

Supplementary material 1.txt

EXPDTA	MODEL	MODELLER	Version	6v2	2002/09/07	15:09:35.216					
REMARK	MODELLER	OBJECTIVE	FUNCTION:	3215.4875							
ATOM	1	N	MET	1	100.386	62.875	55.401	1.00	78.92	1SG	2
ATOM	2	CA	MET	1	100.695	61.441	55.212	1.00	78.92	1SG	3
ATOM	3	CB	MET	1	101.458	61.231	53.894	1.00	78.92	1SG	4
ATOM	4	CG	MET	1	100.655	61.667	52.668	1.00	78.92	1SG	5
ATOM	5	SD	MET	1	101.490	61.428	51.072	1.00	78.92	1SG	6
ATOM	6	CE	MET	1	100.223	62.319	50.124	1.00	78.92	1SG	7
ATOM	7	C	MET	1	101.566	60.972	56.326	1.00	78.92	1SG	8
ATOM	8	O	MET	1	102.777	61.183	56.311	1.00	78.92	1SG	9
ATOM	9	N	ALA	2	100.959	60.340	57.345	1.00	210.12	1SG	10
ATOM	10	CA	ALA	2	101.742	59.856	58.439	1.00	210.12	1SG	11
ATOM	11	CB	ALA	2	100.926	59.595	59.717	1.00	210.12	1SG	12
ATOM	12	C	ALA	2	102.364	58.569	58.011	1.00	210.12	1SG	13
ATOM	13	O	ALA	2	101.858	57.884	57.123	1.00	210.12	1SG	14
ATOM	14	N	GLN	3	103.513	58.222	58.620	1.00	238.96	1SG	15
ATOM	15	CA	GLN	3	104.147	56.985	58.283	1.00	238.96	1SG	16
ATOM	16	CB	GLN	3	105.525	57.153	57.624	1.00	238.96	1SG	17
ATOM	17	CG	GLN	3	105.470	57.879	56.279	1.00	238.96	1SG	18
ATOM	18	CD	GLN	3	106.883	57.928	55.715	1.00	238.96	1SG	19
ATOM	19	OE1	GLN	3	107.815	57.373	56.295	1.00	238.96	1SG	20
ATOM	20	NE2	GLN	3	107.049	58.603	54.546	1.00	238.96	1SG	21
ATOM	21	C	GLN	3	104.353	56.251	59.565	1.00	238.96	1SG	22
ATOM	22	O	GLN	3	104.569	56.860	60.611	1.00	238.96	1SG	23
ATOM	23	N	ILE	4	104.270	54.909	59.525	1.00	126.58	1SG	24
ATOM	24	CA	ILE	4	104.446	54.185	60.745	1.00	126.58	1SG	25
ATOM	25	CB	ILE	4	104.256	52.707	60.556	1.00	126.58	1SG	26
ATOM	26	CG2	ILE	4	104.649	51.990	61.858	1.00	126.58	1SG	27
ATOM	27	CG1	ILE	4	102.813	52.420	60.104	1.00	126.58	1SG	28
ATOM	28	CD1	ILE	4	102.589	50.998	59.588	1.00	126.58	1SG	29
ATOM	29	C	ILE	4	105.844	54.429	61.211	1.00	126.58	1SG	30
ATOM	30	O	ILE	4	106.060	54.852	62.347	1.00	126.58	1SG	31
ATOM	31	N	SER	5	106.837	54.198	60.330	1.00	98.97	1SG	32
ATOM	32	CA	SER	5	108.197	54.471	60.692	1.00	98.97	1SG	33
ATOM	33	CB	SER	5	108.617	53.906	62.058	1.00	98.97	1SG	34
ATOM	34	OG	SER	5	109.974	54.233	62.317	1.00	98.97	1SG	35
ATOM	35	C	SER	5	109.071	53.829	59.672	1.00	98.97	1SG	36
ATOM	36	O	SER	5	108.685	52.838	59.055	1.00	98.97	1SG	37
ATOM	37	N	GLU	6	110.286	54.375	59.475	1.00	66.59	1SG	38
ATOM	38	CA	GLU	6	111.170	53.817	58.496	1.00	66.59	1SG	39
ATOM	39	CB	GLU	6	112.484	54.605	58.383	1.00	66.59	1SG	40
ATOM	40	CG	GLU	6	112.297	56.014	57.820	1.00	66.59	1SG	41
ATOM	41	CD	GLU	6	113.623	56.741	57.970	1.00	66.59	1SG	42
ATOM	42	OE1	GLU	6	114.545	56.153	58.595	1.00	66.59	1SG	43
ATOM	43	OE2	GLU	6	113.731	57.894	57.471	1.00	66.59	1SG	44
ATOM	44	C	GLU	6	111.507	52.414	58.898	1.00	66.59	1SG	45
ATOM	45	O	GLU	6	111.272	51.469	58.149	1.00	66.59	1SG	46
ATOM	46	N	SER	7	112.070	52.247	60.107	1.00	156.47	1SG	47
ATOM	47	CA	SER	7	112.336	50.954	60.671	1.00	156.47	1SG	48
ATOM	48	CB	SER	7	111.052	50.199	61.053	1.00	156.47	1SG	49
ATOM	49	OG	SER	7	110.342	50.923	62.049	1.00	156.47	1SG	50
ATOM	50	C	SER	7	113.124	50.088	59.730	1.00	156.47	1SG	51
ATOM	51	O	SER	7	113.081	48.864	59.856	1.00	156.47	1SG	52
ATOM	52	N	VAL	8	113.885	50.664	58.778	1.00	110.72	1SG	53
ATOM	53	CA	VAL	8	114.665	49.812	57.922	1.00	110.72	1SG	54
ATOM	54	CB	VAL	8	114.363	49.983	56.461	1.00	110.72	1SG	55
ATOM	55	CG1	VAL	8	114.723	51.420	56.044	1.00	110.72	1SG	56
ATOM	56	CG2	VAL	8	115.125	48.902	55.676	1.00	110.72	1SG	57
ATOM	57	C	VAL	8	116.097	50.173	58.128	1.00	110.72	1SG	58
ATOM	58	O	VAL	8	116.439	51.350	58.226	1.00	110.72	1SG	59
ATOM	59	N	SER	9	116.979	49.157	58.209	1.00	38.37	1SG	60
ATOM	60	CA	SER	9	118.364	49.450	58.423	1.00	38.37	1SG	61
ATOM	61	CB	SER	9	119.220	48.217	58.761	1.00	38.37	1SG	62
ATOM	62	OG	SER	9	119.275	47.335	57.650	1.00	38.37	1SG	63
ATOM	63	C	SER	9	118.885	50.044	57.163	1.00	38.37	1SG	64
ATOM	64	O	SER	9	118.583	49.600	56.055	1.00	38.37	1SG	65
ATOM	65	N	PRO	10	119.656	51.070	57.333	1.00	100.34	1SG	66
ATOM	66	CA	PRO	10	120.201	51.741	56.196	1.00	100.34	1SG	67
ATOM	67	CD	PRO	10	119.468	51.969	58.457	1.00	100.34	1SG	68
ATOM	68	CB	PRO	10	120.503	53.174	56.643	1.00	100.34	1SG	69
ATOM	69	CG	PRO	10	120.442	53.121	58.178	1.00	100.34	1SG	70

Supplementary material 1.txt

ATOM	70	C	PRO	10	121.383	51.034	55.654	1.00100.34	1SG	71
ATOM	71	O	PRO	10	122.032	50.272	56.367	1.00100.34	1SG	72
ATOM	72	N	SER	11	121.633	51.239	54.359	1.00209.78	1SG	73
ATOM	73	CA	SER	11	122.834	50.780	53.759	1.00209.78	1SG	74
ATOM	74	CB	SER	11	122.777	51.059	52.277	1.00209.78	1SG	75
ATOM	75	OG	SER	11	121.535	50.587	51.812	1.00209.78	1SG	76
ATOM	76	C	SER	11	123.843	51.724	54.344	1.00209.78	1SG	77
ATOM	77	O	SER	11	124.987	51.377	54.605	1.00209.78	1SG	78
ATOM	78	N	THR	12	123.394	52.957	54.649	1.00149.24	1SG	79
ATOM	79	CA	THR	12	124.288	54.006	55.048	1.00149.24	1SG	80
ATOM	80	CB	THR	12	123.655	55.367	54.871	1.00149.24	1SG	81
ATOM	81	OG1	THR	12	123.079	55.438	53.574	1.00149.24	1SG	82
ATOM	82	CG2	THR	12	124.739	56.463	54.930	1.00149.24	1SG	83
ATOM	83	C	THR	12	124.711	53.779	56.479	1.00149.24	1SG	84
ATOM	84	O	THR	12	124.803	52.639	56.935	1.00149.24	1SG	85
ATOM	85	N	ASP	13	124.972	54.873	57.223	1.00195.40	1SG	86
ATOM	86	CA	ASP	13	125.539	54.894	58.543	1.00195.40	1SG	87
ATOM	87	CB	ASP	13	125.996	56.316	58.950	1.00195.40	1SG	88
ATOM	88	CG	ASP	13	126.978	56.275	60.117	1.00195.40	1SG	89
ATOM	89	OD1	ASP	13	127.713	55.261	60.256	1.00195.40	1SG	90
ATOM	90	OD2	ASP	13	126.992	57.262	60.902	1.00195.40	1SG	91
ATOM	91	C	ASP	13	124.518	54.409	59.524	1.00195.40	1SG	92
ATOM	92	O	ASP	13	123.571	53.715	59.154	1.00195.40	1SG	93
ATOM	93	N	LEU	14	124.707	54.771	60.811	1.00234.76	1SG	94
ATOM	94	CA	LEU	14	123.906	54.288	61.894	1.00234.76	1SG	95
ATOM	95	CB	LEU	14	124.200	54.971	63.240	1.00234.76	1SG	96
ATOM	96	CG	LEU	14	125.623	54.672	63.752	1.00234.76	1SG	97
ATOM	97	CD2	LEU	14	125.797	55.042	65.227	1.00234.76	1SG	98
ATOM	98	CD1	LEU	14	126.689	55.331	62.876	1.00234.76	1SG	99
ATOM	99	C	LEU	14	122.469	54.443	61.546	1.00234.76	1SG	100
ATOM	100	O	LEU	14	122.051	55.404	60.901	1.00234.76	1SG	101
ATOM	101	N	LYS	15	121.698	53.422	61.954	1.00160.87	1SG	102
ATOM	102	CA	LYS	15	120.332	53.237	61.584	1.00160.87	1SG	103
ATOM	103	CB	LYS	15	119.783	51.897	62.100	1.00160.87	1SG	104
ATOM	104	CG	LYS	15	118.357	51.596	61.642	1.00160.87	1SG	105
ATOM	105	CD	LYS	15	117.981	50.116	61.750	1.00160.87	1SG	106
ATOM	106	CE	LYS	15	118.073	49.547	63.168	1.00160.87	1SG	107
ATOM	107	NZ	LYS	15	116.786	49.732	63.875	1.00160.87	1SG	108
ATOM	108	C	LYS	15	119.431	54.336	62.046	1.00160.87	1SG	109
ATOM	109	O	LYS	15	118.657	54.847	61.238	1.00160.87	1SG	110
ATOM	110	N	SER	16	119.478	54.776	63.319	1.00229.10	1SG	111
ATOM	111	CA	SER	16	118.431	55.726	63.554	1.00229.10	1SG	112
ATOM	112	CB	SER	16	117.057	55.030	63.652	1.00229.10	1SG	113
ATOM	113	OG	SER	16	116.019	55.971	63.877	1.00229.10	1SG	114
ATOM	114	C	SER	16	118.635	56.517	64.812	1.00229.10	1SG	115
ATOM	115	O	SER	16	119.483	56.217	65.650	1.00229.10	1SG	116
ATOM	116	N	THR	17	117.842	57.605	64.907	1.00270.77	1SG	117
ATOM	117	CA	THR	17	117.701	58.489	66.028	1.00270.77	1SG	118
ATOM	118	CB	THR	17	118.625	59.669	66.024	1.00270.77	1SG	119
ATOM	119	OG1	THR	17	118.389	60.486	64.887	1.00270.77	1SG	120
ATOM	120	CG2	THR	17	120.072	59.161	66.038	1.00270.77	1SG	121
ATOM	121	C	THR	17	116.315	59.033	65.891	1.00270.77	1SG	122
ATOM	122	O	THR	17	115.520	58.505	65.115	1.00270.77	1SG	123
ATOM	123	N	GLU	18	115.962	60.087	66.652	1.00157.85	1SG	124
ATOM	124	CA	GLU	18	114.653	60.631	66.447	1.00157.85	1SG	125
ATOM	125	CB	GLU	18	114.328	61.825	67.360	1.00157.85	1SG	126
ATOM	126	CG	GLU	18	112.834	62.160	67.386	1.00157.85	1SG	127
ATOM	127	CD	GLU	18	112.116	61.044	68.140	1.00157.85	1SG	128
ATOM	128	OE1	GLU	18	112.819	60.178	68.726	1.00157.85	1SG	129
ATOM	129	OE2	GLU	18	110.855	61.042	68.140	1.00157.85	1SG	130
ATOM	130	C	GLU	18	114.668	61.114	65.036	1.00157.85	1SG	131
ATOM	131	O	GLU	18	113.732	60.885	64.274	1.00157.85	1SG	132
ATOM	132	N	SER	19	115.773	61.789	64.663	1.00194.78	1SG	133
ATOM	133	CA	SER	19	116.010	62.212	63.315	1.00194.78	1SG	134
ATOM	134	CB	SER	19	115.560	61.199	62.247	1.00194.78	1SG	135
ATOM	135	OG	SER	19	116.328	60.008	62.353	1.00194.78	1SG	136
ATOM	136	C	SER	19	115.346	63.522	63.045	1.00194.78	1SG	137
ATOM	137	O	SER	19	114.518	64.004	63.817	1.00194.78	1SG	138
ATOM	138	N	SER	20	115.745	64.133	61.910	1.00182.91	1SG	139
ATOM	139	CA	SER	20	115.223	65.376	61.426	1.00182.91	1SG	140
ATOM	140	CB	SER	20	116.060	66.602	61.838	1.00182.91	1SG	141

Supplementary material 1.txt

ATOM	141	OG	SER	20	115.479	67.796	61.334	1.00182.91	1SG	142
ATOM	142	C	SER	20	115.290	65.243	59.937	1.00182.91	1SG	143
ATOM	143	O	SER	20	115.599	64.166	59.431	1.00182.91	1SG	144
ATOM	144	N	ILE	21	114.992	66.316	59.179	1.0076.89	1SG	145
ATOM	145	CA	ILE	21	115.032	66.152	57.756	1.0076.89	1SG	146
ATOM	146	CB	ILE	21	113.998	66.967	57.032	1.0076.89	1SG	147
ATOM	147	CG2	ILE	21	114.274	66.869	55.522	1.0076.89	1SG	148
ATOM	148	CG1	ILE	21	112.585	66.512	57.436	1.0076.89	1SG	149
ATOM	149	CD1	ILE	21	111.475	67.428	56.923	1.0076.89	1SG	150
ATOM	150	C	ILE	21	116.374	66.600	57.281	1.0076.89	1SG	151
ATOM	151	O	ILE	21	116.703	67.785	57.322	1.0076.89	1SG	152
ATOM	152	N	THR	22	117.192	65.626	56.835	1.00264.57	1SG	153
ATOM	153	CA	THR	22	118.500	65.904	56.327	1.00264.57	1SG	154
ATOM	154	CB	THR	22	119.592	65.735	57.345	1.00264.57	1SG	155
ATOM	155	OG1	THR	22	119.635	64.393	57.807	1.00264.57	1SG	156
ATOM	156	CG2	THR	22	119.328	66.694	58.519	1.00264.57	1SG	157
ATOM	157	C	THR	22	118.752	64.923	55.230	1.00264.57	1SG	158
ATOM	158	O	THR	22	117.964	64.001	55.014	1.00264.57	1SG	159
ATOM	159	N	SER	23	119.860	65.111	54.490	1.00210.73	1SG	160
ATOM	160	CA	SER	23	120.148	64.198	53.426	1.00210.73	1SG	161
ATOM	161	CB	SER	23	120.017	64.819	52.024	1.00210.73	1SG	162
ATOM	162	OG	SER	23	120.320	63.846	51.035	1.00210.73	1SG	163
ATOM	163	C	SER	23	121.565	63.754	53.584	1.00210.73	1SG	164
ATOM	164	O	SER	23	122.388	64.441	54.190	1.00210.73	1SG	165
ATOM	165	N	ASN	24	121.876	62.558	53.050	1.00248.18	1SG	166
ATOM	166	CA	ASN	24	123.209	62.043	53.113	1.00248.18	1SG	167
ATOM	167	CB	ASN	24	123.366	60.836	54.052	1.00248.18	1SG	168
ATOM	168	CG	ASN	24	122.511	59.709	53.493	1.00248.18	1SG	169
ATOM	169	OD1	ASN	24	121.323	59.891	53.230	1.00248.18	1SG	170
ATOM	170	ND2	ASN	24	123.130	58.515	53.295	1.00248.18	1SG	171
ATOM	171	C	ASN	24	123.558	61.579	51.737	1.00248.18	1SG	172
ATOM	172	O	ASN	24	122.693	61.462	50.870	1.00248.18	1SG	173
ATOM	173	N	ARG	25	124.859	61.324	51.502	1.00280.11	1SG	174
ATOM	174	CA	ARG	25	125.307	60.882	50.216	1.00280.11	1SG	175
ATOM	175	CB	ARG	25	126.830	60.967	50.013	1.00280.11	1SG	176
ATOM	176	CG	ARG	25	127.309	62.372	49.651	1.00280.11	1SG	177
ATOM	177	CD	ARG	25	127.014	63.421	50.721	1.00280.11	1SG	178
ATOM	178	NE	ARG	25	127.357	64.748	50.139	1.00280.11	1SG	179
ATOM	179	CZ	ARG	25	126.445	65.396	49.358	1.00280.11	1SG	180
ATOM	180	NH1	ARG	25	125.240	64.815	49.085	1.00280.11	1SG	181
ATOM	181	NH2	ARG	25	126.739	66.624	48.841	1.00280.11	1SG	182
ATOM	182	C	ARG	25	124.900	59.463	50.016	1.00280.11	1SG	183
ATOM	183	O	ARG	25	124.659	58.720	50.967	1.00280.11	1SG	184
ATOM	184	N	HIS	26	124.796	59.071	48.733	1.00248.77	1SG	185
ATOM	185	CA	HIS	26	124.419	57.749	48.333	1.00248.77	1SG	186
ATOM	186	ND1	HIS	26	124.044	55.918	44.948	1.00248.77	1SG	187
ATOM	187	CG	HIS	26	124.016	56.245	46.284	1.00248.77	1SG	188
ATOM	188	CB	HIS	26	124.402	57.600	46.800	1.00248.77	1SG	189
ATOM	189	NE2	HIS	26	123.343	54.106	46.025	1.00248.77	1SG	190
ATOM	190	CD2	HIS	26	123.584	55.127	46.929	1.00248.77	1SG	191
ATOM	191	CE1	HIS	26	123.632	54.629	44.849	1.00248.77	1SG	192
ATOM	192	C	HIS	26	125.445	56.806	48.863	1.00248.77	1SG	193
ATOM	193	O	HIS	26	126.639	57.103	48.852	1.00248.77	1SG	194
ATOM	194	N	GLY	27	124.994	55.639	49.365	1.00132.98	1SG	195
ATOM	195	CA	GLY	27	125.922	54.670	49.863	1.00132.98	1SG	196
ATOM	196	C	GLY	27	125.159	53.436	50.221	1.00132.98	1SG	197
ATOM	197	O	GLY	27	123.930	53.439	50.267	1.00132.98	1SG	198
ATOM	198	N	ASN	28	125.900	52.343	50.483	1.00184.90	1SG	199
ATOM	199	CA	ASN	28	125.336	51.089	50.879	1.00184.90	1SG	200
ATOM	200	CB	ASN	28	125.584	49.936	49.891	1.00184.90	1SG	201
ATOM	201	CG	ASN	28	124.672	50.135	48.690	1.00184.90	1SG	202
ATOM	202	OD1	ASN	28	124.635	49.316	47.773	1.00184.90	1SG	203
ATOM	203	ND2	ASN	28	123.911	51.262	48.693	1.00184.90	1SG	204
ATOM	204	C	ASN	28	126.005	50.730	52.161	1.00184.90	1SG	205
ATOM	205	O	ASN	28	126.813	51.510	52.664	1.00184.90	1SG	206
ATOM	206	N	MET	29	125.667	49.557	52.754	1.00125.90	1SG	207
ATOM	207	CA	MET	29	126.378	49.140	53.931	1.00125.90	1SG	208
ATOM	208	CB	MET	29	125.947	47.766	54.461	1.00125.90	1SG	209
ATOM	209	CG	MET	29	124.511	47.774	54.988	1.00125.90	1SG	210
ATOM	210	SD	MET	29	123.996	46.230	55.790	1.00125.90	1SG	211
ATOM	211	CE	MET	29	122.213	46.558	55.678	1.00125.90	1SG	212

Supplementary material 1.txt

ATOM	212	C	MET	29	127.758	49.055	53.414	1.00125.90	1SG	213
ATOM	213	O	MET	29	128.735	49.396	54.078	1.00125.90	1SG	214
ATOM	214	N	TRP	30	127.826	48.590	52.161	1.00138.66	1SG	215
ATOM	215	CA	TRP	30	129.030	48.534	51.415	1.00138.66	1SG	216
ATOM	216	CB	TRP	30	128.776	47.833	50.073	1.00138.66	1SG	217
ATOM	217	CG	TRP	30	128.047	46.542	50.345	1.00138.66	1SG	218
ATOM	218	CD2	TRP	30	128.565	45.507	51.189	1.00138.66	1SG	219
ATOM	219	CD1	TRP	30	126.777	46.169	50.009	1.00138.66	1SG	220
ATOM	220	NE1	TRP	30	126.467	44.969	50.603	1.00138.66	1SG	221
ATOM	221	CE2	TRP	30	127.560	44.552	51.335	1.00138.66	1SG	222
ATOM	222	CE3	TRP	30	129.772	45.381	51.814	1.00138.66	1SG	223
ATOM	223	CZ2	TRP	30	127.749	43.451	52.119	1.00138.66	1SG	224
ATOM	224	CZ3	TRP	30	129.972	44.257	52.581	1.00138.66	1SG	225
ATOM	225	CH2	TRP	30	128.977	43.315	52.732	1.00138.66	1SG	226
ATOM	226	C	TRP	30	129.456	49.942	51.172	1.00138.66	1SG	227
ATOM	227	O	TRP	30	130.606	50.297	51.424	1.00138.66	1SG	228
ATOM	228	N	GLU	31	128.506	50.774	50.688	1.00215.36	1SG	229
ATOM	229	CA	GLU	31	128.717	52.169	50.416	1.00215.36	1SG	230
ATOM	230	CB	GLU	31	129.781	52.896	51.262	1.00215.36	1SG	231
ATOM	231	CG	GLU	31	129.363	53.145	52.712	1.00215.36	1SG	232
ATOM	232	CD	GLU	31	130.309	54.184	53.298	1.00215.36	1SG	233
ATOM	233	OE1	GLU	31	131.151	54.720	52.528	1.00215.36	1SG	234
ATOM	234	OE2	GLU	31	130.196	54.461	54.522	1.00215.36	1SG	235
ATOM	235	C	GLU	31	129.071	52.356	48.977	1.00215.36	1SG	236
ATOM	236	O	GLU	31	128.684	51.588	48.098	1.00215.36	1SG	237
ATOM	237	N	ASP	32	129.822	53.443	48.748	1.00140.79	1SG	238
ATOM	238	CA	ASP	32	130.306	53.972	47.507	1.00140.79	1SG	239
ATOM	239	CB	ASP	32	130.979	55.343	47.722	1.00140.79	1SG	240
ATOM	240	CG	ASP	32	131.371	55.968	46.393	1.00140.79	1SG	241
ATOM	241	OD1	ASP	32	132.402	55.537	45.812	1.00140.79	1SG	242
ATOM	242	OD2	ASP	32	130.645	56.897	45.947	1.00140.79	1SG	243
ATOM	243	C	ASP	32	131.305	53.031	46.904	1.00140.79	1SG	244
ATOM	244	O	ASP	32	131.614	53.132	45.718	1.00140.79	1SG	245
ATOM	245	N	ASP	33	131.819	52.070	47.696	1.0074.54	1SG	246
ATOM	246	CA	ASP	33	132.921	51.240	47.290	1.0074.54	1SG	247
ATOM	247	CB	ASP	33	133.199	50.085	48.269	1.0074.54	1SG	248
ATOM	248	CG	ASP	33	133.740	50.670	49.565	1.0074.54	1SG	249
ATOM	249	OD1	ASP	33	133.244	51.751	49.980	1.0074.54	1SG	250
ATOM	250	OD2	ASP	33	134.646	50.032	50.166	1.0074.54	1SG	251
ATOM	251	C	ASP	33	132.673	50.617	45.944	1.0074.54	1SG	252
ATOM	252	O	ASP	33	133.608	50.463	45.162	1.0074.54	1SG	253
ATOM	253	N	ARG	34	131.422	50.218	45.662	1.00154.57	1SG	254
ATOM	254	CA	ARG	34	130.969	49.587	44.449	1.00154.57	1SG	255
ATOM	255	CB	ARG	34	129.552	49.024	44.641	1.00154.57	1SG	256
ATOM	256	CG	ARG	34	128.598	50.082	45.201	1.00154.57	1SG	257
ATOM	257	CD	ARG	34	127.178	49.589	45.474	1.00154.57	1SG	258
ATOM	258	NE	ARG	34	126.574	50.562	46.428	1.00154.57	1SG	259
ATOM	259	CZ	ARG	34	126.054	51.746	45.992	1.00154.57	1SG	260
ATOM	260	NH1	ARG	34	126.068	52.057	44.665	1.00154.57	1SG	261
ATOM	261	NH2	ARG	34	125.529	52.634	46.886	1.00154.57	1SG	262
ATOM	262	C	ARG	34	130.954	50.487	43.242	1.00154.57	1SG	263
ATOM	263	O	ARG	34	131.141	50.022	42.117	1.00154.57	1SG	264
ATOM	264	N	ILE	35	130.730	51.798	43.434	1.00100.76	1SG	265
ATOM	265	CA	ILE	35	130.488	52.698	42.340	1.00100.76	1SG	266
ATOM	266	CB	ILE	35	130.267	54.113	42.791	1.00100.76	1SG	267
ATOM	267	CG2	ILE	35	131.594	54.654	43.344	1.00100.76	1SG	268
ATOM	268	CG1	ILE	35	129.683	54.955	41.645	1.00100.76	1SG	269
ATOM	269	CD1	ILE	35	129.127	56.302	42.104	1.00100.76	1SG	270
ATOM	270	C	ILE	35	131.605	52.711	41.340	1.00100.76	1SG	271
ATOM	271	O	ILE	35	131.344	52.746	40.140	1.00100.76	1SG	272
ATOM	272	N	GLN	36	132.882	52.704	41.756	1.00103.74	1SG	273
ATOM	273	CA	GLN	36	133.847	52.779	40.697	1.00103.74	1SG	274
ATOM	274	CB	GLN	36	134.719	54.045	40.752	1.00103.74	1SG	275
ATOM	275	CG	GLN	36	135.592	54.168	41.999	1.00103.74	1SG	276
ATOM	276	CD	GLN	36	136.326	55.496	41.892	1.00103.74	1SG	277
ATOM	277	OE1	GLN	36	137.192	55.814	42.707	1.00103.74	1SG	278
ATOM	278	NE2	GLN	36	135.969	56.298	40.853	1.00103.74	1SG	279
ATOM	279	C	GLN	36	134.721	51.572	40.691	1.00103.74	1SG	280
ATOM	280	O	GLN	36	135.132	51.070	41.736	1.00103.74	1SG	281
ATOM	281	N	SER	37	134.980	51.044	39.477	1.0045.55	1SG	282
ATOM	282	CA	SER	37	135.875	49.937	39.347	1.0045.55	1SG	283

