu Asp Asn Thr Val Tyr
        115                 120                 125

Leu Leu Val Val Asn His Pro Asp Ser Ser Ser Thr Val Glu Val Phe
    130                 135                 140

Lys Phe Gln Glu Glu Glu Arg Ser Leu Leu His Leu Lys Thr Ile Thr
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-continued

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145                 150                 155                 160

His Glu Leu Leu Pro Ser Ile Asn Asp Ile Ala Ala Ile Gly Pro Glu
                165                 170                 175

Ser Phe Tyr Ala Thr Asn Asp His Tyr Phe Ala Asp Pro Tyr Leu Arg
            180                 185                 190

Ser Trp Glu Met Tyr Leu Gly Leu Ser Trp Ser Asn Val Val Tyr Tyr
        195                 200                 205

Ser Pro Asp Lys Val Gln Val Val Ala Glu Gly Phe Asp Phe Ala Asn
    210                 215                 220

Gly Ile Gly Ile Ser Leu Asp Gly Lys Tyr Val Tyr Ile Ala Glu Leu
225                 230                 235                 240

Leu Ala His Lys Ile His Val Tyr Glu Lys His Ala Asn Trp Thr Leu
                245                 250                 255

Thr Pro Leu Lys Val Leu Asn Phe Asp Thr Leu Val Asp Asn Ile Ser
            260                 265                 270

Val Asp Pro Val Thr Gly Asp Leu Trp Val Gly Cys His Pro Asn Gly
        275                 280                 285

Met Arg Ile Phe Phe Tyr Asp Ala Glu Asn Pro Pro Gly Ser Glu Val
    290                 295                 300

Leu Arg Ile Gln Asn Ile Leu Ser Glu Asp Pro Lys Ile Thr Val Val
305                 310                 315                 320

Tyr Ala Glu Asn Gly Thr Val Leu Gln Gly Thr Thr Val Ala Ser Val
                325                 330                 335

Tyr Lys Gly Lys Leu Leu Ile Gly Thr Val Phe His Lys Ala Leu Tyr
            340                 345                 350

Cys Asp Leu
        355


<210> SEQ ID NO 10
<211> LENGTH: 354
<212> TYPE: PRT
<213> ORGANISM: Mus musculus

<400> SEQUENCE: 10

Met Gly Arg Met Val Ala Leu Gly Phe Ala Gly His Arg Val Ala Leu
1               5                   10                  15

Leu Gly Glu Arg Phe Leu Ala Leu Ser Ser Arg Leu Lys Gly Ser Arg
            20                  25                  30

Glu Val Glu Ser Val Asp Leu Pro Asn Cys His Leu Ile Lys Gly Ile
        35                  40                  45

Glu Thr Gly Ala Glu Asp Ile Asp Ile Leu Pro Asn Gly Leu Ala Phe
    50                  55                  60

Phe Ser Val Gly Leu Lys Phe Pro Gly Leu His Ser Phe Ala Pro Asp
65                  70                  75                  80

Lys Pro Gly Gly Ile Leu Met Met Asp Leu Asp Glu Arg Pro Pro Ser
                85                  90                  95

Leu Glu Glu Leu Arg Val Ser Trp Gly Phe Asp Leu Ala Ser Phe Asn
            100                 105                 110

Pro His Gly Ile Ser Thr Phe Ile Asp Asp Asp Asp Thr Val Tyr Leu
        115                 120                 125

Phe Val Val Asn His Pro Gln Phe Ser Asn Thr Val Glu Ile Phe Lys
    130                 135                 140
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Phe Gln Glu Ala Glu Asn Ser Leu Leu His Leu Lys Thr Ile Lys His
145                 150                 155                 160

Glu Leu Leu Pro Ser Val Asn Asp Ile Ile Ala Val Gly Pro Ala His
                165                 170                 175

Phe Tyr Ala Thr Asn Asp His Tyr Phe Ser Asp Pro Phe Leu Lys Tyr
            180                 185                 190

Leu Glu Thr Tyr Leu Asn Leu His Trp Ala Asn Val Val Tyr Tyr Ser
        195                 200                 205

Pro Glu Glu Val Lys Leu Val Ala Glu Gly Phe Asp Ser Ala Asn Gly
    210                 215                 220

Ile Asn Ile Ser Pro Asp Lys Lys Tyr Val Tyr Val Ala Asp Ile Leu
225                 230                 235                 240