Supplementary material 1.txt

ATOM	283	CB	SER	37	135.189	48.564	39.424	1.00	45.55	1SG	284
ATOM	284	OG	SER	37	134.370	48.346	38.284	1.00	45.55	1SG	285
ATOM	285	C	SER	37	136.515	50.057	38.006	1.00	45.55	1SG	286
ATOM	286	O	SER	37	135.835	50.096	36.981	1.00	45.55	1SG	287
ATOM	287	N	LEU	38	137.860	50.108	37.987	1.00	37.42	1SG	288
ATOM	288	CA	LEU	38	138.558	50.218	36.744	1.00	37.42	1SG	289
ATOM	289	CB	LEU	38	139.646	51.307	36.740	1.00	37.42	1SG	290
ATOM	290	CG	LEU	38	139.100	52.734	36.934	1.00	37.42	1SG	291
ATOM	291	CD2	LEU	38	137.894	53.003	36.020	1.00	37.42	1SG	292
ATOM	292	CD1	LEU	38	140.216	53.781	36.778	1.00	37.42	1SG	293
ATOM	293	C	LEU	38	139.240	48.911	36.528	1.00	37.42	1SG	294
ATOM	294	O	LEU	38	140.046	48.477	37.349	1.00	37.42	1SG	295
ATOM	295	N	ASN	39	138.924	48.248	35.402	1.00	34.97	1SG	296
ATOM	296	CA	ASN	39	139.525	46.978	35.130	1.00	34.97	1SG	297
ATOM	297	CB	ASN	39	138.725	46.135	34.117	1.00	34.97	1SG	298
ATOM	298	CG	ASN	39	139.331	44.740	34.040	1.00	34.97	1SG	299
ATOM	299	OD1	ASN	39	140.548	44.569	33.981	1.00	34.97	1SG	300
ATOM	300	ND2	ASN	39	138.453	43.702	34.042	1.00	34.97	1SG	301
ATOM	301	C	ASN	39	140.871	47.232	34.540	1.00	34.97	1SG	302
ATOM	302	O	ASN	39	141.004	47.963	33.557	1.00	34.97	1SG	303
ATOM	303	N	SER	40	141.920	46.638	35.142	1.00	83.69	1SG	304
ATOM	304	CA	SER	40	143.223	46.816	34.578	1.00	83.69	1SG	305
ATOM	305	CB	SER	40	144.367	46.410	35.525	1.00	83.69	1SG	306
ATOM	306	OG	SER	40	144.286	45.027	35.836	1.00	83.69	1SG	307
ATOM	307	C	SER	40	143.278	45.938	33.374	1.00	83.69	1SG	308
ATOM	308	O	SER	40	143.348	44.713	33.452	1.00	83.69	1SG	309
ATOM	309	N	PRO	41	143.261	46.585	32.251	1.00	70.57	1SG	310
ATOM	310	CA	PRO	41	143.242	45.920	30.982	1.00	70.57	1SG	311
ATOM	311	CD	PRO	41	143.723	47.959	32.148	1.00	70.57	1SG	312
ATOM	312	CB	PRO	41	143.283	47.043	29.950	1.00	70.57	1SG	313
ATOM	313	CG	PRO	41	144.090	48.142	30.666	1.00	70.57	1SG	314
ATOM	314	C	PRO	41	144.426	45.026	30.821	1.00	70.57	1SG	315
ATOM	315	O	PRO	41	144.345	44.090	30.033	1.00	70.57	1SG	316
ATOM	316	N	TYR	42	145.568	45.307	31.465	1.00	84.20	1SG	317
ATOM	317	CA	TYR	42	146.662	44.405	31.255	1.00	84.20	1SG	318
ATOM	318	CB	TYR	42	148.001	44.905	31.821	1.00	84.20	1SG	319
ATOM	319	CG	TYR	42	148.525	45.950	30.897	1.00	84.20	1SG	320
ATOM	320	CD1	TYR	42	148.150	47.268	31.015	1.00	84.20	1SG	321
ATOM	321	CD2	TYR	42	149.402	45.593	29.899	1.00	84.20	1SG	322
ATOM	322	CE1	TYR	42	148.649	48.213	30.149	1.00	84.20	1SG	323
ATOM	323	CE2	TYR	42	149.904	46.531	29.031	1.00	84.20	1SG	324
ATOM	324	CZ	TYR	42	149.526	47.845	29.155	1.00	84.20	1SG	325
ATOM	325	OH	TYR	42	150.040	48.811	28.264	1.00	84.20	1SG	326
ATOM	326	C	TYR	42	146.370	43.081	31.882	1.00	84.20	1SG	327
ATOM	327	O	TYR	42	146.560	42.035	31.264	1.00	84.20	1SG	328
ATOM	328	N	GLY	43	145.880	43.104	33.133	1.00	28.38	1SG	329
ATOM	329	CA	GLY	43	145.673	41.900	33.883	1.00	28.38	1SG	330
ATOM	330	C	GLY	43	144.614	41.033	33.274	1.00	28.38	1SG	331
ATOM	331	O	GLY	43	144.765	39.813	33.237	1.00	28.38	1SG	332
ATOM	332	N	ALA	44	143.501	41.624	32.797	1.00	44.92	1SG	333
ATOM	333	CA	ALA	44	142.429	40.785	32.342	1.00	44.92	1SG	334
ATOM	334	CB	ALA	44	141.141	41.564	32.005	1.00	44.92	1SG	335
ATOM	335	C	ALA	44	142.850	39.956	31.162	1.00	44.92	1SG	336
ATOM	336	O	ALA	44	142.617	38.749	31.170	1.00	44.92	1SG	337
ATOM	337	N	PRO	45	143.459	40.511	30.146	1.00	103.73	1SG	338
ATOM	338	CA	PRO	45	143.907	39.651	29.090	1.00	103.73	1SG	339
ATOM	339	CD	PRO	45	142.920	41.735	29.582	1.00	103.73	1SG	340
ATOM	340	CB	PRO	45	144.217	40.556	27.903	1.00	103.73	1SG	341
ATOM	341	CG	PRO	45	143.183	41.680	28.068	1.00	103.73	1SG	342
ATOM	342	C	PRO	45	145.008	38.730	29.497	1.00	103.73	1SG	343
ATOM	343	O	PRO	45	145.170	37.695	28.855	1.00	103.73	1SG	344
ATOM	344	N	ALA	46	145.795	39.082	30.530	1.00	23.95	1SG	345
ATOM	345	CA	ALA	46	146.848	38.199	30.938	1.00	23.95	1SG	346
ATOM	346	CB	ALA	46	147.688	38.774	32.092	1.00	23.95	1SG	347
ATOM	347	C	ALA	46	146.218	36.936	31.431	1.00	23.95	1SG	348
ATOM	348	O	ALA	46	146.638	35.836	31.075	1.00	23.95	1SG	349
ATOM	349	N	TYR	47	145.167	37.077	32.261	1.00	53.63	1SG	350
ATOM	350	CA	TYR	47	144.472	35.951	32.813	1.00	53.63	1SG	351
ATOM	351	CB	TYR	47	143.387	36.346	33.831	1.00	53.63	1SG	352
ATOM	352	CG	TYR	47	144.046	36.654	35.132	1.00	53.63	1SG	353
ATOM	353	CD1	TYR	47	144.770	37.808	35.327	1.00	53.63	1SG	354

Supplementary material 1.txt

ATOM	354	CD2	TYR	47	143.914	35.768	36.176	1.00	53.63	1SG	355
ATOM	355	CE1	TYR	47	145.364	38.060	36.544	1.00	53.63	1SG	356
ATOM	356	CE2	TYR	47	144.505	36.015	37.393	1.00	53.63	1SG	357
ATOM	357	CZ	TYR	47	145.233	37.164	37.578	1.00	53.63	1SG	358
ATOM	358	OH	TYR	47	145.840	37.420	38.826	1.00	53.63	1SG	359
ATOM	359	C	TYR	47	143.797	35.191	31.722	1.00	53.63	1SG	360
ATOM	360	O	TYR	47	143.847	33.962	31.692	1.00	53.63	1SG	361
ATOM	361	N	GLN	48	143.148	35.906	30.787	1.00	84.14	1SG	362
ATOM	362	CA	GLN	48	142.396	35.234	29.770	1.00	84.14	1SG	363
ATOM	363	CB	GLN	48	141.583	36.184	28.874	1.00	84.14	1SG	364
ATOM	364	CG	GLN	48	142.414	37.143	28.025	1.00	84.14	1SG	365
ATOM	365	CD	GLN	48	141.427	37.972	27.219	1.00	84.14	1SG	366
ATOM	366	OE1	GLN	48	141.403	39.202	27.305	1.00	84.14	1SG	367
ATOM	367	NE2	GLN	48	140.578	37.281	26.415	1.00	84.14	1SG	368
ATOM	368	C	GLN	48	143.295	34.417	28.898	1.00	84.14	1SG	369
ATOM	369	O	GLN	48	142.940	33.301	28.522	1.00	84.14	1SG	370
ATOM	370	N	GLU	49	144.486	34.938	28.552	1.00	35.08	1SG	371
ATOM	371	CA	GLU	49	145.340	34.220	27.647	1.00	35.08	1SG	372
ATOM	372	CB	GLU	49	146.598	35.014	27.261	1.00	35.08	1SG	373
ATOM	373	CG	GLU	49	147.447	34.331	26.188	1.00	35.08	1SG	374
ATOM	374	CD	GLU	49	148.526	35.319	25.775	1.00	35.08	1SG	375
ATOM	375	OE1	GLU	49	148.155	36.434	25.320	1.00	35.08	1SG	376
ATOM	376	OE2	GLU	49	149.731	34.979	25.912	1.00	35.08	1SG	377
ATOM	377	C	GLU	49	145.778	32.920	28.255	1.00	35.08	1SG	378
ATOM	378	O	GLU	49	145.750	31.884	27.593	1.00	35.08	1SG	379
ATOM	379	N	ARG	50	146.192	32.943	29.536	1.00	138.02	1SG	380
ATOM	380	CA	ARG	50	146.667	31.770	30.220	1.00	138.02	1SG	381
ATOM	381	CB	ARG	50	147.192	32.086	31.631	1.00	138.02	1SG	382
ATOM	382	CG	ARG	50	148.483	32.907	31.640	1.00	138.02	1SG	383
ATOM	383	CD	ARG	50	148.974	33.258	33.046	1.00	138.02	1SG	384
ATOM	384	NE	ARG	50	148.940	32.012	33.862	1.00	138.02	1SG	385
ATOM	385	CZ	ARG	50	149.752	31.884	34.952	1.00	138.02	1SG	386
ATOM	386	NH1	ARG	50	150.638	32.875	35.263	1.00	138.02	1SG	387
ATOM	387	NH2	ARG	50	149.679	30.765	35.731	1.00	138.02	1SG	388
ATOM	388	C	ARG	50	145.545	30.793	30.378	1.00	138.02	1SG	389
ATOM	389	O	ARG	50	145.732	29.584	30.246	1.00	138.02	1SG	390
ATOM	390	N	SER	51	144.336	31.302	30.666	1.00	30.14	1SG	391
ATOM	391	CA	SER	51	143.214	30.449	30.919	1.00	30.14	1SG	392
ATOM	392	CB	SER	51	141.926	31.236	31.211	1.00	30.14	1SG	393
ATOM	393	OG	SER	51	142.076	31.992	32.404	1.00	30.14	1SG	394
ATOM	394	C	SER	51	142.963	29.613	29.709	1.00	30.14	1SG	395
ATOM	395	O	SER	51	142.701	28.419	29.819	1.00	30.14	1SG	396
ATOM	396	N	GLU	52	143.093	30.207	28.512	1.00	60.34	1SG	397
ATOM	397	CA	GLU	52	142.769	29.507	27.304	1.00	60.34	1SG	398
ATOM	398	CB	GLU	52	143.044	30.362	26.056	1.00	60.34	1SG	399
ATOM	399	CG	GLU	52	142.189	31.631	26.007	1.00	60.34	1SG	400
ATOM	400	CD	GLU	52	142.546	32.408	24.748	1.00	60.34	1SG	401
ATOM	401	OE1	GLU	52	143.293	31.852	23.900	1.00	60.34	1SG	402
ATOM	402	OE2	GLU	52	142.075	33.569	24.619	1.00	60.34	1SG	403
ATOM	403	C	GLU	52	143.625	28.285	27.217	1.00	60.34	1SG	404
ATOM	404	O	GLU	52	143.146	27.215	26.845	1.00	60.34	1SG	405
ATOM	405	N	LYS	53	144.920	28.410	27.558	1.00	83.40	1SG	406
ATOM	406	CA	LYS	53	145.804	27.282	27.488	1.00	83.40	1SG	407
ATOM	407	CB	LYS	53	147.254	27.634	27.862	1.00	83.40	1SG	408
ATOM	408	CG	LYS	53	147.951	28.553	26.858	1.00	83.40	1SG	409
ATOM	409	CD	LYS	53	149.243	29.173	27.397	1.00	83.40	1SG	410
ATOM	410	CE	LYS	53	150.304	28.144	27.791	1.00	83.40	1SG	411
ATOM	411	NZ	LYS	53	150.865	27.507	26.578	1.00	83.40	1SG	412
ATOM	412	C	LYS	53	145.354	26.246	28.470	1.00	83.40	1SG	413
ATOM	413	O	LYS	53	145.273	25.064	28.144	1.00	83.40	1SG	414
ATOM	414	N	LEU	54	145.027	26.683	29.698	1.00	48.43	1SG	415
ATOM	415	CA	LEU	54	144.648	25.813	30.770	1.00	48.43	1SG	416
ATOM	416	CB	LEU	54	144.378	26.581	32.076	1.00	48.43	1SG	417
ATOM	417	CG	LEU	54	145.613	27.312	32.639	1.00	48.43	1SG	418
ATOM	418	CD2	LEU	54	146.804	26.356	32.815	1.00	48.43	1SG	419
ATOM	419	CD1	LEU	54	145.273	28.059	33.940	1.00	48.43	1SG	420
ATOM	420	C	LEU	54	143.385	25.108	30.401	1.00	48.43	1SG	421
ATOM	421	O	LEU	54	143.199	23.946	30.755	1.00	48.43	1SG	422
ATOM	422	N	ILE	55	142.466	25.806	29.703	1.00	96.54	1SG	423
ATOM	423	CA	ILE	55	141.223	25.193	29.333	1.00	96.54	1SG	424
ATOM	424	CB	ILE	55	140.219	26.122	28.702	1.00	96.54	1SG	425

Supplementary material 1.txt

ATOM	425	CG2	ILE	55	139.329	25.272	27.780	1.00	96.54	1SG	426
ATOM	426	CG1	ILE	55	139.404	26.887	29.769	1.00	96.54	1SG	427
ATOM	427	CD1	ILE	55	140.183	27.826	30.684	1.00	96.54	1SG	428
ATOM	428	C	ILE	55	141.426	24.022	28.421	1.00	96.54	1SG	429
ATOM	429	O	ILE	55	140.795	22.985	28.613	1.00	96.54	1SG	430
ATOM	430	N	GLU	56	142.294	24.133	27.400	1.00	93.34	1SG	431
ATOM	431	CA	GLU	56	142.478	23.015	26.516	1.00	93.34	1SG	432
ATOM	432	CB	GLU	56	143.389	23.313	25.313	1.00	93.34	1SG	433
ATOM	433	CG	GLU	56	142.713	24.145	24.222	1.00	93.34	1SG	434
ATOM	434	CD	GLU	56	141.684	23.262	23.526	1.00	93.34	1SG	435
ATOM	435	OE1	GLU	56	141.592	22.058	23.888	1.00	93.34	1SG	436
ATOM	436	OE2	GLU	56	140.973	23.780	22.624	1.00	93.34	1SG	437
ATOM	437	C	GLU	56	143.096	21.883	27.270	1.00	93.34	1SG	438
ATOM	438	O	GLU	56	142.752	20.724	27.047	1.00	93.34	1SG	439
ATOM	439	N	GLU	57	144.031	22.189	28.189	1.00	35.43	1SG	440
ATOM	440	CA	GLU	57	144.718	21.154	28.906	1.00	35.43	1SG	441
ATOM	441	CB	GLU	57	145.746	21.720	29.901	1.00	35.43	1SG	442
ATOM	442	CG	GLU	57	146.910	22.439	29.219	1.00	35.43	1SG	443
ATOM	443	CD	GLU	57	147.745	23.109	30.299	1.00	35.43	1SG	444
ATOM	444	OE1	GLU	57	147.320	23.067	31.484	1.00	35.43	1SG	445
ATOM	445	OE2	GLU	57	148.818	23.672	29.953	1.00	35.43	1SG	446
ATOM	446	C	GLU	57	143.716	20.371	29.692	1.00	35.43	1SG	447
ATOM	447	O	GLU	57	143.722	19.143	29.665	1.00	35.43	1SG	448
ATOM	448	N	ILE	58	142.810	21.071	30.395	1.00	111.04	1SG	449
ATOM	449	CA	ILE	58	141.802	20.442	31.192	1.00	111.04	1SG	450
ATOM	450	CB	ILE	58	141.083	21.419	32.084	1.00	111.04	1SG	451
ATOM	451	CG2	ILE	58	142.108	21.944	33.102	1.00	111.04	1SG	452
ATOM	452	CG1	ILE	58	140.404	22.542	31.291	1.00	111.04	1SG	453
ATOM	453	CD1	ILE	58	139.662	23.534	32.186	1.00	111.04	1SG	454
ATOM	454	C	ILE	58	140.866	19.686	30.300	1.00	111.04	1SG	455
ATOM	455	O	ILE	58	140.364	18.623	30.667	1.00	111.04	1SG	456
ATOM	456	N	LYS	59	140.598	20.224	29.097	1.00	111.76	1SG	457
ATOM	457	CA	LYS	59	139.723	19.583	28.159	1.00	111.76	1SG	458
ATOM	458	CB	LYS	59	139.629	20.365	26.837	1.00	111.76	1SG	459
ATOM	459	CG	LYS	59	138.524	19.887	25.894	1.00	111.76	1SG	460
ATOM	460	CD	LYS	59	138.351	20.789	24.670	1.00	111.76	1SG	461
ATOM	461	CE	LYS	59	138.546	22.279	24.966	1.00	111.76	1SG	462
ATOM	462	NZ	LYS	59	137.460	22.778	25.838	1.00	111.76	1SG	463
ATOM	463	C	LYS	59	140.292	18.240	27.824	1.00	111.76	1SG	464
ATOM	464	O	LYS	59	139.578	17.241	27.808	1.00	111.76	1SG	465
ATOM	465	N	LEU	60	141.615	18.181	27.593	1.00	40.38	1SG	466
ATOM	466	CA	LEU	60	142.261	16.974	27.167	1.00	40.38	1SG	467
ATOM	467	CB	LEU	60	143.766	17.178	26.920	1.00	40.38	1SG	468
ATOM	468	CG	LEU	60	144.497	15.928	26.399	1.00	40.38	1SG	469
ATOM	469	CD2	LEU	60	146.021	16.132	26.413	1.00	40.38	1SG	470
ATOM	470	CD1	LEU	60	143.970	15.509	25.017	1.00	40.38	1SG	471
ATOM	471	C	LEU	60	142.084	15.927	28.222	1.00	40.38	1SG	472
ATOM	472	O	LEU	60	141.844	14.762	27.909	1.00	40.38	1SG	473
ATOM	473	N	LEU	61	142.180	16.316	29.507	1.00	86.80	1SG	474
ATOM	474	CA	LEU	61	142.046	15.355	30.565	1.00	86.80	1SG	475
ATOM	475	CB	LEU	61	142.236	15.940	31.974	1.00	86.80	1SG	476
ATOM	476	CG	LEU	61	143.711	16.167	32.348	1.00	86.80	1SG	477
ATOM	477	CD2	LEU	61	143.848	16.613	33.812	1.00	86.80	1SG	478
ATOM	478	CD1	LEU	61	144.410	17.115	31.369	1.00	86.80	1SG	479
ATOM	479	C	LEU	61	140.689	14.735	30.509	1.00	86.80	1SG	480
ATOM	480	O	LEU	61	140.541	13.534	30.728	1.00	86.80	1SG	481
ATOM	481	N	PHE	62	139.657	15.536	30.203	1.00	93.35	1SG	482
ATOM	482	CA	PHE	62	138.325	15.011	30.162	1.00	93.35	1SG	483
ATOM	483	CB	PHE	62	137.255	16.064	29.816	1.00	93.35	1SG	484
ATOM	484	CG	PHE	62	137.085	16.967	30.989	1.00	93.35	1SG	485
ATOM	485	CD1	PHE	62	136.320	16.571	32.062	1.00	93.35	1SG	486
ATOM	486	CD2	PHE	62	137.675	18.209	31.017	1.00	93.35	1SG	487
ATOM	487	CE1	PHE	62	136.154	17.395	33.150	1.00	93.35	1SG	488
ATOM	488	CE2	PHE	62	137.513	19.038	32.103	1.00	93.35	1SG	489
ATOM	489	CZ	PHE	62	136.752	18.632	33.172	1.00	93.35	1SG	490
ATOM	490	C	PHE	62	138.244	13.953	29.114	1.00	93.35	1SG	491
ATOM	491	O	PHE	62	137.636	12.908	29.340	1.00	93.35	1SG	492
ATOM	492	N	LEU	63	138.844	14.184	27.930	1.00	98.65	1SG	493
ATOM	493	CA	LEU	63	138.727	13.172	26.923	1.00	98.65	1SG	494
ATOM	494	CB	LEU	63	139.404	13.538	25.589	1.00	98.65	1SG	495
ATOM	495	CG	LEU	63	138.666	14.641	24.806	1.00	98.65	1SG	496

Supplementary material 1.txt

ATOM	496	CD2	LEU	63	138.609	15.956	25.593	1.00	98.65	1SG	497
ATOM	497	CD1	LEU	63	137.275	14.170	24.354	1.00	98.65	1SG	498
ATOM	498	C	LEU	63	139.364	11.930	27.448	1.00	98.65	1SG	499
ATOM	499	O	LEU	63	138.770	10.856	27.384	1.00	98.65	1SG	500
ATOM	500	N	SER	64	140.583	12.058	28.007	1.00166.68		1SG	501
ATOM	501	CA	SER	64	141.270	10.932	28.568	1.00166.68		1SG	502
ATOM	502	CB	SER	64	140.569	10.364	29.818	1.00166.68		1SG	503
ATOM	503	OG	SER	64	141.289	9.252	30.332	1.00166.68		1SG	504
ATOM	504	C	SER	64	141.318	9.884	27.514	1.00166.68		1SG	505
ATOM	505	O	SER	64	141.283	8.691	27.814	1.00166.68		1SG	506
ATOM	506	N	ASP	65	141.362	10.332	26.245	1.00203.79		1SG	507
ATOM	507	CA	ASP	65	141.425	9.456	25.115	1.00203.79		1SG	508
ATOM	508	CB	ASP	65	140.060	9.175	24.463	1.00203.79		1SG	509
ATOM	509	CG	ASP	65	139.253	8.262	25.375	1.00203.79		1SG	510
ATOM	510	OD1	ASP	65	139.774	7.174	25.740	1.00203.79		1SG	511
ATOM	511	OD2	ASP	65	138.098	8.636	25.708	1.00203.79		1SG	512
ATOM	512	C	ASP	65	142.245	10.154	24.082	1.00203.79		1SG	513
ATOM	513	O	ASP	65	142.322	11.381	24.062	1.00203.79		1SG	514
ATOM	514	N	MET	66	142.902	9.378	23.202	1.00	93.81	1SG	515
ATOM	515	CA	MET	66	143.659	9.999	22.158	1.00	93.81	1SG	516
ATOM	516	CB	MET	66	144.364	8.990	21.234	1.00	93.81	1SG	517
ATOM	517	CG	MET	66	145.465	8.172	21.914	1.00	93.81	1SG	518
ATOM	518	SD	MET	66	146.293	6.982	20.815	1.00	93.81	1SG	519
ATOM	519	CE	MET	66	147.295	6.193	22.108	1.00	93.81	1SG	520
ATOM	520	C	MET	66	142.676	10.746	21.319	1.00	93.81	1SG	521
ATOM	521	O	MET	66	142.910	11.891	20.933	1.00	93.81	1SG	522
ATOM	522	N	ASP	67	141.524	10.109	21.036	1.00180.14		1SG	523
ATOM	523	CA	ASP	67	140.519	10.732	20.227	1.00180.14		1SG	524
ATOM	524	CB	ASP	67	139.514	9.737	19.621	1.00180.14		1SG	525
ATOM	525	CG	ASP	67	138.705	10.449	18.545	1.00180.14		1SG	526
ATOM	526	OD1	ASP	67	139.148	11.535	18.084	1.00180.14		1SG	527
ATOM	527	OD2	ASP	67	137.636	9.905	18.161	1.00180.14		1SG	528
ATOM	528	C	ASP	67	139.748	11.653	21.109	1.00180.14		1SG	529
ATOM	529	O	ASP	67	139.896	11.632	22.330	1.00180.14		1SG	530
ATOM	530	N	ASP	68	138.908	12.511	20.502	1.00113.19		1SG	531
ATOM	531	CA	ASP	68	138.123	13.401	21.297	1.00113.19		1SG	532
ATOM	532	CB	ASP	68	137.807	14.724	20.583	1.00113.19		1SG	533
ATOM	533	CG	ASP	68	139.107	15.486	20.380	1.00113.19		1SG	534
ATOM	534	OD1	ASP	68	139.901	15.590	21.353	1.00113.19		1SG	535
ATOM	535	OD2	ASP	68	139.318	15.984	19.242	1.00113.19		1SG	536
ATOM	536	C	ASP	68	136.818	12.717	21.521	1.00113.19		1SG	537
ATOM	537	O	ASP	68	135.758	13.336	21.440	1.00113.19		1SG	538
ATOM	538	N	SER	69	136.865	11.409	21.825	1.00133.57		1SG	539
ATOM	539	CA	SER	69	135.643	10.710	22.073	1.00133.57		1SG	540
ATOM	540	CB	SER	69	135.537	9.367	21.331	1.00133.57		1SG	541
ATOM	541	OG	SER	69	135.503	9.586	19.928	1.00133.57		1SG	542
ATOM	542	C	SER	69	135.633	10.420	23.532	1.00133.57		1SG	543
ATOM	543	O	SER	69	136.657	10.051	24.105	1.00133.57		1SG	544
ATOM	544	N	CYS	70	134.470	10.598	24.181	1.00	90.08	1SG	545
ATOM	545	CA	CYS	70	134.440	10.363	25.590	1.00	90.08	1SG	546
ATOM	546	CB	CYS	70	133.252	11.034	26.303	1.00	90.08	1SG	547
ATOM	547	SG	CYS	70	131.635	10.490	25.672	1.00	90.08	1SG	548
ATOM	548	C	CYS	70	134.362	8.892	25.818	1.00	90.08	1SG	549
ATOM	549	O	CYS	70	133.388	8.235	25.454	1.00	90.08	1SG	550
ATOM	550	N	ASN	71	135.429	8.330	26.412	1.00159.29		1SG	551
ATOM	551	CA	ASN	71	135.428	6.939	26.730	1.00159.29		1SG	552
ATOM	552	CB	ASN	71	136.254	6.084	25.757	1.00159.29		1SG	553
ATOM	553	CG	ASN	71	135.858	4.632	25.993	1.00159.29		1SG	554
ATOM	554	OD1	ASN	71	136.673	3.718	25.892	1.00159.29		1SG	555
ATOM	555	ND2	ASN	71	134.555	4.408	26.312	1.00159.29		1SG	556
ATOM	556	C	ASN	71	136.079	6.831	28.065	1.00159.29		1SG	557
ATOM	557	O	ASN	71	135.733	5.967	28.870	1.00159.29		1SG	558
ATOM	558	N	ASP	72	137.023	7.758	28.335	1.00192.67		1SG	559
ATOM	559	CA	ASP	72	137.768	7.721	29.557	1.00192.67		1SG	560
ATOM	560	CB	ASP	72	136.903	7.984	30.799	1.00192.67		1SG	561
ATOM	561	CG	ASP	72	136.508	9.455	30.784	1.00192.67		1SG	562
ATOM	562	OD1	ASP	72	137.222	10.253	30.119	1.00192.67		1SG	563
ATOM	563	OD2	ASP	72	135.489	9.803	31.437	1.00192.67		1SG	564
ATOM	564	C	ASP	72	138.335	6.350	29.636	1.00192.67		1SG	565
ATOM	565	O	ASP	72	138.267	5.681	30.667	1.00192.67		1SG	566
ATOM	566	N	SER	73	138.917	5.908	28.509	1.00121.09		1SG	567

Supplementary material 1.txt

ATOM	567	CA	SER	73	139.420	4.575	28.398	1.00121.09	1SG	568
ATOM	568	CB	SER	73	140.084	4.304	27.039	1.00121.09	1SG	569
ATOM	569	OG	SER	73	139.137	4.469	25.995	1.00121.09	1SG	570
ATOM	570	C	SER	73	140.458	4.348	29.444	1.00121.09	1SG	571
ATOM	571	O	SER	73	140.340	3.444	30.269	1.00121.09	1SG	572
ATOM	572	N	ASP	74	141.503	5.190	29.446	1.00 73.81	1SG	573
ATOM	573	CA	ASP	74	142.577	5.022	30.376	1.00 73.81	1SG	574
ATOM	574	CB	ASP	74	143.715	6.034	30.138	1.00 73.81	1SG	575
ATOM	575	CG	ASP	74	144.863	5.757	31.104	1.00 73.81	1SG	576
ATOM	576	OD1	ASP	74	144.649	5.853	32.343	1.00 73.81	1SG	577
ATOM	577	OD2	ASP	74	145.983	5.461	30.609	1.00 73.81	1SG	578
ATOM	578	C	ASP	74	142.047	5.243	31.752	1.00 73.81	1SG	579
ATOM	579	O	ASP	74	142.424	4.550	32.695	1.00 73.81	1SG	580
ATOM	580	N	ARG	75	141.136	6.219	31.887	1.00118.30	1SG	581
ATOM	581	CA	ARG	75	140.642	6.633	33.165	1.00118.30	1SG	582
ATOM	582	CB	ARG	75	139.894	7.969	33.077	1.00118.30	1SG	583
ATOM	583	CG	ARG	75	139.616	8.628	34.422	1.00118.30	1SG	584
ATOM	584	CD	ARG	75	138.837	9.931	34.272	1.00118.30	1SG	585
ATOM	585	NE	ARG	75	139.608	10.811	33.353	1.00118.30	1SG	586
ATOM	586	CZ	ARG	75	140.620	11.574	33.851	1.00118.30	1SG	587
ATOM	587	NH1	ARG	75	140.955	11.471	35.171	1.00118.30	1SG	588
ATOM	588	NH2	ARG	75	141.296	12.434	33.036	1.00118.30	1SG	589
ATOM	589	C	ARG	75	139.696	5.621	33.734	1.00118.30	1SG	590
ATOM	590	O	ARG	75	138.945	4.969	33.011	1.00118.30	1SG	591
ATOM	591	N	ASP	76	139.727	5.471	35.076	1.00 34.83	1SG	592
ATOM	592	CA	ASP	76	138.856	4.571	35.780	1.00 34.83	1SG	593
ATOM	593	CB	ASP	76	139.366	4.214	37.188	1.00 34.83	1SG	594
ATOM	594	CG	ASP	76	140.664	3.433	37.048	1.00 34.83	1SG	595
ATOM	595	OD1	ASP	76	140.969	2.994	35.908	1.00 34.83	1SG	596
ATOM	596	OD2	ASP	76	141.367	3.267	38.080	1.00 34.83	1SG	597
ATOM	597	C	ASP	76	137.546	5.276	35.965	1.00 34.83	1SG	598
ATOM	598	O	ASP	76	137.439	6.478	35.730	1.00 34.83	1SG	599
ATOM	599	N	LEU	77	136.499	4.531	36.377	1.00103.14	1SG	600
ATOM	600	CA	LEU	77	135.211	5.126	36.595	1.00103.14	1SG	601
ATOM	601	CB	LEU	77	134.133	4.068	36.928	1.00103.14	1SG	602
ATOM	602	CG	LEU	77	132.669	4.564	37.033	1.00103.14	1SG	603
ATOM	603	CD2	LEU	77	132.463	5.657	38.092	1.00103.14	1SG	604
ATOM	604	CD1	LEU	77	131.725	3.384	37.296	1.00103.14	1SG	605
ATOM	605	C	LEU	77	135.343	6.075	37.744	1.00103.14	1SG	606
ATOM	606	O	LEU	77	134.873	7.210	37.684	1.00103.14	1SG	607
ATOM	607	N	ILE	78	136.033	5.635	38.811	1.00 93.27	1SG	608
ATOM	608	CA	ILE	78	136.156	6.419	40.005	1.00 93.27	1SG	609
ATOM	609	CB	ILE	78	137.030	5.758	41.031	1.00 93.27	1SG	610
ATOM	610	CG2	ILE	78	137.064	6.672	42.268	1.00 93.27	1SG	611
ATOM	611	CG1	ILE	78	136.558	4.325	41.327	1.00 93.27	1SG	612
ATOM	612	CD1	ILE	78	135.129	4.234	41.850	1.00 93.27	1SG	613
ATOM	613	C	ILE	78	136.864	7.688	39.653	1.00 93.27	1SG	614
ATOM	614	O	ILE	78	136.449	8.775	40.052	1.00 93.27	1SG	615
ATOM	615	N	LYS	79	137.961	7.572	38.882	1.00132.37	1SG	616
ATOM	616	CA	LYS	79	138.764	8.712	38.543	1.00132.37	1SG	617
ATOM	617	CB	LYS	79	140.036	8.346	37.761	1.00132.37	1SG	618
ATOM	618	CG	LYS	79	141.016	9.515	37.632	1.00132.37	1SG	619
ATOM	619	CD	LYS	79	141.654	9.920	38.963	1.00132.37	1SG	620
ATOM	620	CE	LYS	79	140.658	10.516	39.961	1.00132.37	1SG	621
ATOM	621	NZ	LYS	79	141.344	10.828	41.235	1.00132.37	1SG	622
ATOM	622	C	LYS	79	137.968	9.659	37.698	1.00132.37	1SG	623
ATOM	623	O	LYS	79	138.074	10.874	37.856	1.00132.37	1SG	624
ATOM	624	N	ARG	80	137.156	9.123	36.767	1.00164.81	1SG	625
ATOM	625	CA	ARG	80	136.375	9.945	35.883	1.00164.81	1SG	626
ATOM	626	CB	ARG	80	135.519	9.116	34.913	1.00164.81	1SG	627
ATOM	627	CG	ARG	80	134.607	9.973	34.032	1.00164.81	1SG	628
ATOM	628	CD	ARG	80	133.367	9.240	33.507	1.00164.81	1SG	629
ATOM	629	NE	ARG	80	133.809	8.118	32.630	1.00164.81	1SG	630
ATOM	630	CZ	ARG	80	134.077	6.886	33.156	1.00164.81	1SG	631
ATOM	631	NH1	ARG	80	133.983	6.676	34.501	1.00164.81	1SG	632
ATOM	632	NH2	ARG	80	134.441	5.862	32.329	1.00164.81	1SG	633
ATOM	633	C	ARG	80	135.404	10.759	36.675	1.00164.81	1SG	634
ATOM	634	O	ARG	80	135.237	11.953	36.430	1.00164.81	1SG	635
ATOM	635	N	LEU	81	134.723	10.121	37.642	1.00 52.45	1SG	636
ATOM	636	CA	LEU	81	133.731	10.804	38.424	1.00 52.45	1SG	637
ATOM	637	CB	LEU	81	132.992	9.880	39.413	1.00 52.45	1SG	638

Supplementary material 1.txt

ATOM	638	CG	LEU	81	132.211	8.734	38.740	1.00	52.45	1SG	639
ATOM	639	CD2	LEU	81	131.288	9.254	37.627	1.00	52.45	1SG	640
ATOM	640	CD1	LEU	81	131.467	7.883	39.780	1.00	52.45	1SG	641
ATOM	641	C	LEU	81	134.398	11.863	39.242	1.00	52.45	1SG	642
ATOM	642	O	LEU	81	133.881	12.970	39.386	1.00	52.45	1SG	643
ATOM	643	N	GLU	82	135.572	11.540	39.811	1.00	65.26	1SG	644
ATOM	644	CA	GLU	82	136.257	12.465	40.665	1.00	65.26	1SG	645
ATOM	645	CB	GLU	82	137.527	11.866	41.290	1.00	65.26	1SG	646
ATOM	646	CG	GLU	82	137.239	10.752	42.297	1.00	65.26	1SG	647
ATOM	647	CD	GLU	82	136.596	11.387	43.522	1.00	65.26	1SG	648
ATOM	648	OE1	GLU	82	136.884	12.584	43.788	1.00	65.26	1SG	649
ATOM	649	OE2	GLU	82	135.805	10.683	44.205	1.00	65.26	1SG	650
ATOM	650	C	GLU	82	136.670	13.666	39.877	1.00	65.26	1SG	651
ATOM	651	O	GLU	82	136.548	14.793	40.354	1.00	65.26	1SG	652
ATOM	652	N	ILE	83	137.170	13.468	38.643	1.00	85.41	1SG	653
ATOM	653	CA	ILE	83	137.637	14.596	37.888	1.00	85.41	1SG	654
ATOM	654	CB	ILE	83	138.328	14.219	36.604	1.00	85.41	1SG	655
ATOM	655	CG2	ILE	83	137.311	13.571	35.653	1.00	85.41	1SG	656
ATOM	656	CG1	ILE	83	139.045	15.443	36.012	1.00	85.41	1SG	657
ATOM	657	CD1	ILE	83	140.031	15.093	34.899	1.00	85.41	1SG	658
ATOM	658	C	ILE	83	136.490	15.513	37.575	1.00	85.41	1SG	659
ATOM	659	O	ILE	83	136.600	16.725	37.756	1.00	85.41	1SG	660
ATOM	660	N	VAL	84	135.346	14.961	37.122	1.00	95.11	1SG	661
ATOM	661	CA	VAL	84	134.218	15.778	36.774	1.00	95.11	1SG	662
ATOM	662	CB	VAL	84	133.071	15.008	36.182	1.00	95.11	1SG	663
ATOM	663	CG1	VAL	84	133.540	14.371	34.863	1.00	95.11	1SG	664
ATOM	664	CG2	VAL	84	132.556	13.995	37.216	1.00	95.11	1SG	665
ATOM	665	C	VAL	84	133.723	16.494	37.993	1.00	95.11	1SG	666
ATOM	666	O	VAL	84	133.338	17.660	37.925	1.00	95.11	1SG	667
ATOM	667	N	ASP	85	133.710	15.811	39.151	1.00	49.31	1SG	668
ATOM	668	CA	ASP	85	133.221	16.404	40.365	1.00	49.31	1SG	669
ATOM	669	CB	ASP	85	133.251	15.415	41.545	1.00	49.31	1SG	670
ATOM	670	CG	ASP	85	132.544	16.044	42.737	1.00	49.31	1SG	671
ATOM	671	OD1	ASP	85	131.936	17.133	42.562	1.00	49.31	1SG	672
ATOM	672	OD2	ASP	85	132.607	15.444	43.843	1.00	49.31	1SG	673
ATOM	673	C	ASP	85	134.085	17.579	40.739	1.00	49.31	1SG	674
ATOM	674	O	ASP	85	133.576	18.641	41.098	1.00	49.31	1SG	675
ATOM	675	N	THR	86	135.421	17.418	40.651	1.00	108.62	1SG	676
ATOM	676	CA	THR	86	136.350	18.439	41.054	1.00	108.62	1SG	677
ATOM	677	CB	THR	86	137.776	17.978	40.997	1.00	108.62	1SG	678
ATOM	678	OG1	THR	86	138.139	17.666	39.660	1.00	108.62	1SG	679
ATOM	679	CG2	THR	86	137.925	16.736	41.891	1.00	108.62	1SG	680
ATOM	680	C	THR	86	136.229	19.643	40.173	1.00	108.62	1SG	681
ATOM	681	O	THR	86	136.226	20.776	40.656	1.00	108.62	1SG	682
ATOM	682	N	VAL	87	136.123	19.426	38.848	1.00	99.85	1SG	683
ATOM	683	CA	VAL	87	136.058	20.517	37.923	1.00	99.85	1SG	684
ATOM	684	CB	VAL	87	136.014	20.080	36.484	1.00	99.85	1SG	685
ATOM	685	CG1	VAL	87	137.294	19.285	36.177	1.00	99.85	1SG	686
ATOM	686	CG2	VAL	87	134.708	19.313	36.225	1.00	99.85	1SG	687
ATOM	687	C	VAL	87	134.817	21.308	38.197	1.00	99.85	1SG	688
ATOM	688	O	VAL	87	134.821	22.533	38.086	1.00	99.85	1SG	689
ATOM	689	N	GLU	88	133.706	20.620	38.527	1.00	49.07	1SG	690
ATOM	690	CA	GLU	88	132.454	21.279	38.779	1.00	49.07	1SG	691
ATOM	691	CB	GLU	88	131.287	20.279	38.898	1.00	49.07	1SG	692
ATOM	692	CG	GLU	88	131.021	19.548	37.576	1.00	49.07	1SG	693
ATOM	693	CD	GLU	88	129.862	18.574	37.750	1.00	49.07	1SG	694
ATOM	694	OE1	GLU	88	129.373	18.425	38.901	1.00	49.07	1SG	695
ATOM	695	OE2	GLU	88	129.449	17.967	36.725	1.00	49.07	1SG	696
ATOM	696	C	GLU	88	132.529	22.118	40.025	1.00	49.07	1SG	697
ATOM	697	O	GLU	88	132.084	23.265	40.029	1.00	49.07	1SG	698
ATOM	698	N	CYS	89	133.123	21.582	41.108	1.00	48.53	1SG	699
ATOM	699	CA	CYS	89	133.202	22.274	42.369	1.00	48.53	1SG	700
ATOM	700	CB	CYS	89	133.819	21.412	43.481	1.00	48.53	1SG	701
ATOM	701	SG	CYS	89	132.781	19.979	43.896	1.00	48.53	1SG	702
ATOM	702	C	CYS	89	134.063	23.497	42.214	1.00	48.53	1SG	703
ATOM	703	O	CYS	89	133.869	24.507	42.892	1.00	48.53	1SG	704
ATOM	704	N	LEU	90	135.071	23.402	41.330	1.00	83.96	1SG	705
ATOM	705	CA	LEU	90	136.021	24.443	41.041	1.00	83.96	1SG	706
ATOM	706	CB	LEU	90	137.174	23.957	40.142	1.00	83.96	1SG	707
ATOM	707	CG	LEU	90	138.071	22.912	40.832	1.00	83.96	1SG	708
ATOM	708	CD2	LEU	90	138.581	23.427	42.188	1.00	83.96	1SG	709

Supplementary material 1.txt

ATOM	709	CD1	LEU	90	139.211	22.449	39.909	1.00	83.96	1SG	710
ATOM	710	C	LEU	90	135.334	25.595	40.362	1.00	83.96	1SG	711
ATOM	711	O	LEU	90	135.869	26.703	40.340	1.00	83.96	1SG	712
ATOM	712	N	GLY	91	134.180	25.345	39.706	1.00	47.68	1SG	713
ATOM	713	CA	GLY	91	133.406	26.401	39.101	1.00	47.68	1SG	714
ATOM	714	C	GLY	91	133.805	26.603	37.664	1.00	47.68	1SG	715
ATOM	715	O	GLY	91	133.378	27.565	37.028	1.00	47.68	1SG	716
ATOM	716	N	ILE	92	134.719	25.755	37.164	1.00	117.17	1SG	717
ATOM	717	CA	ILE	92	135.236	25.699	35.820	1.00	117.17	1SG	718
ATOM	718	CB	ILE	92	136.631	25.145	35.752	1.00	117.17	1SG	719
ATOM	719	CG2	ILE	92	137.551	26.140	36.476	1.00	117.17	1SG	720
ATOM	720	CG1	ILE	92	136.698	23.710	36.294	1.00	117.17	1SG	721
ATOM	721	CD1	ILE	92	138.069	23.063	36.100	1.00	117.17	1SG	722
ATOM	722	C	ILE	92	134.353	24.987	34.829	1.00	117.17	1SG	723
ATOM	723	O	ILE	92	134.500	25.181	33.625	1.00	117.17	1SG	724
ATOM	724	N	ASP	93	133.456	24.101	35.303	1.00	135.79	1SG	725
ATOM	725	CA	ASP	93	132.691	23.167	34.511	1.00	135.79	1SG	726
ATOM	726	CB	ASP	93	131.664	22.384	35.348	1.00	135.79	1SG	727
ATOM	727	CG	ASP	93	131.033	21.327	34.453	1.00	135.79	1SG	728
ATOM	728	OD1	ASP	93	131.753	20.796	33.566	1.00	135.79	1SG	729
ATOM	729	OD2	ASP	93	129.825	21.028	34.651	1.00	135.79	1SG	730
ATOM	730	C	ASP	93	131.929	23.820	33.389	1.00	135.79	1SG	731
ATOM	731	O	ASP	93	131.636	23.168	32.389	1.00	135.79	1SG	732
ATOM	732	N	ARG	94	131.585	25.111	33.501	1.00	178.21	1SG	733
ATOM	733	CA	ARG	94	130.780	25.788	32.518	1.00	178.21	1SG	734
ATOM	734	CB	ARG	94	130.586	27.283	32.814	1.00	178.21	1SG	735
ATOM	735	CG	ARG	94	129.885	28.002	31.663	1.00	178.21	1SG	736
ATOM	736	CD	ARG	94	130.006	29.524	31.707	1.00	178.21	1SG	737
ATOM	737	NE	ARG	94	131.446	29.877	31.559	1.00	178.21	1SG	738
ATOM	738	CZ	ARG	94	132.132	30.416	32.608	1.00	178.21	1SG	739
ATOM	739	NH1	ARG	94	131.495	30.669	33.789	1.00	178.21	1SG	740
ATOM	740	NH2	ARG	94	133.457	30.716	32.473	1.00	178.21	1SG	741
ATOM	741	C	ARG	94	131.413	25.723	31.156	1.00	178.21	1SG	742
ATOM	742	O	ARG	94	130.706	25.817	30.154	1.00	178.21	1SG	743
ATOM	743	N	HIS	95	132.757	25.662	31.076	1.00	82.00	1SG	744
ATOM	744	CA	HIS	95	133.461	25.612	29.820	1.00	82.00	1SG	745
ATOM	745	ND1	HIS	95	135.405	28.283	29.918	1.00	82.00	1SG	746
ATOM	746	CG	HIS	95	135.354	27.097	30.616	1.00	82.00	1SG	747
ATOM	747	CB	HIS	95	134.980	25.777	30.005	1.00	82.00	1SG	748
ATOM	748	NE2	HIS	95	135.969	28.759	32.015	1.00	82.00	1SG	749
ATOM	749	CD2	HIS	95	135.700	27.407	31.897	1.00	82.00	1SG	750
ATOM	750	CE1	HIS	95	135.778	29.243	30.801	1.00	82.00	1SG	751
ATOM	751	C	HIS	95	133.226	24.301	29.107	1.00	82.00	1SG	752
ATOM	752	O	HIS	95	133.180	24.235	27.881	1.00	82.00	1SG	753
ATOM	753	N	PHE	96	133.159	23.226	29.901	1.00	161.01	1SG	754
ATOM	754	CA	PHE	96	133.067	21.818	29.628	1.00	161.01	1SG	755
ATOM	755	CB	PHE	96	133.850	21.007	30.655	1.00	161.01	1SG	756
ATOM	756	CG	PHE	96	135.245	21.438	30.400	1.00	161.01	1SG	757
ATOM	757	CD1	PHE	96	135.968	20.867	29.382	1.00	161.01	1SG	758
ATOM	758	CD2	PHE	96	135.815	22.426	31.162	1.00	161.01	1SG	759
ATOM	759	CE1	PHE	96	137.255	21.268	29.130	1.00	161.01	1SG	760
ATOM	760	CE2	PHE	96	137.101	22.831	30.914	1.00	161.01	1SG	761
ATOM	761	CZ	PHE	96	137.824	22.250	29.900	1.00	161.01	1SG	762
ATOM	762	C	PHE	96	131.713	21.211	29.415	1.00	161.01	1SG	763
ATOM	763	O	PHE	96	131.639	19.988	29.429	1.00	161.01	1SG	764
ATOM	764	N	GLN	97	130.607	21.973	29.345	1.00	122.07	1SG	765
ATOM	765	CA	GLN	97	129.288	21.387	29.358	1.00	122.07	1SG	766
ATOM	766	CB	GLN	97	128.199	22.422	29.027	1.00	122.07	1SG	767
ATOM	767	CG	GLN	97	128.216	23.641	29.952	1.00	122.07	1SG	768
ATOM	768	CD	GLN	97	127.919	23.174	31.367	1.00	122.07	1SG	769
ATOM	769	OE1	GLN	97	128.828	23.009	32.179	1.00	122.07	1SG	770
ATOM	770	NE2	GLN	97	126.613	22.947	31.672	1.00	122.07	1SG	771
ATOM	771	C	GLN	97	129.143	20.261	28.362	1.00	122.07	1SG	772
ATOM	772	O	GLN	97	128.588	19.230	28.735	1.00	122.07	1SG	773
ATOM	773	N	PRO	98	129.568	20.358	27.132	1.00	158.43	1SG	774
ATOM	774	CA	PRO	98	129.420	19.219	26.261	1.00	158.43	1SG	775
ATOM	775	CD	PRO	98	129.480	21.613	26.402	1.00	158.43	1SG	776
ATOM	776	CB	PRO	98	129.655	19.746	24.847	1.00	158.43	1SG	777
ATOM	777	CG	PRO	98	129.221	21.222	24.937	1.00	158.43	1SG	778
ATOM	778	C	PRO	98	130.242	18.005	26.606	1.00	158.43	1SG	779
ATOM	779	O	PRO	98	129.722	16.894	26.515	1.00	158.43	1SG	780