Ala His Glu Ile His Val Leu Glu Lys Gln Pro Asn Met Asn Leu Thr
                245                 250                 255

Gln Leu Lys Val Leu Gln Leu Gly Thr Leu Val Asp Asn Leu Ser Ile
            260                 265                 270

Asp Pro Ser Ser Gly Asp Ile Trp Val Gly Cys His Pro Asn Gly Gln
        275                 280                 285

Arg Leu Phe Val Tyr His Pro Asn His Pro Pro Thr Ser Glu Val Leu
    290                 295                 300

Arg Ile Gln Asn Ile Leu Ser Glu Lys Pro Ser Val Thr Thr Val Tyr
305                 310                 315                 320

Ile Asn Asn Gly Ser Val Leu Gln Gly Ser Ser Val Ala Thr Ile Tyr
                325                 330                 335

Asp Arg Lys Leu Leu Val Gly Thr Leu Tyr Gln Lys Ala Leu Tyr Cys
            340                 345                 350

Glu Leu
```

<210> SEQ ID NO 11
<211> LENGTH: 354
<212> TYPE: PRT
<213> ORGANISM: Mus musculus

<400> SEQUENCE: 11

```
Met Gly Lys Leu Val Ala Leu Thr Leu Leu Gly Ala Cys Leu Ala Leu
1               5                   10                  15

Ile Gly Glu Arg Leu Leu Asn Phe Arg Glu Arg Val Ser Thr Thr Arg
            20                  25                  30

Glu Ile Lys Ala Thr Glu Pro Gln Asn Cys His Leu Ile Glu Gly Leu
        35                  40                  45

Glu Asn Gly Ser Glu Asp Ile Asp Ile Leu Pro Ser Gly Leu Ala Phe
    50                  55                  60

Ile Ser Thr Gly Leu Lys Tyr Pro Gly Met Pro Ala Phe Ala Pro Asp
65                  70                  75                  80

Lys Pro Gly Arg Ile Phe Leu Met Asp Leu Asn Glu Gln Asn Pro Glu
                85                  90                  95

Ala Gln Ala Leu Glu Ile Ser Gly Gly Leu Asp Gln Glu Ser Leu Asn
            100                 105                 110

Pro His Gly Ile Ser Thr Phe Ile Asp Lys Asp Asn Thr Ala Tyr Leu
        115                 120                 125

Tyr Val Val Asn His Pro Asn Met Asp Ser Thr Val Glu Ile Phe Lys
    130                 135                 140
```

-continued

```
Phe Glu Glu Gln Gln Arg Ser Leu Ile His Leu Lys Thr Leu Lys His
145                 150                 155                 160

Glu Leu Leu Lys Ser Val Asn Asp Ile Val Val Leu Gly Pro Glu Gln
                165                 170                 175

Phe Tyr Ala Thr Arg Asp His Tyr Phe Thr Ser Tyr Phe Leu Val Leu
            180                 185                 190

Leu Glu Met Ile Leu Asp Pro His Trp Thr Ser Val Val Phe Tyr Ser
        195                 200                 205

Pro Lys Glu Val Lys Val Val Ala Gln Gly Phe Ser Ser Ala Asn Gly
    210                 215                 220

Ile Thr Val Ser Leu Asp Gln Lys Phe Val Tyr Val Ala Asp Val Thr
225                 230                 235                 240

Ala Lys Asn Ile His Ile Met Lys Lys His Asp Asn Trp Asp Leu Thr
                245                 250                 255

Pro Val Lys Val Ile Gln Leu Gly Thr Leu Val Asp Asn Leu Thr Val
            260                 265                 270

Asp Pro Ala Thr Gly Asp Ile Leu Ala Gly Cys His Pro Asn Pro Met
        275                 280                 285

Lys Leu Leu Ile Tyr Asn Pro Glu Asp Pro Pro Gly Ser Glu Val Leu
    290                 295                 300

Arg Ile Gln Asp Ser Leu Ser Asp Lys Pro Arg Val Ser Thr Leu Tyr
305                 310                 315                 320

Ala Asn Asn Gly Ser Val Leu Gln Gly Ser Thr Val Ala Ser Val Tyr
                325                 330                 335

His Lys Arg Met Leu Ile Gly Thr Ile Phe His Lys Ala Leu Tyr Cys
            340                 345                 350