Supplementary material 1.txt

ATOM	780	N	GLU	99	131.515	18.186	27.011	1.00	79.18	1SG	781
ATOM	781	CA	GLU	99	132.391	17.082	27.292	1.00	79.18	1SG	782
ATOM	782	CB	GLU	99	133.828	17.520	27.625	1.00	79.18	1SG	783
ATOM	783	CG	GLU	99	134.606	18.052	26.419	1.00	79.18	1SG	784
ATOM	784	CD	GLU	99	134.127	19.465	26.113	1.00	79.18	1SG	785
ATOM	785	OE1	GLU	99	133.416	20.053	26.972	1.00	79.18	1SG	786
ATOM	786	OE2	GLU	99	134.470	19.976	25.014	1.00	79.18	1SG	787
ATOM	787	C	GLU	99	131.877	16.311	28.467	1.00	79.18	1SG	788
ATOM	788	O	GLU	99	131.847	15.082	28.443	1.00	79.18	1SG	789
ATOM	789	N	ILE	100	131.452	17.015	29.530	1.00106.18		1SG	790
ATOM	790	CA	ILE	100	130.958	16.353	30.701	1.00106.18		1SG	791
ATOM	791	CB	ILE	100	130.655	17.262	31.858	1.00106.18		1SG	792
ATOM	792	CG2	ILE	100	129.655	16.537	32.772	1.00106.18		1SG	793
ATOM	793	CG1	ILE	100	131.947	17.661	32.585	1.00106.18		1SG	794
ATOM	794	CD1	ILE	100	132.934	18.434	31.730	1.00106.18		1SG	795
ATOM	795	C	ILE	100	129.712	15.592	30.389	1.00106.18		1SG	796
ATOM	796	O	ILE	100	129.513	14.497	30.910	1.00106.18		1SG	797
ATOM	797	N	LYS	101	128.826	16.157	29.551	1.00123.20		1SG	798
ATOM	798	CA	LYS	101	127.577	15.504	29.289	1.00123.20		1SG	799
ATOM	799	CB	LYS	101	126.669	16.314	28.349	1.00123.20		1SG	800
ATOM	800	CG	LYS	101	125.274	15.710	28.172	1.00123.20		1SG	801
ATOM	801	CD	LYS	101	124.274	16.658	27.505	1.00123.20		1SG	802
ATOM	802	CE	LYS	101	123.896	17.859	28.373	1.00123.20		1SG	803
ATOM	803	NZ	LYS	101	123.191	17.402	29.591	1.00123.20		1SG	804
ATOM	804	C	LYS	101	127.816	14.171	28.649	1.00123.20		1SG	805
ATOM	805	O	LYS	101	127.259	13.160	29.076	1.00123.20		1SG	806
ATOM	806	N	LEU	102	128.695	14.124	27.634	1.00	40.72	1SG	807
ATOM	807	CA	LEU	102	128.896	12.910	26.898	1.00	40.72	1SG	808
ATOM	808	CB	LEU	102	129.896	13.076	25.740	1.00	40.72	1SG	809
ATOM	809	CG	LEU	102	129.418	14.066	24.661	1.00	40.72	1SG	810
ATOM	810	CD2	LEU	102	128.008	13.709	24.160	1.00	40.72	1SG	811
ATOM	811	CD1	LEU	102	130.444	14.198	23.523	1.00	40.72	1SG	812
ATOM	812	C	LEU	102	129.421	11.845	27.808	1.00	40.72	1SG	813
ATOM	813	O	LEU	102	128.999	10.694	27.721	1.00	40.72	1SG	814
ATOM	814	N	ALA	103	130.361	12.196	28.705	1.00	35.92	1SG	815
ATOM	815	CA	ALA	103	130.953	11.214	29.571	1.00	35.92	1SG	816
ATOM	816	CB	ALA	103	132.063	11.799	30.460	1.00	35.92	1SG	817
ATOM	817	C	ALA	103	129.907	10.634	30.477	1.00	35.92	1SG	818
ATOM	818	O	ALA	103	129.843	9.420	30.666	1.00	35.92	1SG	819
ATOM	819	N	LEU	104	129.054	11.494	31.064	1.00	51.83	1SG	820
ATOM	820	CA	LEU	104	128.015	11.039	31.943	1.00	51.83	1SG	821
ATOM	821	CB	LEU	104	127.264	12.190	32.626	1.00	51.83	1SG	822
ATOM	822	CG	LEU	104	128.147	12.976	33.611	1.00	51.83	1SG	823
ATOM	823	CD2	LEU	104	128.798	12.050	34.652	1.00	51.83	1SG	824
ATOM	824	CD1	LEU	104	127.356	14.112	34.271	1.00	51.83	1SG	825
ATOM	825	C	LEU	104	127.040	10.256	31.132	1.00	51.83	1SG	826
ATOM	826	O	LEU	104	126.438	9.295	31.613	1.00	51.83	1SG	827
ATOM	827	N	ASP	105	126.848	10.692	29.873	1.00	88.00	1SG	828
ATOM	828	CA	ASP	105	125.978	10.046	28.937	1.00	88.00	1SG	829
ATOM	829	CB	ASP	105	125.914	10.757	27.572	1.00	88.00	1SG	830
ATOM	830	CG	ASP	105	124.983	11.958	27.653	1.00	88.00	1SG	831
ATOM	831	OD1	ASP	105	123.797	11.755	28.021	1.00	88.00	1SG	832
ATOM	832	OD2	ASP	105	125.431	13.089	27.323	1.00	88.00	1SG	833
ATOM	833	C	ASP	105	126.522	8.686	28.668	1.00	88.00	1SG	834
ATOM	834	O	ASP	105	125.759	7.768	28.404	1.00	88.00	1SG	835
ATOM	835	N	TYR	106	127.856	8.527	28.651	1.00	47.22	1SG	836
ATOM	836	CA	TYR	106	128.438	7.234	28.425	1.00	47.22	1SG	837
ATOM	837	CB	TYR	106	129.972	7.318	28.323	1.00	47.22	1SG	838
ATOM	838	CG	TYR	106	130.528	5.940	28.228	1.00	47.22	1SG	839
ATOM	839	CD1	TYR	106	130.576	5.282	27.022	1.00	47.22	1SG	840
ATOM	840	CD2	TYR	106	131.012	5.311	29.352	1.00	47.22	1SG	841
ATOM	841	CE1	TYR	106	131.095	4.011	26.940	1.00	47.22	1SG	842
ATOM	842	CE2	TYR	106	131.531	4.041	29.276	1.00	47.22	1SG	843
ATOM	843	CZ	TYR	106	131.571	3.390	28.068	1.00	47.22	1SG	844
ATOM	844	OH	TYR	106	132.104	2.086	27.988	1.00	47.22	1SG	845
ATOM	845	C	TYR	106	128.108	6.346	29.587	1.00	47.22	1SG	846
ATOM	846	O	TYR	106	127.656	5.215	29.414	1.00	47.22	1SG	847
ATOM	847	N	VAL	107	128.315	6.865	30.813	1.00	43.46	1SG	848
ATOM	848	CA	VAL	107	128.099	6.109	32.015	1.00	43.46	1SG	849
ATOM	849	CB	VAL	107	128.478	6.870	33.251	1.00	43.46	1SG	850
ATOM	850	CG1	VAL	107	128.103	6.029	34.483	1.00	43.46	1SG	851

Supplementary material 1.txt

ATOM	851	CG2	VAL	107	129.971	7.226	33.166	1.00	43.46	1SG	852
ATOM	852	C	VAL	107	126.643	5.769	32.135	1.00	43.46	1SG	853
ATOM	853	O	VAL	107	126.285	4.655	32.512	1.00	43.46	1SG	854
ATOM	854	N	TYR	108	125.779	6.762	31.861	1.00111.39		1SG	855
ATOM	855	CA	TYR	108	124.342	6.694	31.922	1.00111.39		1SG	856
ATOM	856	CB	TYR	108	123.685	8.083	31.860	1.00111.39		1SG	857
ATOM	857	CG	TYR	108	122.206	7.894	31.822	1.00111.39		1SG	858
ATOM	858	CD1	TYR	108	121.497	7.632	32.972	1.00111.39		1SG	859
ATOM	859	CD2	TYR	108	121.526	7.990	30.630	1.00111.39		1SG	860
ATOM	860	CE1	TYR	108	120.133	7.460	32.929	1.00111.39		1SG	861
ATOM	861	CE2	TYR	108	120.163	7.819	30.580	1.00111.39		1SG	862
ATOM	862	CZ	TYR	108	119.464	7.556	31.733	1.00111.39		1SG	863
ATOM	863	OH	TYR	108	118.065	7.381	31.690	1.00111.39		1SG	864
ATOM	864	C	TYR	108	123.759	5.885	30.803	1.00111.39		1SG	865
ATOM	865	O	TYR	108	122.706	5.276	30.965	1.00111.39		1SG	866
ATOM	866	N	ARG	109	124.390	5.966	29.618	1.00265.47		1SG	867
ATOM	867	CA	ARG	109	124.040	5.348	28.365	1.00265.47		1SG	868
ATOM	868	CB	ARG	109	124.592	3.934	28.101	1.00265.47		1SG	869
ATOM	869	CG	ARG	109	126.037	3.910	27.603	1.00265.47		1SG	870
ATOM	870	CD	ARG	109	126.140	4.106	26.088	1.00265.47		1SG	871
ATOM	871	NE	ARG	109	127.581	4.065	25.712	1.00265.47		1SG	872
ATOM	872	CZ	ARG	109	127.952	4.233	24.409	1.00265.47		1SG	873
ATOM	873	NH1	ARG	109	127.010	4.487	23.453	1.00265.47		1SG	874
ATOM	874	NH2	ARG	109	129.269	4.153	24.059	1.00265.47		1SG	875
ATOM	875	C	ARG	109	122.572	5.370	28.114	1.00265.47		1SG	876
ATOM	876	O	ARG	109	121.895	4.352	28.248	1.00265.47		1SG	877
ATOM	877	N	CYS	110	122.034	6.549	27.752	1.00115.27		1SG	878
ATOM	878	CA	CYS	110	120.645	6.609	27.412	1.00115.27		1SG	879
ATOM	879	CB	CYS	110	120.129	8.038	27.171	1.00115.27		1SG	880
ATOM	880	SG	CYS	110	118.361	8.080	26.746	1.00115.27		1SG	881
ATOM	881	C	CYS	110	120.494	5.851	26.134	1.00115.27		1SG	882
ATOM	882	O	CYS	110	121.361	5.906	25.264	1.00115.27		1SG	883
ATOM	883	N	TRP	111	119.387	5.098	25.999	1.00271.66		1SG	884
ATOM	884	CA	TRP	111	119.184	4.325	24.810	1.00271.66		1SG	885
ATOM	885	CB	TRP	111	119.389	2.816	25.045	1.00271.66		1SG	886
ATOM	886	CG	TRP	111	119.268	1.933	23.826	1.00271.66		1SG	887
ATOM	887	CD2	TRP	111	119.065	0.514	23.900	1.00271.66		1SG	888
ATOM	888	CD1	TRP	111	119.319	2.246	22.498	1.00271.66		1SG	889
ATOM	889	NE1	TRP	111	119.162	1.110	21.741	1.00271.66		1SG	890
ATOM	890	CE2	TRP	111	119.004	0.036	22.592	1.00271.66		1SG	891
ATOM	891	CE3	TRP	111	118.939	-0.321	24.973	1.00271.66		1SG	892
ATOM	892	CZ2	TRP	111	118.816	-1.292	22.336	1.00271.66		1SG	893
ATOM	893	CZ3	TRP	111	118.749	-1.659	24.711	1.00271.66		1SG	894
ATOM	894	CH2	TRP	111	118.688	-2.135	23.417	1.00271.66		1SG	895
ATOM	895	C	TRP	111	117.760	4.526	24.402	1.00271.66		1SG	896
ATOM	896	O	TRP	111	116.926	4.929	25.210	1.00271.66		1SG	897
ATOM	897	N	ASN	112	117.451	4.272	23.116	1.00185.35		1SG	898
ATOM	898	CA	ASN	112	116.098	4.412	22.668	1.00185.35		1SG	899
ATOM	899	CB	ASN	112	115.969	4.820	21.189	1.00185.35		1SG	900
ATOM	900	CG	ASN	112	116.336	6.292	21.059	1.00185.35		1SG	901
ATOM	901	OD1	ASN	112	115.782	7.138	21.758	1.00185.35		1SG	902
ATOM	902	ND2	ASN	112	117.289	6.610	20.142	1.00185.35		1SG	903
ATOM	903	C	ASN	112	115.464	3.071	22.810	1.00185.35		1SG	904
ATOM	904	O	ASN	112	115.871	2.107	22.164	1.00185.35		1SG	905
ATOM	905	N	GLU	113	114.453	2.980	23.692	1.00318.80		1SG	906
ATOM	906	CA	GLU	113	113.777	1.738	23.905	1.00318.80		1SG	907
ATOM	907	CB	GLU	113	114.360	0.922	25.073	1.00318.80		1SG	908
ATOM	908	CG	GLU	113	113.862	-0.524	25.136	1.00318.80		1SG	909
ATOM	909	CD	GLU	113	114.583	-1.309	24.048	1.00318.80		1SG	910
ATOM	910	OE1	GLU	113	115.237	-0.660	23.188	1.00318.80		1SG	911
ATOM	911	OE2	GLU	113	114.491	-2.566	24.062	1.00318.80		1SG	912
ATOM	912	C	GLU	113	112.368	2.086	24.255	1.00318.80		1SG	913
ATOM	913	O	GLU	113	112.059	3.247	24.520	1.00318.80		1SG	914
ATOM	914	N	ARG	114	111.463	1.090	24.236	1.00269.60		1SG	915
ATOM	915	CA	ARG	114	110.111	1.381	24.604	1.00269.60		1SG	916
ATOM	916	CB	ARG	114	109.049	0.655	23.759	1.00269.60		1SG	917
ATOM	917	CG	ARG	114	107.611	0.981	24.171	1.00269.60		1SG	918
ATOM	918	CD	ARG	114	106.952	-0.097	25.035	1.00269.60		1SG	919
ATOM	919	NE	ARG	114	105.569	0.358	25.353	1.00269.60		1SG	920
ATOM	920	CZ	ARG	114	105.216	0.650	26.640	1.00269.60		1SG	921
ATOM	921	NH1	ARG	114	106.118	0.492	27.652	1.00269.60		1SG	922

Supplementary material 1.txt

ATOM	922	NH2	ARG	114	103.955	1.093	26.914	1.00269.60	1SG	923
ATOM	923	C	ARG	114	109.937	0.922	26.011	1.00269.60	1SG	924
ATOM	924	O	ARG	114	110.563	-0.045	26.444	1.00269.60	1SG	925
ATOM	925	N	GLY	115	109.091	1.635	26.775	1.00 77.20	1SG	926
ATOM	926	CA	GLY	115	108.861	1.254	28.135	1.00 77.20	1SG	927
ATOM	927	C	GLY	115	110.116	1.535	28.888	1.00 77.20	1SG	928
ATOM	928	O	GLY	115	110.816	2.508	28.613	1.00 77.20	1SG	929
ATOM	929	N	ILE	116	110.430	0.674	29.872	1.00 89.92	1SG	930
ATOM	930	CA	ILE	116	111.619	0.874	30.640	1.00 89.92	1SG	931
ATOM	931	CB	ILE	116	111.396	0.856	32.127	1.00 89.92	1SG	932
ATOM	932	CG2	ILE	116	110.918	-0.548	32.531	1.00 89.92	1SG	933
ATOM	933	CG1	ILE	116	112.665	1.320	32.863	1.00 89.92	1SG	934
ATOM	934	CD1	ILE	116	112.441	1.602	34.348	1.00 89.92	1SG	935
ATOM	935	C	ILE	116	112.552	-0.242	30.316	1.00 89.92	1SG	936
ATOM	936	O	ILE	116	112.156	-1.404	30.238	1.00 89.92	1SG	937
ATOM	937	N	GLY	117	113.830	0.105	30.084	1.00119.68	1SG	938
ATOM	938	CA	GLY	117	114.823	-0.878	29.783	1.00119.68	1SG	939
ATOM	939	C	GLY	117	116.103	-0.338	30.320	1.00119.68	1SG	940
ATOM	940	O	GLY	117	116.213	0.856	30.595	1.00119.68	1SG	941
ATOM	941	N	GLU	118	117.115	-1.209	30.482	1.00213.44	1SG	942
ATOM	942	CA	GLU	118	118.355	-0.742	31.021	1.00213.44	1SG	943
ATOM	943	CB	GLU	118	119.338	-1.867	31.384	1.00213.44	1SG	944
ATOM	944	CG	GLU	118	118.956	-2.655	32.639	1.00213.44	1SG	945
ATOM	945	CD	GLU	118	120.022	-3.724	32.837	1.00213.44	1SG	946
ATOM	946	OE1	GLU	118	120.783	-3.973	31.864	1.00213.44	1SG	947
ATOM	947	OE2	GLU	118	120.089	-4.306	33.952	1.00213.44	1SG	948
ATOM	948	C	GLU	118	119.019	0.119	30.000	1.00213.44	1SG	949
ATOM	949	O	GLU	118	118.964	-0.152	28.802	1.00213.44	1SG	950
ATOM	950	N	GLY	119	119.657	1.206	30.474	1.00141.15	1SG	951
ATOM	951	CA	GLY	119	120.388	2.085	29.613	1.00141.15	1SG	952
ATOM	952	C	GLY	119	121.462	2.674	30.464	1.00141.15	1SG	953
ATOM	953	O	GLY	119	121.167	3.328	31.463	1.00141.15	1SG	954
ATOM	954	N	SER	120	122.730	2.432	30.069	1.00283.87	1SG	955
ATOM	955	CA	SER	120	123.915	2.867	30.737	1.00283.87	1SG	956
ATOM	956	CB	SER	120	123.764	3.038	32.259	1.00283.87	1SG	957
ATOM	957	OG	SER	120	123.345	1.814	32.842	1.00283.87	1SG	958
ATOM	958	C	SER	120	124.951	1.836	30.513	1.00283.87	1SG	959
ATOM	959	O	SER	120	124.650	0.694	30.172	1.00283.87	1SG	960
ATOM	960	N	ARG	121	126.221	2.236	30.677	1.00150.12	1SG	961
ATOM	961	CA	ARG	121	127.244	1.248	30.647	1.00150.12	1SG	962
ATOM	962	CB	ARG	121	128.650	1.844	30.836	1.00150.12	1SG	963
ATOM	963	CG	ARG	121	129.796	0.908	30.443	1.00150.12	1SG	964
ATOM	964	CD	ARG	121	130.014	-0.267	31.397	1.00150.12	1SG	965
ATOM	965	NE	ARG	121	129.335	-1.455	30.806	1.00150.12	1SG	966
ATOM	966	CZ	ARG	121	129.131	-2.568	31.568	1.00150.12	1SG	967
ATOM	967	NH1	ARG	121	129.567	-2.595	32.861	1.00150.12	1SG	968
ATOM	968	NH2	ARG	121	128.494	-3.654	31.039	1.00150.12	1SG	969
ATOM	969	C	ARG	121	126.890	0.458	31.859	1.00150.12	1SG	970
ATOM	970	O	ARG	121	127.017	-0.763	31.910	1.00150.12	1SG	971
ATOM	971	N	ASP	122	126.382	1.195	32.866	1.00 90.75	1SG	972
ATOM	972	CA	ASP	122	125.943	0.638	34.106	1.00 90.75	1SG	973
ATOM	973	CB	ASP	122	124.735	-0.307	33.983	1.00 90.75	1SG	974
ATOM	974	CG	ASP	122	124.206	-0.559	35.388	1.00 90.75	1SG	975
ATOM	975	OD1	ASP	122	124.811	-0.014	36.350	1.00 90.75	1SG	976
ATOM	976	OD2	ASP	122	123.190	-1.292	35.522	1.00 90.75	1SG	977
ATOM	977	C	ASP	122	127.066	-0.142	34.682	1.00 90.75	1SG	978
ATOM	978	O	ASP	122	126.866	-1.237	35.204	1.00 90.75	1SG	979
ATOM	979	N	SER	123	128.291	0.403	34.597	1.00 90.25	1SG	980
ATOM	980	CA	SER	123	129.377	-0.304	35.195	1.00 90.25	1SG	981
ATOM	981	CB	SER	123	130.746	0.353	34.941	1.00 90.25	1SG	982
ATOM	982	OG	SER	123	131.778	-0.395	35.566	1.00 90.25	1SG	983
ATOM	983	C	SER	123	129.110	-0.246	36.657	1.00 90.25	1SG	984
ATOM	984	O	SER	123	128.679	0.786	37.174	1.00 90.25	1SG	985
ATOM	985	N	LEU	124	129.343	-1.357	37.375	1.00 98.33	1SG	986
ATOM	986	CA	LEU	124	129.034	-1.281	38.766	1.00 98.33	1SG	987
ATOM	987	CB	LEU	124	128.358	-2.543	39.326	1.00 98.33	1SG	988
ATOM	988	CG	LEU	124	126.979	-2.822	38.703	1.00 98.33	1SG	989
ATOM	989	CD2	LEU	124	127.097	-3.111	37.198	1.00 98.33	1SG	990
ATOM	990	CD1	LEU	124	125.983	-1.696	39.026	1.00 98.33	1SG	991
ATOM	991	C	LEU	124	130.300	-1.095	39.521	1.00 98.33	1SG	992
ATOM	992	O	LEU	124	130.990	-2.062	39.842	1.00 98.33	1SG	993

Supplementary material 1.txt

ATOM	993	N	LYS	125	130.650	0.169	39.824	1.00112.90	1SG 994
ATOM	994	CA	LYS	125	131.777	0.318	40.686	1.00112.90	1SG 995
ATOM	995	CB	LYS	125	132.458	1.695	40.647	1.00112.90	1SG 996
ATOM	996	CG	LYS	125	133.869	1.634	41.237	1.00112.90	1SG 997
ATOM	997	CD	LYS	125	134.791	0.718	40.425	1.00112.90	1SG 998
ATOM	998	CE	LYS	125	136.213	0.591	40.975	1.00112.90	1SG 999
ATOM	999	NZ	LYS	125	136.979	-0.381	40.163	1.00112.90	1SG1000
ATOM	1000	C	LYS	125	131.151	0.115	42.025	1.00112.90	1SG1001
ATOM	1001	O	LYS	125	130.246	0.848	42.418	1.00112.90	1SG1002
ATOM	1002	N	LYS	126	131.633	-0.909	42.744	1.00 62.63	1SG1003
ATOM	1003	CA	LYS	126	131.042	-1.436	43.940	1.00 62.63	1SG1004
ATOM	1004	CB	LYS	126	131.723	-2.751	44.359	1.00 62.63	1SG1005
ATOM	1005	CG	LYS	126	131.458	-3.874	43.351	1.00 62.63	1SG1006
ATOM	1006	CD	LYS	126	132.387	-5.083	43.475	1.00 62.63	1SG1007
ATOM	1007	CE	LYS	126	132.082	-6.180	42.450	1.00 62.63	1SG1008
ATOM	1008	NZ	LYS	126	133.184	-7.165	42.409	1.00 62.63	1SG1009
ATOM	1009	C	LYS	126	131.011	-0.505	45.120	1.00 62.63	1SG1010
ATOM	1010	O	LYS	126	130.056	-0.552	45.893	1.00 62.63	1SG1011
ATOM	1011	N	ASP	127	132.027	0.356	45.318	1.00 52.56	1SG1012
ATOM	1012	CA	ASP	127	132.086	1.120	46.541	1.00 52.56	1SG1013
ATOM	1013	CB	ASP	127	133.459	1.771	46.803	1.00 52.56	1SG1014
ATOM	1014	CG	ASP	127	133.765	2.745	45.676	1.00 52.56	1SG1015
ATOM	1015	OD1	ASP	127	133.406	2.434	44.509	1.00 52.56	1SG1016
ATOM	1016	OD2	ASP	127	134.359	3.817	45.967	1.00 52.56	1SG1017
ATOM	1017	C	ASP	127	131.028	2.185	46.636	1.00 52.56	1SG1018
ATOM	1018	O	ASP	127	130.515	2.689	45.640	1.00 52.56	1SG1019
ATOM	1019	N	LEU	128	130.690	2.544	47.898	1.00 54.28	1SG1020
ATOM	1020	CA	LEU	128	129.688	3.515	48.253	1.00 54.28	1SG1021
ATOM	1021	CB	LEU	128	129.483	3.613	49.774	1.00 54.28	1SG1022
ATOM	1022	CG	LEU	128	128.421	4.645	50.197	1.00 54.28	1SG1023
ATOM	1023	CD2	LEU	128	128.439	4.854	51.719	1.00 54.28	1SG1024
ATOM	1024	CD1	LEU	128	127.025	4.278	49.667	1.00 54.28	1SG1025
ATOM	1025	C	LEU	128	130.084	4.879	47.767	1.00 54.28	1SG1026
ATOM	1026	O	LEU	128	129.243	5.633	47.280	1.00 54.28	1SG1027
ATOM	1027	N	ASN	129	131.381	5.228	47.883	1.00 70.76	1SG1028
ATOM	1028	CA	ASN	129	131.856	6.537	47.516	1.00 70.76	1SG1029
ATOM	1029	CB	ASN	129	133.392	6.622	47.437	1.00 70.76	1SG1030
ATOM	1030	CG	ASN	129	134.059	6.099	48.690	1.00 70.76	1SG1031
ATOM	1031	OD1	ASN	129	133.949	6.684	49.762	1.00 70.76	1SG1032
ATOM	1032	ND2	ASN	129	134.798	4.965	48.548	1.00 70.76	1SG1033
ATOM	1033	C	ASN	129	131.521	6.766	46.077	1.00 70.76	1SG1034
ATOM	1034	O	ASN	129	130.892	7.756	45.708	1.00 70.76	1SG1035
ATOM	1035	N	ALA	130	131.966	5.825	45.227	1.00 40.59	1SG1036
ATOM	1036	CA	ALA	130	131.834	5.927	43.804	1.00 40.59	1SG1037
ATOM	1037	CB	ALA	130	132.501	4.757	43.066	1.00 40.59	1SG1038
ATOM	1038	C	ALA	130	130.395	5.906	43.417	1.00 40.59	1SG1039
ATOM	1039	O	ALA	130	129.975	6.663	42.543	1.00 40.59	1SG1040
ATOM	1040	N	THR	131	129.608	5.019	44.055	1.00106.52	1SG1041
ATOM	1041	CA	THR	131	128.225	4.856	43.708	1.00106.52	1SG1042
ATOM	1042	CB	THR	131	127.551	3.755	44.474	1.00106.52	1SG1043
ATOM	1043	OG1	THR	131	127.616	4.016	45.868	1.00106.52	1SG1044
ATOM	1044	CG2	THR	131	128.235	2.420	44.139	1.00106.52	1SG1045
ATOM	1045	C	THR	131	127.461	6.112	43.986	1.00106.52	1SG1046
ATOM	1046	O	THR	131	126.702	6.580	43.139	1.00106.52	1SG1047
ATOM	1047	N	ALA	132	127.657	6.701	45.179	1.00 31.73	1SG1048
ATOM	1048	CA	ALA	132	126.919	7.868	45.570	1.00 31.73	1SG1049
ATOM	1049	CB	ALA	132	127.261	8.335	46.995	1.00 31.73	1SG1050
ATOM	1050	C	ALA	132	127.238	8.994	44.635	1.00 31.73	1SG1051
ATOM	1051	O	ALA	132	126.351	9.749	44.235	1.00 31.73	1SG1052
ATOM	1052	N	LEU	133	128.525	9.137	44.272	1.00107.34	1SG1053
ATOM	1053	CA	LEU	133	128.974	10.200	43.415	1.00107.34	1SG1054
ATOM	1054	CB	LEU	133	130.504	10.178	43.222	1.00107.34	1SG1055
ATOM	1055	CG	LEU	133	131.127	11.450	42.602	1.00107.34	1SG1056
ATOM	1056	CD2	LEU	133	131.110	12.610	43.601	1.00107.34	1SG1057
ATOM	1057	CD1	LEU	133	130.528	11.827	41.239	1.00107.34	1SG1058
ATOM	1058	C	LEU	133	128.362	10.005	42.059	1.00107.34	1SG1059
ATOM	1059	O	LEU	133	127.902	10.958	41.433	1.00107.34	1SG1060
ATOM	1060	N	GLY	134	128.337	8.746	41.574	1.00 29.29	1SG1061
ATOM	1061	CA	GLY	134	127.833	8.454	40.262	1.00 29.29	1SG1062
ATOM	1062	C	GLY	134	126.384	8.828	40.199	1.00 29.29	1SG1063
ATOM	1063	O	GLY	134	125.903	9.329	39.183	1.00 29.29	1SG1064

Supplementary material 1.txt

ATOM	1064	N	PHE	135	125.649	8.548	41.289	1.00	63.38	1SG1065
ATOM	1065	CA	PHE	135	124.245	8.821	41.393	1.00	63.38	1SG1066
ATOM	1066	CB	PHE	135	123.702	8.319	42.747	1.00	63.38	1SG1067
ATOM	1067	CG	PHE	135	122.259	8.657	42.901	1.00	63.38	1SG1068
ATOM	1068	CD1	PHE	135	121.280	7.862	42.352	1.00	63.38	1SG1069
ATOM	1069	CD2	PHE	135	121.886	9.770	43.621	1.00	63.38	1SG1070
ATOM	1070	CE1	PHE	135	119.951	8.182	42.511	1.00	63.38	1SG1071
ATOM	1071	CE2	PHE	135	120.560	10.095	43.783	1.00	63.38	1SG1072
ATOM	1072	CZ	PHE	135	119.590	9.300	43.225	1.00	63.38	1SG1073
ATOM	1073	C	PHE	135	123.989	10.299	41.310	1.00	63.38	1SG1074
ATOM	1074	O	PHE	135	123.213	10.759	40.474	1.00	63.38	1SG1075
ATOM	1075	N	ARG	136	124.683	11.087	42.153	1.00	134.11	1SG1076
ATOM	1076	CA	ARG	136	124.456	12.501	42.264	1.00	134.11	1SG1077
ATOM	1077	CB	ARG	136	125.375	13.134	43.320	1.00	134.11	1SG1078
ATOM	1078	CG	ARG	136	125.209	14.644	43.481	1.00	134.11	1SG1079
ATOM	1079	CD	ARG	136	126.388	15.279	44.219	1.00	134.11	1SG1080
ATOM	1080	NE	ARG	136	127.621	14.761	43.560	1.00	134.11	1SG1081
ATOM	1081	CZ	ARG	136	128.728	15.546	43.429	1.00	134.11	1SG1082
ATOM	1082	NH1	ARG	136	128.736	16.814	43.932	1.00	134.11	1SG1083
ATOM	1083	NH2	ARG	136	129.834	15.061	42.793	1.00	134.11	1SG1084
ATOM	1084	C	ARG	136	124.732	13.200	40.969	1.00	134.11	1SG1085
ATOM	1085	O	ARG	136	123.913	13.985	40.491	1.00	134.11	1SG1086
ATOM	1086	N	ALA	137	125.887	12.910	40.349	1.00	41.62	1SG1087
ATOM	1087	CA	ALA	137	126.283	13.620	39.168	1.00	41.62	1SG1088
ATOM	1088	CB	ALA	137	127.662	13.182	38.646	1.00	41.62	1SG1089
ATOM	1089	C	ALA	137	125.294	13.380	38.071	1.00	41.62	1SG1090
ATOM	1090	O	ALA	137	124.886	14.317	37.390	1.00	41.62	1SG1091
ATOM	1091	N	LEU	138	124.869	12.118	37.881	1.00	52.86	1SG1092
ATOM	1092	CA	LEU	138	123.981	11.772	36.807	1.00	52.86	1SG1093
ATOM	1093	CB	LEU	138	123.732	10.254	36.724	1.00	52.86	1SG1094
ATOM	1094	CG	LEU	138	124.996	9.450	36.359	1.00	52.86	1SG1095
ATOM	1095	CD2	LEU	138	125.639	9.986	35.070	1.00	52.86	1SG1096
ATOM	1096	CD1	LEU	138	124.711	7.941	36.282	1.00	52.86	1SG1097
ATOM	1097	C	LEU	138	122.648	12.439	36.990	1.00	52.86	1SG1098
ATOM	1098	O	LEU	138	122.085	12.978	36.040	1.00	52.86	1SG1099
ATOM	1099	N	ARG	139	122.110	12.424	38.226	1.00	129.73	1SG1100
ATOM	1100	CA	ARG	139	120.809	12.976	38.482	1.00	129.73	1SG1101
ATOM	1101	CB	ARG	139	120.321	12.745	39.923	1.00	129.73	1SG1102
ATOM	1102	CG	ARG	139	119.858	11.311	40.196	1.00	129.73	1SG1103
ATOM	1103	CD	ARG	139	118.526	10.970	39.520	1.00	129.73	1SG1104
ATOM	1104	NE	ARG	139	118.124	9.599	39.950	1.00	129.73	1SG1105
ATOM	1105	CZ	ARG	139	117.355	9.433	41.066	1.00	129.73	1SG1106
ATOM	1106	NH1	ARG	139	116.956	10.521	41.788	1.00	129.73	1SG1107
ATOM	1107	NH2	ARG	139	116.978	8.181	41.457	1.00	129.73	1SG1108
ATOM	1108	C	ARG	139	120.794	14.451	38.225	1.00	129.73	1SG1109
ATOM	1109	O	ARG	139	119.866	14.970	37.607	1.00	129.73	1SG1110
ATOM	1110	N	LEU	140	121.847	15.163	38.656	1.00	70.45	1SG1111
ATOM	1111	CA	LEU	140	121.898	16.593	38.529	1.00	70.45	1SG1112
ATOM	1112	CB	LEU	140	123.185	17.190	39.116	1.00	70.45	1SG1113
ATOM	1113	CG	LEU	140	123.299	16.973	40.634	1.00	70.45	1SG1114
ATOM	1114	CD2	LEU	140	121.999	17.374	41.346	1.00	70.45	1SG1115
ATOM	1115	CD1	LEU	140	124.543	17.667	41.208	1.00	70.45	1SG1116
ATOM	1116	C	LEU	140	121.841	16.940	37.073	1.00	70.45	1SG1117
ATOM	1117	O	LEU	140	121.386	18.017	36.690	1.00	70.45	1SG1118
ATOM	1118	N	HIS	141	122.391	16.046	36.241	1.00	118.97	1SG1119
ATOM	1119	CA	HIS	141	122.469	16.138	34.812	1.00	118.97	1SG1120
ATOM	1120	ND1	HIS	141	125.480	17.050	33.567	1.00	118.97	1SG1121
ATOM	1121	CG	HIS	141	124.929	16.182	34.482	1.00	118.97	1SG1122
ATOM	1122	CB	HIS	141	123.675	15.391	34.231	1.00	118.97	1SG1123
ATOM	1123	NE2	HIS	141	126.766	17.138	35.379	1.00	118.97	1SG1124
ATOM	1124	CD2	HIS	141	125.725	16.249	35.583	1.00	118.97	1SG1125
ATOM	1125	CE1	HIS	141	126.577	17.594	34.156	1.00	118.97	1SG1126
ATOM	1126	C	HIS	141	121.200	15.775	34.093	1.00	118.97	1SG1127
ATOM	1127	O	HIS	141	121.143	15.952	32.877	1.00	118.97	1SG1128
ATOM	1128	N	ARG	142	120.178	15.242	34.802	1.00	171.14	1SG1129
ATOM	1129	CA	ARG	142	118.909	14.830	34.252	1.00	171.14	1SG1130
ATOM	1130	CB	ARG	142	118.445	15.696	33.064	1.00	171.14	1SG1131
ATOM	1131	CG	ARG	142	118.694	17.193	33.279	1.00	171.14	1SG1132
ATOM	1132	CD	ARG	142	117.971	18.084	32.265	1.00	171.14	1SG1133
ATOM	1133	NE	ARG	142	118.503	17.756	30.913	1.00	171.14	1SG1134
ATOM	1134	CZ	ARG	142	117.791	18.096	29.800	1.00	171.14	1SG1135

Supplementary material 1.txt

ATOM	1135	NH1	ARG	142	116.594	18.741	29.924	1.00171.14	1SG1136
ATOM	1136	NH2	ARG	142	118.276	17.788	28.562	1.00171.14	1SG1137
ATOM	1137	C	ARG	142	118.931	13.407	33.766	1.00171.14	1SG1138
ATOM	1138	O	ARG	142	118.024	12.987	33.048	1.00171.14	1SG1139
ATOM	1139	N	TYR	143	119.915	12.597	34.203	1.0098.17	1SG1140
ATOM	1140	CA	TYR	143	119.935	11.213	33.807	1.0098.17	1SG1141
ATOM	1141	CB	TYR	143	121.356	10.633	33.686	1.0098.17	1SG1142
ATOM	1142	CG	TYR	143	122.119	11.447	32.696	1.0098.17	1SG1143
ATOM	1143	CD1	TYR	143	121.840	11.381	31.351	1.0098.17	1SG1144
ATOM	1144	CD2	TYR	143	123.141	12.264	33.121	1.0098.17	1SG1145
ATOM	1145	CE1	TYR	143	122.558	12.135	30.453	1.0098.17	1SG1146
ATOM	1146	CE2	TYR	143	123.862	13.019	32.226	1.0098.17	1SG1147
ATOM	1147	CZ	TYR	143	123.570	12.957	30.887	1.0098.17	1SG1148
ATOM	1148	OH	TYR	143	124.306	13.729	29.963	1.0098.17	1SG1149
ATOM	1149	C	TYR	143	119.270	10.468	34.927	1.0098.17	1SG1150
ATOM	1150	O	TYR	143	119.754	10.469	36.057	1.0098.17	1SG1151
ATOM	1151	N	ASN	144	118.126	9.808	34.645	1.0068.62	1SG1152
ATOM	1152	CA	ASN	144	117.400	9.155	35.703	1.0068.62	1SG1153
ATOM	1153	CB	ASN	144	115.911	8.948	35.364	1.0068.62	1SG1154
ATOM	1154	CG	ASN	144	115.158	8.516	36.620	1.0068.62	1SG1155
ATOM	1155	OD1	ASN	144	115.734	8.332	37.691	1.0068.62	1SG1156
ATOM	1156	ND2	ASN	144	113.817	8.339	36.484	1.0068.62	1SG1157
ATOM	1157	C	ASN	144	117.996	7.806	35.955	1.0068.62	1SG1158
ATOM	1158	O	ASN	144	117.552	6.803	35.397	1.0068.62	1SG1159
ATOM	1159	N	VAL	145	119.013	7.752	36.836	1.0050.66	1SG1160
ATOM	1160	CA	VAL	145	119.639	6.502	37.170	1.0050.66	1SG1161
ATOM	1161	CB	VAL	145	121.067	6.650	37.594	1.0050.66	1SG1162
ATOM	1162	CG1	VAL	145	121.590	5.281	38.060	1.0050.66	1SG1163
ATOM	1163	CG2	VAL	145	121.849	7.254	36.419	1.0050.66	1SG1164
ATOM	1164	C	VAL	145	118.890	5.898	38.315	1.0050.66	1SG1165
ATOM	1165	O	VAL	145	118.497	6.594	39.249	1.0050.66	1SG1166
ATOM	1166	N	SER	146	118.693	4.565	38.277	1.0038.45	1SG1167
ATOM	1167	CA	SER	146	117.933	3.892	39.294	1.0038.45	1SG1168
ATOM	1168	CB	SER	146	117.664	2.412	38.976	1.0038.45	1SG1169
ATOM	1169	OG	SER	146	116.911	1.820	40.024	1.0038.45	1SG1170
ATOM	1170	C	SER	146	118.668	3.958	40.597	1.0038.45	1SG1171
ATOM	1171	O	SER	146	119.889	3.823	40.645	1.0038.45	1SG1172
ATOM	1172	N	SER	147	117.907	4.186	41.690	1.0092.80	1SG1173
ATOM	1173	CA	SER	147	118.417	4.303	43.030	1.0092.80	1SG1174
ATOM	1174	CB	SER	147	117.450	5.016	43.989	1.0092.80	1SG1175
ATOM	1175	OG	SER	147	118.066	5.164	45.259	1.0092.80	1SG1176
ATOM	1176	C	SER	147	118.712	2.946	43.598	1.0092.80	1SG1177
ATOM	1177	O	SER	147	119.176	2.825	44.729	1.0092.80	1SG1178
ATOM	1178	N	GLY	148	118.441	1.887	42.819	1.0046.40	1SG1179
ATOM	1179	CA	GLY	148	118.605	0.512	43.210	1.0046.40	1SG1180
ATOM	1180	C	GLY	148	120.042	0.247	43.530	1.0046.40	1SG1181
ATOM	1181	O	GLY	148	120.361	-0.700	44.246	1.0046.40	1SG1182
ATOM	1182	N	VAL	149	120.950	1.063	42.970	1.00116.11	1SG1183
ATOM	1183	CA	VAL	149	122.366	0.884	43.121	1.00116.11	1SG1184
ATOM	1184	CB	VAL	149	123.165	1.985	42.486	1.00116.11	1SG1185
ATOM	1185	CG1	VAL	149	122.910	1.965	40.970	1.00116.11	1SG1186
ATOM	1186	CG2	VAL	149	122.794	3.314	43.163	1.00116.11	1SG1187
ATOM	1187	C	VAL	149	122.703	0.870	44.583	1.00116.11	1SG1188
ATOM	1188	O	VAL	149	123.715	0.300	44.978	1.00116.11	1SG1189
ATOM	1189	N	LEU	150	121.887	1.554	45.402	1.00127.18	1SG1190
ATOM	1190	CA	LEU	150	121.998	1.691	46.831	1.00127.18	1SG1191
ATOM	1191	CB	LEU	150	121.064	2.769	47.414	1.00127.18	1SG1192
ATOM	1192	CG	LEU	150	121.419	4.205	46.985	1.00127.18	1SG1193
ATOM	1193	CD2	LEU	150	120.601	5.242	47.771	1.00127.18	1SG1194
ATOM	1194	CD1	LEU	150	121.298	4.384	45.466	1.00127.18	1SG1195
ATOM	1195	C	LEU	150	121.702	0.406	47.555	1.00127.18	1SG1196
ATOM	1196	O	LEU	150	121.971	0.305	48.751	1.00127.18	1SG1197
ATOM	1197	N	GLU	151	121.053	-0.571	46.891	1.0049.37	1SG1198
ATOM	1198	CA	GLU	151	120.626	-1.797	47.520	1.0049.37	1SG1199
ATOM	1199	CB	GLU	151	119.906	-2.749	46.546	1.0049.37	1SG1200
ATOM	1200	CG	GLU	151	118.544	-2.249	46.060	1.0049.37	1SG1201
ATOM	1201	CD	GLU	151	117.983	-3.306	45.115	1.0049.37	1SG1202
ATOM	1202	OE1	GLU	151	118.420	-4.482	45.226	1.0049.37	1SG1203
ATOM	1203	OE2	GLU	151	117.115	-2.954	44.272	1.0049.37	1SG1204
ATOM	1204	C	GLU	151	121.775	-2.580	48.098	1.0049.37	1SG1205
ATOM	1205	O	GLU	151	121.669	-3.098	49.209	1.0049.37	1SG1206

Supplementary material 1.txt

ATOM	1206	N	ASN	152	122.915	-2.673	47.392	1.00106.23	1SG1207
ATOM	1207	CA	ASN	152	123.997	-3.509	47.841	1.00106.23	1SG1208
ATOM	1208	CB	ASN	152	125.208	-3.528	46.890	1.00106.23	1SG1209
ATOM	1209	CG	ASN	152	125.820	-2.141	46.844	1.00106.23	1SG1210
ATOM	1210	OD1	ASN	152	125.210	-1.196	46.354	1.00106.23	1SG1211
ATOM	1211	ND2	ASN	152	127.067	-2.010	47.371	1.00106.23	1SG1212
ATOM	1212	C	ASN	152	124.475	-3.045	49.181	1.00106.23	1SG1213
ATOM	1213	O	ASN	152	125.032	-3.823	49.953	1.00106.23	1SG1214
ATOM	1214	N	PHE	153	124.339	-1.739	49.451	1.00 91.71	1SG1215
ATOM	1215	CA	PHE	153	124.748	-1.106	50.669	1.00 91.71	1SG1216
ATOM	1216	CB	PHE	153	124.823	0.418	50.519	1.00 91.71	1SG1217
ATOM	1217	CG	PHE	153	125.774	0.638	49.394	1.00 91.71	1SG1218
ATOM	1218	CD1	PHE	153	127.112	0.360	49.547	1.00 91.71	1SG1219
ATOM	1219	CD2	PHE	153	125.328	1.129	48.188	1.00 91.71	1SG1220
ATOM	1220	CE1	PHE	153	127.991	0.559	48.510	1.00 91.71	1SG1221
ATOM	1221	CE2	PHE	153	126.203	1.332	47.147	1.00 91.71	1SG1222
ATOM	1222	CZ	PHE	153	127.538	1.045	47.306	1.00 91.71	1SG1223
ATOM	1223	C	PHE	153	123.826	-1.440	51.811	1.00 91.71	1SG1224
ATOM	1224	O	PHE	153	124.250	-1.435	52.965	1.00 91.71	1SG1225
ATOM	1225	N	ARG	154	122.529	-1.686	51.532	1.00137.06	1SG1226
ATOM	1226	CA	ARG	154	121.538	-1.880	52.555	1.00137.06	1SG1227
ATOM	1227	CB	ARG	154	120.183	-1.237	52.196	1.00137.06	1SG1228
ATOM	1228	CG	ARG	154	119.592	-1.726	50.868	1.00137.06	1SG1229
ATOM	1229	CD	ARG	154	119.115	-3.180	50.885	1.00137.06	1SG1230
ATOM	1230	NE	ARG	154	118.589	-3.507	49.529	1.00137.06	1SG1231
ATOM	1231	CZ	ARG	154	117.314	-3.966	49.378	1.00137.06	1SG1232
ATOM	1232	NH1	ARG	154	116.496	-4.100	50.464	1.00137.06	1SG1233
ATOM	1233	NH2	ARG	154	116.855	-4.299	48.135	1.00137.06	1SG1234
ATOM	1234	C	ARG	154	121.295	-3.327	52.861	1.00137.06	1SG1235
ATOM	1235	O	ARG	154	121.656	-4.230	52.108	1.00137.06	1SG1236
ATOM	1236	N	ASP	155	120.671	-3.541	54.037	1.00125.63	1SG1237
ATOM	1237	CA	ASP	155	120.315	-4.807	54.607	1.00125.63	1SG1238
ATOM	1238	CB	ASP	155	120.116	-4.664	56.128	1.00125.63	1SG1239
ATOM	1239	CG	ASP	155	119.960	-6.024	56.779	1.00125.63	1SG1240
ATOM	1240	OD1	ASP	155	120.366	-7.027	56.137	1.00125.63	1SG1241
ATOM	1241	OD2	ASP	155	119.421	-6.079	57.916	1.00125.63	1SG1242
ATOM	1242	C	ASP	155	119.005	-5.230	54.000	1.00125.63	1SG1243
ATOM	1243	O	ASP	155	118.431	-4.526	53.173	1.00125.63	1SG1244
ATOM	1244	N	ASP	156	118.507	-6.418	54.401	1.00 39.02	1SG1245
ATOM	1245	CA	ASP	156	117.257	-6.955	53.949	1.00 39.02	1SG1246
ATOM	1246	CB	ASP	156	116.927	-8.328	54.558	1.00 39.02	1SG1247
ATOM	1247	CG	ASP	156	117.920	-9.348	54.022	1.00 39.02	1SG1248
ATOM	1248	OD1	ASP	156	119.001	-8.924	53.534	1.00 39.02	1SG1249
ATOM	1249	OD2	ASP	156	117.611	-10.567	54.101	1.00 39.02	1SG1250
ATOM	1250	C	ASP	156	116.208	-6.013	54.429	1.00 39.02	1SG1251
ATOM	1251	O	ASP	156	115.167	-5.836	53.797	1.00 39.02	1SG1252
ATOM	1252	N	ASN	157	116.479	-5.374	55.579	1.00 46.31	1SG1253
ATOM	1253	CA	ASN	157	115.555	-4.455	56.168	1.00 46.31	1SG1254
ATOM	1254	CB	ASN	157	116.114	-3.776	57.433	1.00 46.31	1SG1255
ATOM	1255	CG	ASN	157	115.027	-2.900	58.047	1.00 46.31	1SG1256
ATOM	1256	OD1	ASN	157	114.453	-2.031	57.392	1.00 46.31	1SG1257
ATOM	1257	ND2	ASN	157	114.725	-3.140	59.351	1.00 46.31	1SG1258
ATOM	1258	C	ASN	157	115.298	-3.396	55.150	1.00 46.31	1SG1259
ATOM	1259	O	ASN	157	114.177	-2.907	55.025	1.00 46.31	1SG1260
ATOM	1260	N	GLY	158	116.328	-3.035	54.360	1.00 28.66	1SG1261
ATOM	1261	CA	GLY	158	116.132	-2.016	53.373	1.00 28.66	1SG1262
ATOM	1262	C	GLY	158	116.790	-0.768	53.854	1.00 28.66	1SG1263
ATOM	1263	O	GLY	158	116.698	0.280	53.217	1.00 28.66	1SG1264
ATOM	1264	N	GLN	159	117.468	-0.842	55.012	1.00 99.74	1SG1265
ATOM	1265	CA	GLN	159	118.147	0.325	55.481	1.00 99.74	1SG1266
ATOM	1266	CB	GLN	159	117.715	0.764	56.888	1.00 99.74	1SG1267
ATOM	1267	CG	GLN	159	116.234	1.138	56.942	1.00 99.74	1SG1268
ATOM	1268	CD	GLN	159	115.938	2.060	55.769	1.00 99.74	1SG1269
ATOM	1269	OE1	GLN	159	116.674	3.005	55.492	1.00 99.74	1SG1270
ATOM	1270	NE2	GLN	159	114.825	1.765	55.046	1.00 99.74	1SG1271
ATOM	1271	C	GLN	159	119.602	0.005	55.516	1.00 99.74	1SG1272
ATOM	1272	O	GLN	159	119.990	-1.148	55.334	1.00 99.74	1SG1273
ATOM	1273	N	PHE	160	120.454	1.038	55.681	1.00127.50	1SG1274
ATOM	1274	CA	PHE	160	121.845	0.754	55.858	1.00127.50	1SG1275
ATOM	1275	CB	PHE	160	122.716	2.024	55.875	1.00127.50	1SG1276
ATOM	1276	CG	PHE	160	122.520	2.724	54.574	1.00127.50	1SG1277