Asp Leu
```

1-15. (canceled)

16. A protein characterized in that it comprises or is constituted by:

the sequence SEQ ID NO:1,

or any sequence derived from the sequence SEQ ID NO: 1, in particular by substitution, suppression or addition of one or more amino acids, providing that said derived sequence binds to phosphate,

or any sequence homologous to the sequence SEQ ID NO: 1, preferable having a homology of at least approximately 80% with the sequence SEQ ID NO: 1, providing that said homologous sequence binds to phosphate,

or any fragment of one of the sequences defined above, providing that said fragment binds to phosphate, in particular any fragment being constituted by at least approximately 20 contiguous amino acids in the sequence SEQ ID NO: 1.

17. The protein of claim 16, characterized in that it comprises or is constituted by:

the sequence SEQ ID NO: 2 or SEQ ID NO: 3,

or any sequence derived from the sequence SEQ ID NO: 2 or SEQ ID NO: 3, in particular by substitution, suppression or addition of one or more amino acids, providing that said derived sequence binds to phosphate,

or any sequence homologous to the sequence SEQ ID NO: 2 or SEQ ID NO: 3, preferably having a homology of at least approximately 80% with the sequence SEQ ID NO: 2 or SEQ ID NO: 3, providing that said homologous sequence binds to phosphate,

or any fragment of one of the sequences defined above, providing that said fragment binds to phosphate, in particular any fragment being constituted by at least approximately 20 contiguous amino acids in the sequence SEQ ID NO: 2 or SEQ ID NO: 3.

18. A nucleotide sequence encoding a protein as defined in claim 16.

19. A recombinant vector, in particular plasmid, cosmid, phage or virus DNA, containing a nucleotide sequence encoding a protein as defined in claim 16.

20. The recombinant vector according to claim 19, containing the elements necessary for the expression in a host cell of the polypeptides encoded by a nucleotide sequence encoding a protein, inserted into said vector.

21. A host cell, chosen in particular from bacteria, yeasts, fungi cells, plant cells or mammal cells, said host cell being transformed using a recombinant vector containing a nucleotide sequence encoding a protein as defined in claim 16.

22. A pharmaceutical composition comprising as active ingredient a protein according to claim 16, in combination with a pharmaceutically acceptable vehicle.

23. A pharmaceutical composition, comprising as active ingredient a protein represented by the sequence SEQ ID NO: 2 or SEQ ID NO: 3, in combination with a pharmaceutically acceptable vehicle.

24. The pharmaceutical composition according to claim 22, in which the protein, in particular SEQ ID NO: 2 or SEQ ID NO: 3, is in combination with a variant of the paraoxonase protein, in particular SEQ ID NO: 4, SEQ ID NO. 5, SEQ ID NO: 6, SEQ ID NO: 7, SEQ ID NO: 8, SEQ ID NO: 9, SEQ ID NO: 10 or SEQ ID NO: 11.

25. A combination product comprising at least one protein according to claim 16, in particular SEQ ID NO: 2 or SEQ ID NO: 3, and at least one variant of the paraoxonase protein, in particular SEQ ID NO: 4, SEQ ID NO. 5, SEQ ID NO: 6, SEQ ID NO: 7, SEQ ID NO: 8, SEQ ID NO: 9, SEQ ID NO: 10 or SEQ ID NO: 11, for simultaneous or separate use, or use spread over time, intended for the prophylaxis or treatment of intoxications caused by insecticides or nerve agents such as soman, VX, sarin or tabun.

26. An assay method of the protein according to claim 16, in particular SEQ ID NO: 2 or SEQ ID NO: 3, characterized in that it comprises the following stages:

rabbit monoclonal antibodies directed against different epitopes of the protein, in particular SEQ ID NO: 2 or SEQ ID NO: 3, are fixed to a plate and the human serum to be analyzed containing said protein is applied to the above-mentioned plate,