Supplementary material 1.txt

ATOM	1277	CD1	PHE	160	123.289	2.412	53.478	1.00127.50	1SG1278
ATOM	1278	CD2	PHE	160	121.553	3.696	54.449	1.00127.50	1SG1279
ATOM	1279	CE1	PHE	160	123.100	3.065	52.281	1.00127.50	1SG1280
ATOM	1280	CE2	PHE	160	121.359	4.352	53.256	1.00127.50	1SG1281
ATOM	1281	CZ	PHE	160	122.133	4.035	52.166	1.00127.50	1SG1282
ATOM	1282	C	PHE	160	121.825	0.223	57.267	1.00127.50	1SG1283
ATOM	1283	O	PHE	160	122.104	0.950	58.215	1.00127.50	1SG1284
ATOM	1284	N	PHE	161	121.528	-1.081	57.447	1.00221.88	1SG1285
ATOM	1285	CA	PHE	161	121.221	-1.588	58.761	1.00221.88	1SG1286
ATOM	1286	CB	PHE	161	120.597	-2.998	58.730	1.00221.88	1SG1287
ATOM	1287	CG	PHE	161	119.880	-3.245	60.015	1.00221.88	1SG1288
ATOM	1288	CD1	PHE	161	118.588	-2.793	60.160	1.00221.88	1SG1289
ATOM	1289	CD2	PHE	161	120.471	-3.908	61.066	1.00221.88	1SG1290
ATOM	1290	CE1	PHE	161	117.887	-2.999	61.324	1.00221.88	1SG1291
ATOM	1291	CE2	PHE	161	119.772	-4.120	62.233	1.00221.88	1SG1292
ATOM	1292	CZ	PHE	161	118.481	-3.668	62.365	1.00221.88	1SG1293
ATOM	1293	C	PHE	161	122.430	-1.591	59.645	1.00221.88	1SG1294
ATOM	1294	O	PHE	161	123.549	-1.849	59.211	1.00221.88	1SG1295
ATOM	1295	N	CYS	162	122.210	-1.286	60.939	1.0095.35	1SG1296
ATOM	1296	CA	CYS	162	123.266	-1.205	61.904	1.0095.35	1SG1297
ATOM	1297	CB	CYS	162	123.204	0.090	62.731	1.0095.35	1SG1298
ATOM	1298	SG	CYS	162	124.271	0.058	64.201	1.0095.35	1SG1299
ATOM	1299	C	CYS	162	123.113	-2.331	62.872	1.0095.35	1SG1300
ATOM	1300	O	CYS	162	122.008	-2.808	63.117	1.0095.35	1SG1301
ATOM	1301	N	GLY	163	124.243	-2.792	63.443	1.0066.45	1SG1302
ATOM	1302	CA	GLY	163	124.201	-3.824	64.435	1.0066.45	1SG1303
ATOM	1303	C	GLY	163	124.263	-5.139	63.740	1.0066.45	1SG1304
ATOM	1304	O	GLY	163	124.165	-5.220	62.519	1.0066.45	1SG1305
ATOM	1305	N	SER	164	124.432	-6.221	64.526	1.00158.18	1SG1306
ATOM	1306	CA	SER	164	124.487	-7.519	63.928	1.00158.18	1SG1307
ATOM	1307	CB	SER	164	125.841	-8.228	64.097	1.00158.18	1SG1308
ATOM	1308	OG	SER	164	125.801	-9.504	63.476	1.00158.18	1SG1309
ATOM	1309	C	SER	164	123.463	-8.368	64.601	1.00158.18	1SG1310
ATOM	1310	O	SER	164	123.235	-8.262	65.804	1.00158.18	1SG1311
ATOM	1311	N	THR	165	122.796	-9.220	63.807	1.00258.79	1SG1312
ATOM	1312	CA	THR	165	121.822	-10.132	64.319	1.00258.79	1SG1313
ATOM	1313	CB	THR	165	120.418	-9.605	64.246	1.00258.79	1SG1314
ATOM	1314	OG1	THR	165	119.523	-10.481	64.915	1.00258.79	1SG1315
ATOM	1315	CG2	THR	165	120.021	-9.456	62.767	1.00258.79	1SG1316
ATOM	1316	C	THR	165	121.905	-11.313	63.418	1.00258.79	1SG1317
ATOM	1317	O	THR	165	122.708	-11.321	62.486	1.00258.79	1SG1318
ATOM	1318	N	VAL	166	121.110	-12.367	63.675	1.00159.62	1SG1319
ATOM	1319	CA	VAL	166	121.177	-13.425	62.717	1.00159.62	1SG1320
ATOM	1320	CB	VAL	166	120.652	-14.742	63.226	1.00159.62	1SG1321
ATOM	1321	CG1	VAL	166	119.246	-14.551	63.820	1.00159.62	1SG1322
ATOM	1322	CG2	VAL	166	120.709	-15.757	62.070	1.00159.62	1SG1323
ATOM	1323	C	VAL	166	120.365	-12.949	61.558	1.00159.62	1SG1324
ATOM	1324	O	VAL	166	119.173	-13.226	61.429	1.00159.62	1SG1325
ATOM	1325	N	GLU	167	121.029	-12.190	60.671	1.00309.22	1SG1326
ATOM	1326	CA	GLU	167	120.366	-11.614	59.545	1.00309.22	1SG1327
ATOM	1327	CB	GLU	167	119.532	-10.375	59.918	1.00309.22	1SG1328
ATOM	1328	CG	GLU	167	118.553	-9.925	58.833	1.00309.22	1SG1329
ATOM	1329	CD	GLU	167	117.250	-10.685	59.037	1.00309.22	1SG1330
ATOM	1330	OE1	GLU	167	117.121	-11.374	60.084	1.00309.22	1SG1331
ATOM	1331	OE2	GLU	167	116.363	-10.579	58.150	1.00309.22	1SG1332
ATOM	1332	C	GLU	167	121.453	-11.138	58.645	1.00309.22	1SG1333
ATOM	1333	O	GLU	167	122.629	-11.183	59.004	1.00309.22	1SG1334
ATOM	1334	N	GLU	168	121.088	-10.683	57.434	1.00265.09	1SG1335
ATOM	1335	CA	GLU	168	122.089	-10.156	56.561	1.00265.09	1SG1336
ATOM	1336	CB	GLU	168	121.596	-9.917	55.124	1.00265.09	1SG1337
ATOM	1337	CG	GLU	168	121.200	-11.213	54.409	1.00265.09	1SG1338
ATOM	1338	CD	GLU	168	122.429	-12.108	54.323	1.00265.09	1SG1339
ATOM	1339	OE1	GLU	168	123.525	-11.651	54.743	1.00265.09	1SG1340
ATOM	1340	OE2	GLU	168	122.288	-13.263	53.839	1.00265.09	1SG1341
ATOM	1341	C	GLU	168	122.490	-8.850	57.161	1.00265.09	1SG1342
ATOM	1342	O	GLU	168	121.721	-8.241	57.903	1.00265.09	1SG1343
ATOM	1343	N	GLU	169	123.729	-8.401	56.888	1.00244.93	1SG1344
ATOM	1344	CA	GLU	169	124.204	-7.192	57.494	1.00244.93	1SG1345
ATOM	1345	CB	GLU	169	125.726	-6.991	57.391	1.00244.93	1SG1346
ATOM	1346	CG	GLU	169	126.551	-8.041	58.140	1.00244.93	1SG1347
ATOM	1347	CD	GLU	169	126.845	-9.189	57.185	1.00244.93	1SG1348

Supplementary material 1.txt

ATOM	1348	OE1	GLU	169	127.598	-8.961	56.201	1.00244.93	1SG1349
ATOM	1349	OE2	GLU	169	126.325	-10.311	57.430	1.00244.93	1SG1350
ATOM	1350	C	GLU	169	123.581	-6.013	56.825	1.00244.93	1SG1351
ATOM	1351	O	GLU	169	123.243	-6.049	55.643	1.00244.93	1SG1352
ATOM	1352	N	GLY	170	123.389	-4.932	57.603	1.00157.15	1SG1353
ATOM	1353	CA	GLY	170	122.908	-3.705	57.048	1.00157.15	1SG1354
ATOM	1354	C	GLY	170	124.138	-2.918	56.758	1.00157.15	1SG1355
ATOM	1355	O	GLY	170	125.240	-3.462	56.801	1.00157.15	1SG1356
ATOM	1356	N	ALA	171	124.010	-1.611	56.460	1.00127.08	1SG1357
ATOM	1357	CA	ALA	171	125.259	-0.970	56.199	1.00127.08	1SG1358
ATOM	1358	CB	ALA	171	125.159	0.066	55.070	1.00127.08	1SG1359
ATOM	1359	C	ALA	171	125.704	-0.224	57.417	1.00127.08	1SG1360
ATOM	1360	O	ALA	171	125.878	0.992	57.379	1.00127.08	1SG1361
ATOM	1361	N	GLU	172	125.911	-0.941	58.535	1.00150.31	1SG1362
ATOM	1362	CA	GLU	172	126.454	-0.349	59.721	1.00150.31	1SG1363
ATOM	1363	CB	GLU	172	126.211	-1.181	60.986	1.00150.31	1SG1364
ATOM	1364	CG	GLU	172	127.028	-0.679	62.176	1.00150.31	1SG1365
ATOM	1365	CD	GLU	172	126.670	0.779	62.435	1.00150.31	1SG1366
ATOM	1366	OE1	GLU	172	125.717	1.293	61.790	1.00150.31	1SG1367
ATOM	1367	OE2	GLU	172	127.352	1.398	63.295	1.00150.31	1SG1368
ATOM	1368	C	GLU	172	127.929	-0.210	59.544	1.00150.31	1SG1369
ATOM	1369	O	GLU	172	128.545	0.734	60.035	1.00150.31	1SG1370
ATOM	1370	N	ALA	173	128.522	-1.171	58.812	1.00 46.67	1SG1371
ATOM	1371	CA	ALA	173	129.938	-1.271	58.612	1.00 46.67	1SG1372
ATOM	1372	CB	ALA	173	130.340	-2.463	57.727	1.00 46.67	1SG1373
ATOM	1373	C	ALA	173	130.408	-0.031	57.936	1.00 46.67	1SG1374
ATOM	1374	O	ALA	173	131.524	0.429	58.164	1.00 46.67	1SG1375
ATOM	1375	N	TYR	174	129.540	0.540	57.091	1.00132.03	1SG1376
ATOM	1376	CA	TYR	174	129.804	1.690	56.280	1.00132.03	1SG1377
ATOM	1377	CB	TYR	174	128.658	2.006	55.307	1.00132.03	1SG1378
ATOM	1378	CG	TYR	174	128.711	0.918	54.288	1.00132.03	1SG1379
ATOM	1379	CD1	TYR	174	128.025	-0.258	54.483	1.00132.03	1SG1380
ATOM	1380	CD2	TYR	174	129.473	1.060	53.150	1.00132.03	1SG1381
ATOM	1381	CE1	TYR	174	128.076	-1.268	53.552	1.00132.03	1SG1382
ATOM	1382	CE2	TYR	174	129.529	0.053	52.214	1.00132.03	1SG1383
ATOM	1383	CZ	TYR	174	128.828	-1.113	52.412	1.00132.03	1SG1384
ATOM	1384	OH	TYR	174	128.884	-2.148	51.454	1.00132.03	1SG1385
ATOM	1385	C	TYR	174	130.130	2.893	57.115	1.00132.03	1SG1386
ATOM	1386	O	TYR	174	130.778	3.819	56.631	1.00132.03	1SG1387
ATOM	1387	N	ASN	175	129.681	2.928	58.382	1.00105.05	1SG1388
ATOM	1388	CA	ASN	175	129.871	4.073	59.233	1.00105.05	1SG1389
ATOM	1389	CB	ASN	175	129.480	3.799	60.693	1.00105.05	1SG1390
ATOM	1390	CG	ASN	175	130.492	2.830	61.283	1.00105.05	1SG1391
ATOM	1391	OD1	ASN	175	130.765	1.769	60.725	1.00105.05	1SG1392
ATOM	1392	ND2	ASN	175	131.077	3.215	62.450	1.00105.05	1SG1393
ATOM	1393	C	ASN	175	131.326	4.448	59.246	1.00105.05	1SG1394
ATOM	1394	O	ASN	175	131.673	5.606	59.475	1.00105.05	1SG1395
ATOM	1395	N	LYS	176	132.214	3.458	59.057	1.00139.25	1SG1396
ATOM	1396	CA	LYS	176	133.639	3.642	59.052	1.00139.25	1SG1397
ATOM	1397	CB	LYS	176	134.388	2.306	58.928	1.00139.25	1SG1398
ATOM	1398	CG	LYS	176	133.986	1.531	57.671	1.00139.25	1SG1399
ATOM	1399	CD	LYS	176	134.944	0.403	57.293	1.00139.25	1SG1400
ATOM	1400	CE	LYS	176	135.855	0.752	56.115	1.00139.25	1SG1401
ATOM	1401	NZ	LYS	176	135.057	0.836	54.870	1.00139.25	1SG1402
ATOM	1402	C	LYS	176	134.114	4.498	57.906	1.00139.25	1SG1403
ATOM	1403	O	LYS	176	135.053	5.272	58.085	1.00139.25	1SG1404
ATOM	1404	N	HIS	177	133.508	4.392	56.700	1.00119.24	1SG1405
ATOM	1405	CA	HIS	177	134.083	5.083	55.572	1.00119.24	1SG1406
ATOM	1406	ND1	HIS	177	134.851	6.034	52.575	1.00119.24	1SG1407
ATOM	1407	CG	HIS	177	134.845	4.800	53.183	1.00119.24	1SG1408
ATOM	1408	CB	HIS	177	133.859	4.369	54.229	1.00119.24	1SG1409
ATOM	1409	NE2	HIS	177	136.561	4.901	51.721	1.00119.24	1SG1410
ATOM	1410	CD2	HIS	177	135.895	4.120	52.648	1.00119.24	1SG1411
ATOM	1411	CE1	HIS	177	135.897	6.042	51.711	1.00119.24	1SG1412
ATOM	1412	C	HIS	177	133.539	6.476	55.448	1.00119.24	1SG1413
ATOM	1413	O	HIS	177	132.371	6.697	55.128	1.00119.24	1SG1414
ATOM	1414	N	VAL	178	134.433	7.455	55.689	1.00 70.62	1SG1415
ATOM	1415	CA	VAL	178	134.158	8.863	55.694	1.00 70.62	1SG1416
ATOM	1416	CB	VAL	178	135.402	9.633	56.016	1.00 70.62	1SG1417
ATOM	1417	CG1	VAL	178	135.065	11.132	56.075	1.00 70.62	1SG1418
ATOM	1418	CG2	VAL	178	136.086	9.004	57.239	1.00 70.62	1SG1419

Supplementary material 1.txt

ATOM	1419	C	VAL	178	133.777	9.314	54.319	1.00	70.62	1SG1420
ATOM	1420	O	VAL	178	132.753	9.964	54.117	1.00	70.62	1SG1421
ATOM	1421	N	ARG	179	134.605	8.951	53.323	1.00	110.89	1SG1422
ATOM	1422	CA	ARG	179	134.411	9.405	51.980	1.00	110.89	1SG1423
ATOM	1423	CB	ARG	179	135.541	8.978	51.029	1.00	110.89	1SG1424
ATOM	1424	CG	ARG	179	136.852	9.713	51.314	1.00	110.89	1SG1425
ATOM	1425	CD	ARG	179	136.905	11.119	50.710	1.00	110.89	1SG1426
ATOM	1426	NE	ARG	179	138.102	11.805	51.275	1.00	110.89	1SG1427
ATOM	1427	CZ	ARG	179	138.885	12.594	50.483	1.00	110.89	1SG1428
ATOM	1428	NH1	ARG	179	138.609	12.719	49.150	1.00	110.89	1SG1429
ATOM	1429	NH2	ARG	179	139.944	13.259	51.027	1.00	110.89	1SG1430
ATOM	1430	C	ARG	179	133.119	8.871	51.460	1.00	110.89	1SG1431
ATOM	1431	O	ARG	179	132.460	9.518	50.649	1.00	110.89	1SG1432
ATOM	1432	N	CYS	180	132.752	7.643	51.865	1.00	37.04	1SG1433
ATOM	1433	CA	CYS	180	131.533	7.057	51.389	1.00	37.04	1SG1434
ATOM	1434	CB	CYS	180	131.369	5.582	51.797	1.00	37.04	1SG1435
ATOM	1435	SG	CYS	180	132.610	4.490	51.040	1.00	37.04	1SG1436
ATOM	1436	C	CYS	180	130.370	7.796	51.966	1.00	37.04	1SG1437
ATOM	1437	O	CYS	180	129.406	8.106	51.269	1.00	37.04	1SG1438
ATOM	1438	N	MET	181	130.444	8.095	53.276	1.00	80.22	1SG1439
ATOM	1439	CA	MET	181	129.370	8.721	53.989	1.00	80.22	1SG1440
ATOM	1440	CB	MET	181	129.666	8.851	55.492	1.00	80.22	1SG1441
ATOM	1441	CG	MET	181	129.801	7.498	56.195	1.00	80.22	1SG1442
ATOM	1442	SD	MET	181	130.249	7.606	57.952	1.00	80.22	1SG1443
ATOM	1443	CE	MET	181	131.939	8.184	57.622	1.00	80.22	1SG1444
ATOM	1444	C	MET	181	129.131	10.093	53.444	1.00	80.22	1SG1445
ATOM	1445	O	MET	181	127.985	10.509	53.274	1.00	80.22	1SG1446
ATOM	1446	N	LEU	182	130.216	10.831	53.148	1.00	52.19	1SG1447
ATOM	1447	CA	LEU	182	130.099	12.184	52.688	1.00	52.19	1SG1448
ATOM	1448	CB	LEU	182	131.462	12.873	52.519	1.00	52.19	1SG1449
ATOM	1449	CG	LEU	182	131.345	14.323	52.019	1.00	52.19	1SG1450
ATOM	1450	CD2	LEU	182	132.727	14.902	51.683	1.00	52.19	1SG1451
ATOM	1451	CD1	LEU	182	130.566	15.196	53.016	1.00	52.19	1SG1452
ATOM	1452	C	LEU	182	129.407	12.233	51.358	1.00	52.19	1SG1453
ATOM	1453	O	LEU	182	128.500	13.038	51.153	1.00	52.19	1SG1454
ATOM	1454	N	SER	183	129.810	11.358	50.417	1.00	68.86	1SG1455
ATOM	1455	CA	SER	183	129.265	11.365	49.087	1.00	68.86	1SG1456
ATOM	1456	CB	SER	183	129.969	10.356	48.163	1.00	68.86	1SG1457
ATOM	1457	OG	SER	183	129.403	10.401	46.862	1.00	68.86	1SG1458
ATOM	1458	C	SER	183	127.818	10.998	49.149	1.00	68.86	1SG1459
ATOM	1459	O	SER	183	127.018	11.461	48.337	1.00	68.86	1SG1460
ATOM	1460	N	LEU	184	127.458	10.119	50.102	1.00	51.71	1SG1461
ATOM	1461	CA	LEU	184	126.104	9.680	50.286	1.00	51.71	1SG1462
ATOM	1462	CB	LEU	184	126.012	8.532	51.315	1.00	51.71	1SG1463
ATOM	1463	CG	LEU	184	124.591	7.992	51.575	1.00	51.71	1SG1464
ATOM	1464	CD2	LEU	184	124.592	6.957	52.714	1.00	51.71	1SG1465
ATOM	1465	CD1	LEU	184	123.962	7.431	50.291	1.00	51.71	1SG1466
ATOM	1466	C	LEU	184	125.290	10.842	50.772	1.00	51.71	1SG1467
ATOM	1467	O	LEU	184	124.153	11.041	50.347	1.00	51.71	1SG1468
ATOM	1468	N	SER	185	125.871	11.651	51.680	1.00	33.38	1SG1469
ATOM	1469	CA	SER	185	125.184	12.769	52.261	1.00	33.38	1SG1470
ATOM	1470	CB	SER	185	126.058	13.529	53.274	1.00	33.38	1SG1471
ATOM	1471	OG	SER	185	125.339	14.625	53.822	1.00	33.38	1SG1472
ATOM	1472	C	SER	185	124.805	13.734	51.183	1.00	33.38	1SG1473
ATOM	1473	O	SER	185	123.687	14.247	51.157	1.00	33.38	1SG1474
ATOM	1474	N	ARG	186	125.737	14.017	50.259	1.00	84.52	1SG1475
ATOM	1475	CA	ARG	186	125.477	14.961	49.211	1.00	84.52	1SG1476
ATOM	1476	CB	ARG	186	126.751	15.332	48.433	1.00	84.52	1SG1477
ATOM	1477	CG	ARG	186	127.678	16.156	49.332	1.00	84.52	1SG1478
ATOM	1478	CD	ARG	186	129.032	16.539	48.736	1.00	84.52	1SG1479
ATOM	1479	NE	ARG	186	129.710	17.384	49.762	1.00	84.52	1SG1480
ATOM	1480	CZ	ARG	186	131.043	17.247	50.022	1.00	84.52	1SG1481
ATOM	1481	NH1	ARG	186	131.788	16.329	49.340	1.00	84.52	1SG1482
ATOM	1482	NH2	ARG	186	131.629	18.031	50.973	1.00	84.52	1SG1483
ATOM	1483	C	ARG	186	124.419	14.428	48.293	1.00	84.52	1SG1484
ATOM	1484	O	ARG	186	123.557	15.171	47.830	1.00	84.52	1SG1485
ATOM	1485	N	ALA	187	124.458	13.112	48.022	1.00	43.91	1SG1486
ATOM	1486	CA	ALA	187	123.545	12.444	47.136	1.00	43.91	1SG1487
ATOM	1487	CB	ALA	187	123.907	10.966	46.919	1.00	43.91	1SG1488
ATOM	1488	C	ALA	187	122.143	12.492	47.673	1.00	43.91	1SG1489
ATOM	1489	O	ALA	187	121.182	12.552	46.908	1.00	43.91	1SG1490

Supplementary material 1.txt

ATOM	1490	N	SER	188	121.984	12.448	49.009	1.00	54.18	1SG1491
ATOM	1491	CA	SER	188	120.686	12.366	49.626	1.00	54.18	1SG1492
ATOM	1492	CB	SER	188	120.758	12.261	51.159	1.00	54.18	1SG1493
ATOM	1493	OG	SER	188	121.270	13.465	51.712	1.00	54.18	1SG1494
ATOM	1494	C	SER	188	119.837	13.567	49.295	1.00	54.18	1SG1495
ATOM	1495	O	SER	188	118.614	13.495	49.384	1.00	54.18	1SG1496
ATOM	1496	N	ASN	189	120.457	14.710	48.945	1.00	89.67	1SG1497
ATOM	1497	CA	ASN	189	119.775	15.947	48.647	1.00	89.67	1SG1498
ATOM	1498	CB	ASN	189	120.743	17.141	48.595	1.00	89.67	1SG1499
ATOM	1499	CG	ASN	189	121.401	17.276	49.961	1.00	89.67	1SG1500
ATOM	1500	OD1	ASN	189	122.627	17.259	50.070	1.00	89.67	1SG1501
ATOM	1501	ND2	ASN	189	120.572	17.409	51.030	1.00	89.67	1SG1502
ATOM	1502	C	ASN	189	119.050	15.913	47.323	1.00	89.67	1SG1503
ATOM	1503	O	ASN	189	118.094	16.655	47.123	1.00	89.67	1SG1504
ATOM	1504	N	ILE	190	119.574	15.137	46.360	1.00231.84		1SG1505
ATOM	1505	CA	ILE	190	119.167	14.940	44.986	1.00231.84		1SG1506
ATOM	1506	CB	ILE	190	120.300	14.351	44.165	1.00231.84		1SG1507
ATOM	1507	CG2	ILE	190	119.827	14.010	42.740	1.00231.84		1SG1508
ATOM	1508	CG1	ILE	190	121.489	15.328	44.131	1.00231.84		1SG1509
ATOM	1509	CD1	ILE	190	122.224	15.493	45.458	1.00231.84		1SG1510
ATOM	1510	C	ILE	190	117.908	14.115	44.824	1.00231.84		1SG1511
ATOM	1511	O	ILE	190	117.311	14.114	43.752	1.00231.84		1SG1512
ATOM	1512	N	LEU	191	117.519	13.306	45.828	1.00129.30		1SG1513
ATOM	1513	CA	LEU	191	116.447	12.347	45.685	1.00129.30		1SG1514
ATOM	1514	CB	LEU	191	116.205	11.500	46.945	1.00129.30		1SG1515
ATOM	1515	CG	LEU	191	115.417	12.231	48.051	1.00129.30		1SG1516
ATOM	1516	CD2	LEU	191	116.023	13.604	48.382	1.00129.30		1SG1517
ATOM	1517	CD1	LEU	191	115.243	11.332	49.284	1.00129.30		1SG1518
ATOM	1518	C	LEU	191	115.119	12.953	45.329	1.00129.30		1SG1519
ATOM	1519	O	LEU	191	114.818	14.101	45.649	1.00129.30		1SG1520
ATOM	1520	N	PHE	192	114.284	12.139	44.632	1.00126.36		1SG1521
ATOM	1521	CA	PHE	192	112.963	12.522	44.207	1.00126.36		1SG1522
ATOM	1522	CB	PHE	192	112.756	12.443	42.678	1.00126.36		1SG1523
ATOM	1523	CG	PHE	192	112.863	11.042	42.189	1.00126.36		1SG1524
ATOM	1524	CD1	PHE	192	114.094	10.460	41.997	1.00126.36		1SG1525
ATOM	1525	CD2	PHE	192	111.729	10.310	41.926	1.00126.36		1SG1526
ATOM	1526	CE1	PHE	192	114.196	9.167	41.542	1.00126.36		1SG1527
ATOM	1527	CE2	PHE	192	111.826	9.018	41.468	1.00126.36		1SG1528
ATOM	1528	CZ	PHE	192	113.059	8.444	41.276	1.00126.36		1SG1529
ATOM	1529	C	PHE	192	111.989	11.630	44.930	1.00126.36		1SG1530
ATOM	1530	O	PHE	192	112.385	10.934	45.861	1.00126.36		1SG1531
ATOM	1531	N	PRO	193	110.720	11.664	44.604	1.00119.21		1SG1532
ATOM	1532	CA	PRO	193	109.753	10.852	45.304	1.00119.21		1SG1533
ATOM	1533	CD	PRO	193	110.103	12.863	44.064	1.00119.21		1SG1534
ATOM	1534	CB	PRO	193	108.376	11.390	44.902	1.00119.21		1SG1535
ATOM	1535	CG	PRO	193	108.657	12.426	43.797	1.00119.21		1SG1536
ATOM	1536	C	PRO	193	109.895	9.363	45.149	1.00119.21		1SG1537
ATOM	1537	O	PRO	193	109.434	8.636	46.028	1.00119.21		1SG1538
ATOM	1538	N	GLY	194	110.480	8.891	44.034	1.00	70.01	1SG1539
ATOM	1539	CA	GLY	194	110.687	7.497	43.715	1.00	70.01	1SG1540
ATOM	1540	C	GLY	194	111.740	6.889	44.602	1.00	70.01	1SG1541
ATOM	1541	O	GLY	194	111.859	5.672	44.722	1.00	70.01	1SG1542
ATOM	1542	N	GLU	195	112.577	7.769	45.158	1.00201.20		1SG1543
ATOM	1543	CA	GLU	195	113.797	7.618	45.899	1.00201.20		1SG1544
ATOM	1544	CB	GLU	195	114.599	8.923	45.934	1.00201.20		1SG1545
ATOM	1545	CG	GLU	195	116.089	8.671	46.118	1.00201.20		1SG1546
ATOM	1546	CD	GLU	195	116.620	8.099	44.810	1.00201.20		1SG1547
ATOM	1547	OE1	GLU	195	115.811	7.931	43.859	1.00201.20		1SG1548
ATOM	1548	OE2	GLU	195	117.846	7.821	44.745	1.00201.20		1SG1549
ATOM	1549	C	GLU	195	113.687	7.088	47.309	1.00201.20		1SG1550
ATOM	1550	O	GLU	195	114.631	7.260	48.075	1.00201.20		1SG1551
ATOM	1551	N	LYS	196	112.545	6.521	47.739	1.00	78.77	1SG1552
ATOM	1552	CA	LYS	196	112.323	6.121	49.111	1.00	78.77	1SG1553
ATOM	1553	CB	LYS	196	111.023	5.320	49.305	1.00	78.77	1SG1554
ATOM	1554	CG	LYS	196	109.749	6.147	49.117	1.00	78.77	1SG1555
ATOM	1555	CD	LYS	196	108.473	5.302	49.071	1.00	78.77	1SG1556
ATOM	1556	CE	LYS	196	107.191	6.132	48.973	1.00	78.77	1SG1557
ATOM	1557	NZ	LYS	196	106.010	5.240	48.936	1.00	78.77	1SG1558
ATOM	1558	C	LYS	196	113.445	5.277	49.671	1.00	78.77	1SG1559
ATOM	1559	O	LYS	196	113.619	5.237	50.887	1.00	78.77	1SG1560
ATOM	1560	N	VAL	197	114.223	4.555	48.844	1.00118.43		1SG1561