the plate is rinsed and washed,

antibodies directed against rabbit antibodies marked with peroxidase are applied to the plate over 30 minutes, in order to form a ternary complex between a rabbit monoclonal antibody, said protein and an above-mentioned antibody directed against a rabbit antibody,

the plate is rinsed and washed,

the peroxidase fixed to the plate is reacted with its substrate and the reaction is stopped at the end of 30 minutes with 3,3',5,5'-tetramethylbenzidine,

the optical density of the product formed in the preceding stage is measured at 450 nm using a spectrophotometer, and comparison of this measurement with a standard curve makes it possible to determine the concentration of the protein, in particular SEQ ID NO: 2 or SEQ ID NO: 3 present in the serum.

27. A method for the prevention or treatment of arthritis or diseases linked to hyperphosphataemia, such as cardiovascular diseases, comprising the administration of a pharmaceutically acceptable amount of a protein according to claim 16, in particular the protein represented by the sequence SEQ ID NO: 2 or SEQ ID NO: 3.

28. A method for the prophylaxis or treatment of intoxications caused by insecticides or nerve agents such as soman, VX, sarin or tabun, or for the treatment of atherosclerosis, comprising the administration of a pharmaceutically acceptable amount of a protein according to claim 16, in particular the protein represented by the sequence SEQ ID NO: 2 or SEQ ID NO: 3, in combination with a variant of the paraoxonase protein, in particular SEQ ID NO: 4, SEQ ID NO: 5, SEQ ID NO: 6, SEQ ID NO: 7, SEQ ID NO: 8, SEQ ID NO: 9, SEQ ID NO: 10 or SEQ ID NO: 11.

29. A method for the in vitro diagnosis of diseases linked to hyperphosphataemia, comprising the use of the assay method of claim 27, wherein the concentration of protein SEQ ID NO: 2 or SEQ ID NO: 3 as assayed is less than the quantity of this protein normally present in the blood of a healthy individual.

30. A method for the in vitro diagnosis of diseases linked to hypophosphataemia, comprising the use of the assay method of claim 27, wherein the concentration of protein SEQ ID NO: 2 or SEQ ID NO: 3 as assayed is greater than the quantity of this protein normally present in the blood of a healthy individual.

31. A method for the in vitro diagnosis of an individual's predisposition to diseases linked to hyperphosphataemia, comprising the use of the assay method of claim 27.

32. The method of claim 29, wherein the diseases linked to hyperphosphataemia are cardiovascular diseases, in particular cardiovascular diseases linked to the formation of atheroma plaques.

* * * * *

专利名称(译)	新型磷酸盐结合蛋白，含有它们的药物组合物及其用途		
公开(公告)号	US20070196879A1	公开(公告)日	2007-08-23
申请号	US10/577658	申请日	2004-10-29
[标]申请(专利权)人(译)	CHABRIERE ERIC 孔特雷拉斯MARTEL CARLOS FONTECILLA CAMPS JUAN		
申请(专利权)人(译)	CHABRIERE ERIC 孔特雷拉斯MARTEL CARLOS FONTECILLA-CAMPS JUAN		
当前申请(专利权)人(译)	CHABRIERE ERIC 孔特雷拉斯MARTEL CARLOS FONTECILLA-CAMPS JUAN		
[标]发明人	CHABRIERE ERIC CONTRERAS MARTEL CARLOS FONTECILLA CAMPS JUAN		
发明人	CHABRIERE, ERIC CONTRERAS-MARTEL, CARLOS FONTECILLA-CAMPS, JUAN		
IPC分类号	G01N33/53 C07H21/04 C12P21/06 C12N9/02 A61K38/00 C07K14/47 C12N15/12		
CPC分类号	A61K38/00 C07K2299/00 C07K14/47 A61P19/00 A61P19/02		
优先权	2003012729 2003-10-30 FR		
其他公开文献	US7718773		
外部链接	Espacenet USPTO		

摘要(译)

蛋白质包括或由以下物质形成：（i）SEQ ID NO：1;（ii）衍生自序列SEQ ID NO：1的任何序列，例如，在衍生物序列与磷酸酯结合的条件下，通过取代，去除或添加一个或多个氨基酸;（iii）与序列SEQ ID NO：1同源的任何序列，优选与序列SEQ ID NO：1具有至少约80％的同源性，条件是同源序列与磷酸酯结合;或者（iv）上述序列之一的任何片段，条件是片段与磷酸结合，例如序列SEQ ID NO：1中包含至少约20个连续氨基酸的任何片段。

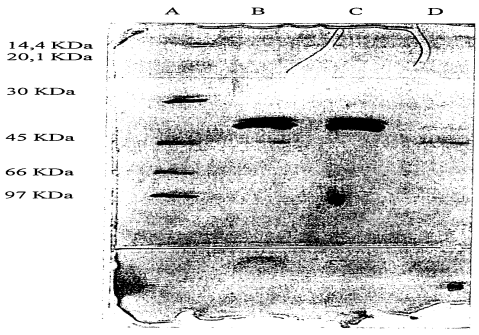

FIGURE 1