Supplementary material 1.txt

ATOM	1561	CA	VAL	197	115.281	3.729	49.373	1.00118.43	1SG1562
ATOM	1562	CB	VAL	197	116.049	3.003	48.311	1.00118.43	1SG1563
ATOM	1563	CG1	VAL	197	116.774	4.044	47.449	1.00118.43	1SG1564
ATOM	1564	CG2	VAL	197	116.992	1.995	48.989	1.00118.43	1SG1565
ATOM	1565	C	VAL	197	116.261	4.583	50.140	1.00118.43	1SG1566
ATOM	1566	O	VAL	197	116.928	4.106	51.056	1.00118.43	1SG1567
ATOM	1567	N	MET	198	116.406	5.847	49.706	1.00168.49	1SG1568
ATOM	1568	CA	MET	198	117.216	6.950	50.165	1.00168.49	1SG1569
ATOM	1569	CB	MET	198	117.317	8.066	49.108	1.00168.49	1SG1570
ATOM	1570	CG	MET	198	118.258	9.212	49.487	1.00168.49	1SG1571
ATOM	1571	SD	MET	198	120.027	8.809	49.380	1.00168.49	1SG1572
ATOM	1572	CE	MET	198	120.066	8.842	47.564	1.00168.49	1SG1573
ATOM	1573	C	MET	198	116.701	7.596	51.426	1.00168.49	1SG1574
ATOM	1574	O	MET	198	117.370	8.468	51.972	1.00168.49	1SG1575
ATOM	1575	N	GLU	199	115.476	7.281	51.881	1.00 69.46	1SG1576
ATOM	1576	CA	GLU	199	114.858	8.024	52.952	1.00 69.46	1SG1577
ATOM	1577	CB	GLU	199	113.538	7.384	53.420	1.00 69.46	1SG1578
ATOM	1578	CG	GLU	199	113.708	5.970	53.986	1.00 69.46	1SG1579
ATOM	1579	CD	GLU	199	112.341	5.445	54.410	1.00 69.46	1SG1580
ATOM	1580	OE1	GLU	199	111.345	6.201	54.260	1.00 69.46	1SG1581
ATOM	1581	OE2	GLU	199	112.274	4.281	54.890	1.00 69.46	1SG1582
ATOM	1582	C	GLU	199	115.747	8.153	54.164	1.00 69.46	1SG1583
ATOM	1583	O	GLU	199	115.824	9.235	54.743	1.00 69.46	1SG1584
ATOM	1584	N	GLU	200	116.398	7.062	54.613	1.00 83.26	1SG1585
ATOM	1585	CA	GLU	200	117.263	7.042	55.771	1.00 83.26	1SG1586
ATOM	1586	CB	GLU	200	117.398	5.654	56.423	1.00 83.26	1SG1587
ATOM	1587	CG	GLU	200	116.108	5.218	57.126	1.00 83.26	1SG1588
ATOM	1588	CD	GLU	200	116.410	4.027	58.027	1.00 83.26	1SG1589
ATOM	1589	OE1	GLU	200	117.601	3.621	58.092	1.00 83.26	1SG1590
ATOM	1590	OE2	GLU	200	115.456	3.512	58.671	1.00 83.26	1SG1591
ATOM	1591	C	GLU	200	118.641	7.600	55.520	1.00 83.26	1SG1592
ATOM	1592	O	GLU	200	119.366	7.888	56.470	1.00 83.26	1SG1593
ATOM	1593	N	ALA	201	119.058	7.733	54.248	1.00 62.52	1SG1594
ATOM	1594	CA	ALA	201	120.412	8.066	53.887	1.00 62.52	1SG1595
ATOM	1595	CB	ALA	201	120.593	8.187	52.364	1.00 62.52	1SG1596
ATOM	1596	C	ALA	201	120.895	9.353	54.499	1.00 62.52	1SG1597
ATOM	1597	O	ALA	201	122.051	9.424	54.914	1.00 62.52	1SG1598
ATOM	1598	N	LYS	202	120.068	10.416	54.549	1.00 63.82	1SG1599
ATOM	1599	CA	LYS	202	120.540	11.655	55.109	1.00 63.82	1SG1600
ATOM	1600	CB	LYS	202	119.533	12.812	54.992	1.00 63.82	1SG1601
ATOM	1601	CG	LYS	202	120.079	14.106	55.599	1.00 63.82	1SG1602
ATOM	1602	CD	LYS	202	119.222	15.343	55.331	1.00 63.82	1SG1603
ATOM	1603	CE	LYS	202	118.259	15.669	56.474	1.00 63.82	1SG1604
ATOM	1604	NZ	LYS	202	117.482	16.887	56.156	1.00 63.82	1SG1605
ATOM	1605	C	LYS	202	120.829	11.503	56.571	1.00 63.82	1SG1606
ATOM	1606	O	LYS	202	121.871	11.939	57.056	1.00 63.82	1SG1607
ATOM	1607	N	ALA	203	119.903	10.877	57.318	1.00 29.95	1SG1608
ATOM	1608	CA	ALA	203	120.058	10.747	58.738	1.00 29.95	1SG1609
ATOM	1609	CB	ALA	203	118.844	10.083	59.409	1.00 29.95	1SG1610
ATOM	1610	C	ALA	203	121.257	9.907	59.040	1.00 29.95	1SG1611
ATOM	1611	O	ALA	203	122.014	10.207	59.961	1.00 29.95	1SG1612
ATOM	1612	N	PHE	204	121.448	8.820	58.270	1.00 69.46	1SG1613
ATOM	1613	CA	PHE	204	122.508	7.885	58.517	1.00 69.46	1SG1614
ATOM	1614	CB	PHE	204	122.414	6.654	57.596	1.00 69.46	1SG1615
ATOM	1615	CG	PHE	204	123.522	5.709	57.920	1.00 69.46	1SG1616
ATOM	1616	CD1	PHE	204	123.432	4.852	58.995	1.00 69.46	1SG1617
ATOM	1617	CD2	PHE	204	124.649	5.669	57.132	1.00 69.46	1SG1618
ATOM	1618	CE1	PHE	204	124.455	3.978	59.285	1.00 69.46	1SG1619
ATOM	1619	CE2	PHE	204	125.673	4.798	57.416	1.00 69.46	1SG1620
ATOM	1620	CZ	PHE	204	125.580	3.953	58.495	1.00 69.46	1SG1621
ATOM	1621	C	PHE	204	123.853	8.529	58.329	1.00 69.46	1SG1622
ATOM	1622	O	PHE	204	124.705	8.465	59.213	1.00 69.46	1SG1623
ATOM	1623	N	THR	205	124.067	9.199	57.179	1.00117.43	1SG1624
ATOM	1624	CA	THR	205	125.338	9.793	56.866	1.00117.43	1SG1625
ATOM	1625	CB	THR	205	125.388	10.383	55.487	1.00117.43	1SG1626
ATOM	1626	OG1	THR	205	124.430	11.425	55.362	1.00117.43	1SG1627
ATOM	1627	CG2	THR	205	125.107	9.273	54.463	1.00117.43	1SG1628
ATOM	1628	C	THR	205	125.645	10.905	57.818	1.00117.43	1SG1629
ATOM	1629	O	THR	205	126.793	11.081	58.224	1.00117.43	1SG1630
ATOM	1630	N	THR	206	124.623	11.701	58.182	1.00112.76	1SG1631
ATOM	1631	CA	THR	206	124.840	12.856	59.004	1.00112.76	1SG1632

Supplementary material 1.txt

ATOM	1632	CB	THR	206	123.607	13.702	59.167	1.00112.76	1SG1633
ATOM	1633	OG1	THR	206	123.942	14.921	59.811	1.00112.76	1SG1634
ATOM	1634	CG2	THR	206	122.547	12.939	59.981	1.00112.76	1SG1635
ATOM	1635	C	THR	206	125.348	12.489	60.366	1.00112.76	1SG1636
ATOM	1636	O	THR	206	126.320	13.075	60.841	1.00112.76	1SG1637
ATOM	1637	N	ASN	207	124.734	11.491	61.026	1.0079.79	1SG1638
ATOM	1638	CA	ASN	207	125.119	11.191	62.375	1.0079.79	1SG1639
ATOM	1639	CB	ASN	207	124.298	10.041	62.982	1.0079.79	1SG1640
ATOM	1640	CG	ASN	207	122.860	10.521	63.118	1.0079.79	1SG1641
ATOM	1641	OD1	ASN	207	121.926	9.723	63.166	1.0079.79	1SG1642
ATOM	1642	ND2	ASN	207	122.676	11.867	63.176	1.0079.79	1SG1643
ATOM	1643	C	ASN	207	126.552	10.773	62.396	1.0079.79	1SG1644
ATOM	1644	O	ASN	207	127.331	11.241	63.224	1.0079.79	1SG1645
ATOM	1645	N	TYR	208	126.931	9.878	61.470	1.00106.36	1SG1646
ATOM	1646	CA	TYR	208	128.265	9.358	61.420	1.00106.36	1SG1647
ATOM	1647	CB	TYR	208	128.394	8.146	60.486	1.00106.36	1SG1648
ATOM	1648	CG	TYR	208	127.611	7.065	61.155	1.00106.36	1SG1649
ATOM	1649	CD1	TYR	208	126.247	6.975	60.990	1.00106.36	1SG1650
ATOM	1650	CD2	TYR	208	128.238	6.147	61.965	1.00106.36	1SG1651
ATOM	1651	CE1	TYR	208	125.526	5.981	61.611	1.00106.36	1SG1652
ATOM	1652	CE2	TYR	208	127.524	5.150	62.590	1.00106.36	1SG1653
ATOM	1653	CZ	TYR	208	126.165	5.066	62.413	1.00106.36	1SG1654
ATOM	1654	OH	TYR	208	125.427	4.046	63.051	1.00106.36	1SG1655
ATOM	1655	C	TYR	208	129.236	10.428	61.026	1.00106.36	1SG1656
ATOM	1656	O	TYR	208	130.366	10.452	61.511	1.00106.36	1SG1657
ATOM	1657	N	LEU	209	128.840	11.322	60.103	1.0052.56	1SG1658
ATOM	1658	CA	LEU	209	129.742	12.354	59.680	1.0052.56	1SG1659
ATOM	1659	CB	LEU	209	129.173	13.244	58.563	1.0052.56	1SG1660
ATOM	1660	CG	LEU	209	129.032	12.526	57.211	1.0052.56	1SG1661
ATOM	1661	CD2	LEU	209	130.365	11.883	56.785	1.0052.56	1SG1662
ATOM	1662	CD1	LEU	209	128.460	13.469	56.141	1.0052.56	1SG1663
ATOM	1663	C	LEU	209	130.035	13.259	60.828	1.0052.56	1SG1664
ATOM	1664	O	LEU	209	131.182	13.645	61.050	1.0052.56	1SG1665
ATOM	1665	N	LYS	210	128.994	13.640	61.589	1.00150.17	1SG1666
ATOM	1666	CA	LYS	210	129.240	14.548	62.663	1.00150.17	1SG1667
ATOM	1667	CB	LYS	210	127.961	14.971	63.403	1.00150.17	1SG1668
ATOM	1668	CG	LYS	210	128.240	15.809	64.654	1.00150.17	1SG1669
ATOM	1669	CD	LYS	210	128.967	17.125	64.371	1.00150.17	1SG1670
ATOM	1670	CE	LYS	210	128.178	18.093	63.491	1.00150.17	1SG1671
ATOM	1671	NZ	LYS	210	128.969	19.325	63.274	1.00150.17	1SG1672
ATOM	1672	C	LYS	210	130.145	13.911	63.653	1.00150.17	1SG1673
ATOM	1673	O	LYS	210	131.180	14.471	64.008	1.00150.17	1SG1674
ATOM	1674	N	LYS	211	129.794	12.708	64.136	1.0097.22	1SG1675
ATOM	1675	CA	LYS	211	130.683	12.199	65.125	1.0097.22	1SG1676
ATOM	1676	CB	LYS	211	130.149	10.932	65.828	1.0097.22	1SG1677
ATOM	1677	CG	LYS	211	129.865	9.736	64.916	1.0097.22	1SG1678
ATOM	1678	CD	LYS	211	129.606	8.443	65.690	1.0097.22	1SG1679
ATOM	1679	CE	LYS	211	129.316	7.234	64.801	1.0097.22	1SG1680
ATOM	1680	NZ	LYS	211	129.030	6.053	65.645	1.0097.22	1SG1681
ATOM	1681	C	LYS	211	132.008	11.902	64.506	1.0097.22	1SG1682
ATOM	1682	O	LYS	211	133.002	12.544	64.828	1.0097.22	1SG1683
ATOM	1683	N	VAL	212	132.033	10.932	63.573	1.00110.24	1SG1684
ATOM	1684	CA	VAL	212	133.233	10.457	62.951	1.00110.24	1SG1685
ATOM	1685	CB	VAL	212	133.021	9.113	62.317	1.00110.24	1SG1686
ATOM	1686	CG1	VAL	212	134.308	8.692	61.589	1.00110.24	1SG1687
ATOM	1687	CG2	VAL	212	132.563	8.128	63.406	1.00110.24	1SG1688
ATOM	1688	C	VAL	212	133.781	11.348	61.896	1.00110.24	1SG1689
ATOM	1689	O	VAL	212	134.935	11.764	61.986	1.00110.24	1SG1690
ATOM	1690	N	LEU	213	132.943	11.714	60.905	1.00230.66	1SG1691
ATOM	1691	CA	LEU	213	133.468	12.333	59.722	1.00230.66	1SG1692
ATOM	1692	CB	LEU	213	134.060	13.739	59.920	1.00230.66	1SG1693
ATOM	1693	CG	LEU	213	134.386	14.531	58.629	1.00230.66	1SG1694
ATOM	1694	CD2	LEU	213	135.239	13.747	57.616	1.00230.66	1SG1695
ATOM	1695	CD1	LEU	213	135.000	15.895	58.979	1.00230.66	1SG1696
ATOM	1696	C	LEU	213	134.558	11.395	59.314	1.00230.66	1SG1697
ATOM	1697	O	LEU	213	134.281	10.302	58.825	1.00230.66	1SG1698
ATOM	1698	N	ALA	214	135.825	11.799	59.535	1.00239.86	1SG1699
ATOM	1699	CA	ALA	214	136.951	10.967	59.252	1.00239.86	1SG1700
ATOM	1700	CB	ALA	214	137.954	11.589	58.265	1.00239.86	1SG1701
ATOM	1701	C	ALA	214	137.659	10.784	60.550	1.00239.86	1SG1702
ATOM	1702	O	ALA	214	137.620	11.655	61.416	1.00239.86	1SG1703

Supplementary material 1.txt

ATOM	1703	N	GLY	215	138.304	9.623	60.742	1.00	89.05	1SG1704
ATOM	1704	CA	GLY	215	138.995	9.430	61.979	1.00	89.05	1SG1705
ATOM	1705	C	GLY	215	137.952	9.241	63.026	1.00	89.05	1SG1706
ATOM	1706	O	GLY	215	136.795	8.953	62.722	1.00	89.05	1SG1707
ATOM	1707	N	ARG	216	138.345	9.394	64.303	1.00170.94		1SG1708
ATOM	1708	CA	ARG	216	137.403	9.212	65.365	1.00170.94		1SG1709
ATOM	1709	CB	ARG	216	138.039	9.230	66.768	1.00170.94		1SG1710
ATOM	1710	CG	ARG	216	138.801	10.508	67.116	1.00170.94		1SG1711
ATOM	1711	CD	ARG	216	140.248	10.487	66.621	1.00170.94		1SG1712
ATOM	1712	NE	ARG	216	140.960	11.643	67.235	1.00170.94		1SG1713
ATOM	1713	CZ	ARG	216	141.550	11.502	68.457	1.00170.94		1SG1714
ATOM	1714	NH1	ARG	216	141.473	10.310	69.119	1.00170.94		1SG1715
ATOM	1715	NH2	ARG	216	142.220	12.552	69.017	1.00170.94		1SG1716
ATOM	1716	C	ARG	216	136.354	10.275	65.302	1.00170.94		1SG1717
ATOM	1717	O	ARG	216	135.172	9.988	65.486	1.00170.94		1SG1718
ATOM	1718	N	GLU	217	136.740	11.537	65.026	1.00217.11		1SG1719
ATOM	1719	CA	GLU	217	135.718	12.542	65.051	1.00217.11		1SG1720
ATOM	1720	CB	GLU	217	135.779	13.421	66.303	1.00217.11		1SG1721
ATOM	1721	CG	GLU	217	135.472	12.671	67.597	1.00217.11		1SG1722
ATOM	1722	CD	GLU	217	135.756	13.621	68.749	1.00217.11		1SG1723
ATOM	1723	OE1	GLU	217	136.956	13.927	68.982	1.00217.11		1SG1724
ATOM	1724	OE2	GLU	217	134.776	14.052	69.413	1.00217.11		1SG1725
ATOM	1725	C	GLU	217	135.854	13.470	63.888	1.00217.11		1SG1726
ATOM	1726	O	GLU	217	136.942	13.648	63.351	1.00217.11		1SG1727
ATOM	1727	N	ALA	218	134.720	14.067	63.446	1.00	88.77	1SG1728
ATOM	1728	CA	ALA	218	134.804	15.063	62.423	1.00	88.77	1SG1729
ATOM	1729	CB	ALA	218	133.453	15.720	62.098	1.00	88.77	1SG1730
ATOM	1730	C	ALA	218	135.680	16.093	63.050	1.00	88.77	1SG1731
ATOM	1731	O	ALA	218	136.522	16.704	62.395	1.00	88.77	1SG1732
ATOM	1732	N	THR	219	135.517	16.278	64.373	1.00116.56		1SG1733
ATOM	1733	CA	THR	219	136.313	17.244	65.062	1.00116.56		1SG1734
ATOM	1734	CB	THR	219	136.004	17.361	66.529	1.00116.56		1SG1735
ATOM	1735	OG1	THR	219	136.634	18.516	67.064	1.00116.56		1SG1736
ATOM	1736	CG2	THR	219	136.503	16.108	67.264	1.00116.56		1SG1737
ATOM	1737	C	THR	219	137.744	16.849	64.902	1.00116.56		1SG1738
ATOM	1738	O	THR	219	138.607	17.706	64.718	1.00116.56		1SG1739
ATOM	1739	N	HIS	220	138.058	15.540	64.978	1.00148.27		1SG1740
ATOM	1740	CA	HIS	220	139.436	15.223	64.761	1.00148.27		1SG1741
ATOM	1741	ND1	HIS	220	139.571	14.867	68.362	1.00148.27		1SG1742
ATOM	1742	CG	HIS	220	140.143	15.249	67.169	1.00148.27		1SG1743
ATOM	1743	CB	HIS	220	140.095	14.437	65.908	1.00148.27		1SG1744
ATOM	1744	NE2	HIS	220	140.480	16.868	68.706	1.00148.27		1SG1745
ATOM	1745	CD2	HIS	220	140.693	16.474	67.398	1.00148.27		1SG1746
ATOM	1746	CE1	HIS	220	139.803	15.871	69.246	1.00148.27		1SG1747
ATOM	1747	C	HIS	220	139.557	14.445	63.491	1.00148.27		1SG1748
ATOM	1748	O	HIS	220	139.631	13.218	63.493	1.00148.27		1SG1749
ATOM	1749	N	VAL	221	139.575	15.180	62.363	1.00	79.73	1SG1750
ATOM	1750	CA	VAL	221	139.749	14.637	61.046	1.00	79.73	1SG1751
ATOM	1751	CB	VAL	221	138.592	14.898	60.117	1.00	79.73	1SG1752
ATOM	1752	CG1	VAL	221	138.935	14.341	58.726	1.00	79.73	1SG1753
ATOM	1753	CG2	VAL	221	137.315	14.295	60.718	1.00	79.73	1SG1754
ATOM	1754	C	VAL	221	140.909	15.413	60.510	1.00	79.73	1SG1755
ATOM	1755	O	VAL	221	141.218	16.486	61.026	1.00	79.73	1SG1756
ATOM	1756	N	ASP	222	141.599	14.894	59.478	1.00	81.33	1SG1757
ATOM	1757	CA	ASP	222	142.731	15.606	58.961	1.00	81.33	1SG1758
ATOM	1758	CB	ASP	222	143.544	14.809	57.927	1.00	81.33	1SG1759
ATOM	1759	CG	ASP	222	142.657	14.536	56.721	1.00	81.33	1SG1760
ATOM	1760	OD1	ASP	222	141.465	14.180	56.923	1.00	81.33	1SG1761
ATOM	1761	OD2	ASP	222	143.168	14.670	55.577	1.00	81.33	1SG1762
ATOM	1762	C	ASP	222	142.236	16.851	58.300	1.00	81.33	1SG1763
ATOM	1763	O	ASP	222	141.083	16.927	57.878	1.00	81.33	1SG1764
ATOM	1764	N	GLU	223	143.111	17.875	58.215	1.00118.95		1SG1765
ATOM	1765	CA	GLU	223	142.730	19.128	57.632	1.00118.95		1SG1766
ATOM	1766	CB	GLU	223	143.720	20.268	57.901	1.00118.95		1SG1767
ATOM	1767	CG	GLU	223	143.815	20.638	59.382	1.00118.95		1SG1768
ATOM	1768	CD	GLU	223	142.448	21.132	59.839	1.00118.95		1SG1769
ATOM	1769	OE1	GLU	223	141.469	20.344	59.747	1.00118.95		1SG1770
ATOM	1770	OE2	GLU	223	142.366	22.307	60.288	1.00118.95		1SG1771
ATOM	1771	C	GLU	223	142.626	18.945	56.166	1.00118.95		1SG1772
ATOM	1772	O	GLU	223	143.443	18.251	55.556	1.00118.95		1SG1773
ATOM	1773	N	SER	224	141.596	19.616	55.613	1.00247.51		1SG1774

Supplementary material 1.txt

ATOM	1774	CA	SER	224	141.086	19.507	54.290	1.00247.51	1SG1775
ATOM	1775	CB	SER	224	141.885	18.592	53.343	1.00247.51	1SG1776
ATOM	1776	OG	SER	224	143.180	19.132	53.122	1.00247.51	1SG1777
ATOM	1777	C	SER	224	139.736	18.900	54.491	1.00247.51	1SG1778
ATOM	1778	O	SER	224	138.704	19.568	54.487	1.00247.51	1SG1779
ATOM	1779	N	LEU	225	139.743	17.581	54.734	1.00 85.86	1SG1780
ATOM	1780	CA	LEU	225	138.562	16.788	54.859	1.00 85.86	1SG1781
ATOM	1781	CB	LEU	225	138.898	15.307	55.085	1.00 85.86	1SG1782
ATOM	1782	CG	LEU	225	137.662	14.407	55.228	1.00 85.86	1SG1783
ATOM	1783	CD2	LEU	225	138.065	12.993	55.672	1.00 85.86	1SG1784
ATOM	1784	CD1	LEU	225	136.825	14.402	53.938	1.00 85.86	1SG1785
ATOM	1785	C	LEU	225	137.704	17.256	56.000	1.00 85.86	1SG1786
ATOM	1786	O	LEU	225	136.479	17.266	55.889	1.00 85.86	1SG1787
ATOM	1787	N	LEU	226	138.309	17.667	57.127	1.00 56.00	1SG1788
ATOM	1788	CA	LEU	226	137.537	18.043	58.280	1.00 56.00	1SG1789
ATOM	1789	CB	LEU	226	138.458	18.476	59.445	1.00 56.00	1SG1790
ATOM	1790	CG	LEU	226	137.809	18.799	60.814	1.00 56.00	1SG1791
ATOM	1791	CD2	LEU	226	136.740	19.904	60.750	1.00 56.00	1SG1792
ATOM	1792	CD1	LEU	226	138.899	19.158	61.838	1.00 56.00	1SG1793
ATOM	1793	C	LEU	226	136.647	19.192	57.909	1.00 56.00	1SG1794
ATOM	1794	O	LEU	226	135.465	19.197	58.255	1.00 56.00	1SG1795
ATOM	1795	N	GLY	227	137.204	20.198	57.205	1.00 35.69	1SG1796
ATOM	1796	CA	GLY	227	136.473	21.377	56.836	1.00 35.69	1SG1797
ATOM	1797	C	GLY	227	135.388	21.043	55.864	1.00 35.69	1SG1798
ATOM	1798	O	GLY	227	134.276	21.565	55.952	1.00 35.69	1SG1799
ATOM	1799	N	GLU	228	135.692	20.158	54.899	1.00 57.19	1SG1800
ATOM	1800	CA	GLU	228	134.752	19.829	53.869	1.00 57.19	1SG1801
ATOM	1801	CB	GLU	228	135.342	18.822	52.865	1.00 57.19	1SG1802
ATOM	1802	CG	GLU	228	134.405	18.441	51.718	1.00 57.19	1SG1803
ATOM	1803	CD	GLU	228	135.154	17.469	50.812	1.00 57.19	1SG1804
ATOM	1804	OE1	GLU	228	135.613	16.414	51.326	1.00 57.19	1SG1805
ATOM	1805	OE2	GLU	228	135.275	17.768	49.594	1.00 57.19	1SG1806
ATOM	1806	C	GLU	228	133.534	19.216	54.490	1.00 57.19	1SG1807
ATOM	1807	O	GLU	228	132.404	19.544	54.128	1.00 57.19	1SG1808
ATOM	1808	N	VAL	229	133.732	18.293	55.445	1.00 58.35	1SG1809
ATOM	1809	CA	VAL	229	132.610	17.649	56.064	1.00 58.35	1SG1810
ATOM	1810	CB	VAL	229	132.997	16.466	56.890	1.00 58.35	1SG1811
ATOM	1811	CG1	VAL	229	131.778	15.979	57.693	1.00 58.35	1SG1812
ATOM	1812	CG2	VAL	229	133.532	15.414	55.906	1.00 58.35	1SG1813
ATOM	1813	C	VAL	229	131.831	18.612	56.900	1.00 58.35	1SG1814
ATOM	1814	O	VAL	229	130.604	18.631	56.840	1.00 58.35	1SG1815
ATOM	1815	N	LYS	230	132.509	19.462	57.689	1.00 81.41	1SG1816
ATOM	1816	CA	LYS	230	131.750	20.333	58.536	1.00 81.41	1SG1817
ATOM	1817	CB	LYS	230	132.586	21.186	59.506	1.00 81.41	1SG1818
ATOM	1818	CG	LYS	230	133.230	20.367	60.627	1.00 81.41	1SG1819
ATOM	1819	CD	LYS	230	134.068	21.202	61.594	1.00 81.41	1SG1820
ATOM	1820	CE	LYS	230	134.951	22.248	60.915	1.00 81.41	1SG1821
ATOM	1821	NZ	LYS	230	135.522	23.156	61.934	1.00 81.41	1SG1822
ATOM	1822	C	LYS	230	130.931	21.246	57.685	1.00 81.41	1SG1823
ATOM	1823	O	LYS	230	129.782	21.537	58.017	1.00 81.41	1SG1824
ATOM	1824	N	TYR	231	131.494	21.723	56.561	1.00 42.15	1SG1825
ATOM	1825	CA	TYR	231	130.778	22.630	55.713	1.00 42.15	1SG1826
ATOM	1826	CB	TYR	231	131.626	23.186	54.556	1.00 42.15	1SG1827
ATOM	1827	CG	TYR	231	130.779	24.177	53.829	1.00 42.15	1SG1828
ATOM	1828	CD1	TYR	231	130.651	25.463	54.302	1.00 42.15	1SG1829
ATOM	1829	CD2	TYR	231	130.112	23.823	52.679	1.00 42.15	1SG1830
ATOM	1830	CE1	TYR	231	129.873	26.384	53.640	1.00 42.15	1SG1831
ATOM	1831	CE2	TYR	231	129.332	24.740	52.012	1.00 42.15	1SG1832
ATOM	1832	CZ	TYR	231	129.210	26.021	52.492	1.00 42.15	1SG1833
ATOM	1833	OH	TYR	231	128.409	26.961	51.808	1.00 42.15	1SG1834
ATOM	1834	C	TYR	231	129.589	21.931	55.121	1.00 42.15	1SG1835
ATOM	1835	O	TYR	231	128.511	22.512	55.017	1.00 42.15	1SG1836
ATOM	1836	N	ALA	232	129.756	20.656	54.716	1.00 33.88	1SG1837
ATOM	1837	CA	ALA	232	128.706	19.917	54.068	1.00 33.88	1SG1838
ATOM	1838	CB	ALA	232	129.143	18.495	53.677	1.00 33.88	1SG1839
ATOM	1839	C	ALA	232	127.529	19.787	54.981	1.00 33.88	1SG1840
ATOM	1840	O	ALA	232	126.388	19.940	54.550	1.00 33.88	1SG1841
ATOM	1841	N	LEU	233	127.764	19.506	56.275	1.00102.39	1SG1842
ATOM	1842	CA	LEU	233	126.645	19.363	57.156	1.00102.39	1SG1843
ATOM	1843	CB	LEU	233	127.012	18.891	58.571	1.00102.39	1SG1844
ATOM	1844	CG	LEU	233	127.341	17.385	58.608	1.00102.39	1SG1845

Supplementary material 1.txt

ATOM	1845	CD2	LEU	233	127.478	16.872	60.047	1.00102.39	1SG1846
ATOM	1846	CD1	LEU	233	128.555	17.046	57.736	1.00102.39	1SG1847
ATOM	1847	C	LEU	233	125.916	20.665	57.225	1.00102.39	1SG1848
ATOM	1848	O	LEU	233	124.692	20.684	57.342	1.00102.39	1SG1849
ATOM	1849	N	GLU	234	126.655	21.789	57.204	1.0044.04	1SG1850
ATOM	1850	CA	GLU	234	126.032	23.082	57.234	1.0044.04	1SG1851
ATOM	1851	CB	GLU	234	127.048	24.212	57.464	1.0044.04	1SG1852
ATOM	1852	CG	GLU	234	127.714	24.132	58.838	1.0044.04	1SG1853
ATOM	1853	CD	GLU	234	128.693	25.291	58.957	1.0044.04	1SG1854
ATOM	1854	OE1	GLU	234	128.715	26.140	58.026	1.0044.04	1SG1855
ATOM	1855	OE2	GLU	234	129.429	25.344	59.978	1.0044.04	1SG1856
ATOM	1856	C	GLU	234	125.318	23.351	55.938	1.0044.04	1SG1857
ATOM	1857	O	GLU	234	124.181	23.827	55.946	1.0044.04	1SG1858
ATOM	1858	N	PHE	235	125.961	23.060	54.784	1.0068.11	1SG1859
ATOM	1859	CA	PHE	235	125.318	23.343	53.528	1.0068.11	1SG1860
ATOM	1860	CB	PHE	235	125.807	24.654	52.890	1.0068.11	1SG1861
ATOM	1861	CG	PHE	235	125.619	25.756	53.874	1.0068.11	1SG1862
ATOM	1862	CD1	PHE	235	126.547	25.948	54.872	1.0068.11	1SG1863
ATOM	1863	CD2	PHE	235	124.537	26.602	53.799	1.0068.11	1SG1864
ATOM	1864	CE1	PHE	235	126.395	26.960	55.789	1.0068.11	1SG1865
ATOM	1865	CE2	PHE	235	124.380	27.617	54.714	1.0068.11	1SG1866
ATOM	1866	CZ	PHE	235	125.310	27.799	55.710	1.0068.11	1SG1867
ATOM	1867	C	PHE	235	125.688	22.270	52.543	1.0068.11	1SG1868
ATOM	1868	O	PHE	235	126.866	22.029	52.289	1.0068.11	1SG1869
ATOM	1869	N	PRO	236	124.702	21.633	51.966	1.00148.11	1SG1870
ATOM	1870	CA	PRO	236	124.981	20.642	50.958	1.00148.11	1SG1871
ATOM	1871	CD	PRO	236	123.534	21.274	52.758	1.00148.11	1SG1872
ATOM	1872	CB	PRO	236	123.746	19.747	50.888	1.00148.11	1SG1873
ATOM	1873	CG	PRO	236	123.132	19.866	52.292	1.00148.11	1SG1874
ATOM	1874	C	PRO	236	125.300	21.310	49.655	1.00148.11	1SG1875
ATOM	1875	O	PRO	236	124.950	22.475	49.481	1.00148.11	1SG1876
ATOM	1876	N	TRP	237	125.972	20.592	48.735	1.00100.97	1SG1877
ATOM	1877	CA	TRP	237	126.370	21.111	47.455	1.00100.97	1SG1878
ATOM	1878	CB	TRP	237	127.238	20.107	46.677	1.00100.97	1SG1879
ATOM	1879	CG	TRP	237	127.651	20.567	45.300	1.00100.97	1SG1880
ATOM	1880	CD2	TRP	237	128.782	21.410	45.032	1.00100.97	1SG1881
ATOM	1881	CD1	TRP	237	127.072	20.299	44.095	1.00100.97	1SG1882
ATOM	1882	NE1	TRP	237	127.775	20.917	43.089	1.00100.97	1SG1883
ATOM	1883	CE2	TRP	237	128.829	21.606	43.651	1.00100.97	1SG1884
ATOM	1884	CE3	TRP	237	129.704	21.974	45.865	1.00100.97	1SG1885
ATOM	1885	CZ2	TRP	237	129.806	22.373	43.082	1.00100.97	1SG1886
ATOM	1886	CZ3	TRP	237	130.688	22.746	45.287	1.00100.97	1SG1887
ATOM	1887	CH2	TRP	237	130.737	22.941	43.923	1.00100.97	1SG1888
ATOM	1888	C	TRP	237	125.182	21.427	46.594	1.00100.97	1SG1889
ATOM	1889	O	TRP	237	125.127	22.486	45.968	1.00100.97	1SG1890
ATOM	1890	N	HIS	238	124.195	20.512	46.545	1.0062.60	1SG1891
ATOM	1891	CA	HIS	238	123.080	20.626	45.645	1.0062.60	1SG1892
ATOM	1892	ND1	HIS	238	121.249	19.304	43.331	1.0062.60	1SG1893
ATOM	1893	CG	HIS	238	121.048	19.439	44.686	1.0062.60	1SG1894
ATOM	1894	CB	HIS	238	122.154	19.396	45.699	1.0062.60	1SG1895
ATOM	1895	NE2	HIS	238	119.059	19.555	43.625	1.0062.60	1SG1896
ATOM	1896	CD2	HIS	238	119.704	19.593	44.848	1.0062.60	1SG1897
ATOM	1897	CE1	HIS	238	120.028	19.381	42.744	1.0062.60	1SG1898
ATOM	1898	C	HIS	238	122.245	21.839	45.925	1.0062.60	1SG1899
ATOM	1899	O	HIS	238	121.856	22.544	44.994	1.0062.60	1SG1900
ATOM	1900	N	CYS	239	121.940	22.130	47.204	1.00136.86	1SG1901
ATOM	1901	CA	CYS	239	121.055	23.236	47.442	1.00136.86	1SG1902
ATOM	1902	CB	CYS	239	120.058	22.958	48.579	1.00136.86	1SG1903
ATOM	1903	SG	CYS	239	120.887	22.555	50.145	1.00136.86	1SG1904
ATOM	1904	C	CYS	239	121.821	24.473	47.805	1.00136.86	1SG1905
ATOM	1905	O	CYS	239	121.297	25.347	48.497	1.00136.86	1SG1906
ATOM	1906	N	SER	240	123.060	24.621	47.298	1.0094.34	1SG1907
ATOM	1907	CA	SER	240	123.814	25.797	47.632	1.0094.34	1SG1908
ATOM	1908	CB	SER	240	125.190	25.512	48.245	1.0094.34	1SG1909
ATOM	1909	OG	SER	240	125.041	25.048	49.578	1.0094.34	1SG1910
ATOM	1910	C	SER	240	124.059	26.587	46.386	1.0094.34	1SG1911
ATOM	1911	O	SER	240	123.879	26.092	45.276	1.0094.34	1SG1912
ATOM	1912	N	VAL	241	124.457	27.867	46.556	1.0049.91	1SG1913
ATOM	1913	CA	VAL	241	124.731	28.727	45.436	1.0049.91	1SG1914
ATOM	1914	CB	VAL	241	124.772	30.183	45.803	1.0049.91	1SG1915
ATOM	1915	CG1	VAL	241	125.157	30.998	44.558	1.0049.91	1SG1916

Supplementary material 1.txt

ATOM	1916	CG2	VAL	241	123.408	30.570	46.399	1.00	49.91	1SG1917
ATOM	1917	C	VAL	241	126.072	28.348	44.870	1.00	49.91	1SG1918
ATOM	1918	O	VAL	241	127.034	28.127	45.602	1.00	49.91	1SG1919
ATOM	1919	N	GLN	242	126.171	28.303	43.526	1.00	60.63	1SG1920
ATOM	1920	CA	GLN	242	127.342	27.821	42.840	1.00	60.63	1SG1921
ATOM	1921	CB	GLN	242	127.167	27.833	41.313	1.00	60.63	1SG1922
ATOM	1922	CG	GLN	242	126.092	26.872	40.803	1.00	60.63	1SG1923
ATOM	1923	CD	GLN	242	126.026	27.016	39.289	1.00	60.63	1SG1924
ATOM	1924	OE1	GLN	242	125.228	26.357	38.625	1.00	60.63	1SG1925
ATOM	1925	NE2	GLN	242	126.880	27.913	38.727	1.00	60.63	1SG1926
ATOM	1926	C	GLN	242	128.574	28.631	43.138	1.00	60.63	1SG1927
ATOM	1927	O	GLN	242	129.618	28.064	43.453	1.00	60.63	1SG1928
ATOM	1928	N	ARG	243	128.504	29.974	43.057	1.00	164.32	1SG1929
ATOM	1929	CA	ARG	243	129.683	30.768	43.268	1.00	164.32	1SG1930
ATOM	1930	CB	ARG	243	129.435	32.263	43.023	1.00	164.32	1SG1931
ATOM	1931	CG	ARG	243	129.181	32.588	41.552	1.00	164.32	1SG1932
ATOM	1932	CD	ARG	243	130.353	33.297	40.872	1.00	164.32	1SG1933
ATOM	1933	NE	ARG	243	131.567	32.443	41.008	1.00	164.32	1SG1934
ATOM	1934	CZ	ARG	243	131.827	31.456	40.101	1.00	164.32	1SG1935
ATOM	1935	NH1	ARG	243	130.904	31.137	39.150	1.00	164.32	1SG1936
ATOM	1936	NH2	ARG	243	133.022	30.799	40.134	1.00	164.32	1SG1937
ATOM	1937	C	ARG	243	130.141	30.610	44.683	1.00	164.32	1SG1938
ATOM	1938	O	ARG	243	131.334	30.455	44.943	1.00	164.32	1SG1939
ATOM	1939	N	TRP	244	129.193	30.623	45.640	1.00	150.06	1SG1940
ATOM	1940	CA	TRP	244	129.563	30.547	47.024	1.00	150.06	1SG1941
ATOM	1941	CB	TRP	244	128.382	30.654	48.002	1.00	150.06	1SG1942
ATOM	1942	CG	TRP	244	128.804	30.407	49.432	1.00	150.06	1SG1943
ATOM	1943	CD2	TRP	244	129.569	31.332	50.221	1.00	150.06	1SG1944
ATOM	1944	CD1	TRP	244	128.616	29.301	50.208	1.00	150.06	1SG1945
ATOM	1945	NE1	TRP	244	129.212	29.480	51.434	1.00	150.06	1SG1946
ATOM	1946	CE2	TRP	244	129.805	30.724	51.454	1.00	150.06	1SG1947
ATOM	1947	CE3	TRP	244	130.044	32.580	49.938	1.00	150.06	1SG1948
ATOM	1948	CZ2	TRP	244	130.523	31.360	52.427	1.00	150.06	1SG1949
ATOM	1949	CZ3	TRP	244	130.761	33.220	50.924	1.00	150.06	1SG1950
ATOM	1950	CH2	TRP	244	130.997	32.622	52.145	1.00	150.06	1SG1951
ATOM	1951	C	TRP	244	130.257	29.256	47.306	1.00	150.06	1SG1952
ATOM	1952	O	TRP	244	131.259	29.230	48.018	1.00	150.06	1SG1953
ATOM	1953	N	GLU	245	129.731	28.141	46.775	1.00	83.85	1SG1954
ATOM	1954	CA	GLU	245	130.336	26.867	47.031	1.00	83.85	1SG1955
ATOM	1955	CB	GLU	245	129.502	25.696	46.485	1.00	83.85	1SG1956
ATOM	1956	CG	GLU	245	128.163	25.558	47.211	1.00	83.85	1SG1957
ATOM	1957	CD	GLU	245	128.474	25.371	48.688	1.00	83.85	1SG1958
ATOM	1958	OE1	GLU	245	129.604	24.903	48.986	1.00	83.85	1SG1959
ATOM	1959	OE2	GLU	245	127.599	25.688	49.537	1.00	83.85	1SG1960
ATOM	1960	C	GLU	245	131.689	26.823	46.390	1.00	83.85	1SG1961
ATOM	1961	O	GLU	245	132.632	26.267	46.951	1.00	83.85	1SG1962
ATOM	1962	N	ALA	246	131.814	27.402	45.182	1.00	41.82	1SG1963
ATOM	1963	CA	ALA	246	133.062	27.357	44.475	1.00	41.82	1SG1964
ATOM	1964	CB	ALA	246	132.974	28.016	43.087	1.00	41.82	1SG1965
ATOM	1965	C	ALA	246	134.111	28.096	45.246	1.00	41.82	1SG1966
ATOM	1966	O	ALA	246	135.214	27.590	45.447	1.00	41.82	1SG1967
ATOM	1967	N	ARG	247	133.790	29.306	45.740	1.00	106.10	1SG1968
ATOM	1968	CA	ARG	247	134.812	30.060	46.402	1.00	106.10	1SG1969
ATOM	1969	CB	ARG	247	134.390	31.482	46.802	1.00	106.10	1SG1970
ATOM	1970	CG	ARG	247	135.498	32.211	47.561	1.00	106.10	1SG1971
ATOM	1971	CD	ARG	247	135.515	33.723	47.348	1.00	106.10	1SG1972
ATOM	1972	NE	ARG	247	136.435	34.292	48.372	1.00	106.10	1SG1973
ATOM	1973	CZ	ARG	247	137.785	34.203	48.211	1.00	106.10	1SG1974
ATOM	1974	NH1	ARG	247	138.301	33.525	47.145	1.00	106.10	1SG1975
ATOM	1975	NH2	ARG	247	138.622	34.773	49.127	1.00	106.10	1SG1976
ATOM	1976	C	ARG	247	135.262	29.326	47.617	1.00	106.10	1SG1977
ATOM	1977	O	ARG	247	136.456	29.269	47.912	1.00	106.10	1SG1978
ATOM	1978	N	SER	248	134.313	28.724	48.350	1.00	76.13	1SG1979
ATOM	1979	CA	SER	248	134.680	28.029	49.541	1.00	76.13	1SG1980
ATOM	1980	CB	SER	248	133.474	27.417	50.272	1.00	76.13	1SG1981
ATOM	1981	OG	SER	248	133.905	26.743	51.445	1.00	76.13	1SG1982
ATOM	1982	C	SER	248	135.586	26.911	49.169	1.00	76.13	1SG1983
ATOM	1983	O	SER	248	136.595	26.699	49.827	1.00	76.13	1SG1984
ATOM	1984	N	PHE	249	135.261	26.178	48.092	1.00	86.68	1SG1985
ATOM	1985	CA	PHE	249	136.009	25.021	47.700	1.00	86.68	1SG1986
ATOM	1986	CB	PHE	249	135.306	24.324	46.519	1.00	86.68	1SG1987

Supplementary material 1.txt

ATOM	1987	CG	PHE	249	135.926	23.005	46.213	1.00	86.68	1SG1988
ATOM	1988	CD1	PHE	249	135.857	21.972	47.120	1.00	86.68	1SG1989
ATOM	1989	CD2	PHE	249	136.525	22.787	44.995	1.00	86.68	1SG1990
ATOM	1990	CE1	PHE	249	136.413	20.749	46.831	1.00	86.68	1SG1991
ATOM	1991	CE2	PHE	249	137.080	21.565	44.700	1.00	86.68	1SG1992
ATOM	1992	CZ	PHE	249	137.029	20.545	45.619	1.00	86.68	1SG1993
ATOM	1993	C	PHE	249	137.416	25.387	47.316	1.00	86.68	1SG1994
ATOM	1994	O	PHE	249	138.368	24.793	47.821	1.00	86.68	1SG1995
ATOM	1995	N	ILE	250	137.604	26.381	46.423	1.00144.79		1SG1996
ATOM	1996	CA	ILE	250	138.945	26.579	45.945	1.00144.79		1SG1997
ATOM	1997	CB	ILE	250	139.053	27.461	44.726	1.00144.79		1SG1998
ATOM	1998	CG2	ILE	250	140.544	27.789	44.543	1.00144.79		1SG1999
ATOM	1999	CG1	ILE	250	138.418	26.834	43.473	1.00144.79		1SG2000
ATOM	2000	CD1	ILE	250	136.904	26.987	43.384	1.00144.79		1SG2001
ATOM	2001	C	ILE	250	139.968	27.161	46.897	1.00144.79		1SG2002
ATOM	2002	O	ILE	250	140.963	26.501	47.190	1.00144.79		1SG2003
ATOM	2003	N	GLU	251	139.776	28.396	47.419	1.00211.44		1SG2004
ATOM	2004	CA	GLU	251	141.012	28.970	47.911	1.00211.44		1SG2005
ATOM	2005	CB	GLU	251	140.975	30.499	47.991	1.00211.44		1SG2006
ATOM	2006	CG	GLU	251	141.102	31.152	46.620	1.00211.44		1SG2007
ATOM	2007	CD	GLU	251	142.475	30.796	46.061	1.00211.44		1SG2008
ATOM	2008	OE1	GLU	251	143.448	31.538	46.360	1.00211.44		1SG2009
ATOM	2009	OE2	GLU	251	142.570	29.770	45.334	1.00211.44		1SG2010
ATOM	2010	C	GLU	251	141.676	28.522	49.172	1.00211.44		1SG2011
ATOM	2011	O	GLU	251	142.003	27.352	49.364	1.00211.44		1SG2012
ATOM	2012	N	ILE	252	141.830	29.506	50.097	1.00240.05		1SG2013
ATOM	2013	CA	ILE	252	142.565	29.298	51.313	1.00240.05		1SG2014
ATOM	2014	CB	ILE	252	143.015	30.586	51.978	1.00240.05		1SG2015
ATOM	2015	CG2	ILE	252	141.798	31.437	52.375	1.00240.05		1SG2016
ATOM	2016	CG1	ILE	252	144.009	30.310	53.124	1.00240.05		1SG2017
ATOM	2017	CD1	ILE	252	143.434	29.538	54.312	1.00240.05		1SG2018
ATOM	2018	C	ILE	252	141.694	28.496	52.180	1.00240.05		1SG2019
ATOM	2019	O	ILE	252	142.086	27.461	52.717	1.00240.05		1SG2020
ATOM	2020	N	PHE	253	140.451	28.972	52.314	1.00289.37		1SG2021
ATOM	2021	CA	PHE	253	139.509	28.150	52.960	1.00289.37		1SG2022
ATOM	2022	CB	PHE	253	138.246	28.884	53.434	1.00289.37		1SG2023
ATOM	2023	CG	PHE	253	137.440	27.901	54.209	1.00289.37		1SG2024
ATOM	2024	CD1	PHE	253	137.694	27.690	55.545	1.00289.37		1SG2025
ATOM	2025	CD2	PHE	253	136.433	27.189	53.602	1.00289.37		1SG2026
ATOM	2026	CE1	PHE	253	136.954	26.783	56.267	1.00289.37		1SG2027
ATOM	2027	CE2	PHE	253	135.690	26.280	54.318	1.00289.37		1SG2028
ATOM	2028	CZ	PHE	253	135.948	26.077	55.652	1.00289.37		1SG2029
ATOM	2029	C	PHE	253	139.162	27.305	51.806	1.00289.37		1SG2030
ATOM	2030	O	PHE	253	139.151	27.781	50.672	1.00289.37		1SG2031
ATOM	2031	N	GLY	254	138.886	26.026	52.028	1.00365.59		1SG2032
ATOM	2032	CA	GLY	254	138.650	25.271	50.854	1.00365.59		1SG2033
ATOM	2033	C	GLY	254	139.524	24.084	50.828	1.00365.59		1SG2034
ATOM	2034	O	GLY	254	140.607	24.052	51.406	1.00365.59		1SG2035
ATOM	2035	N	GLN	255	138.992	23.034	50.193	1.00168.56		1SG2036
ATOM	2036	CA	GLN	255	139.680	21.794	50.108	1.00168.56		1SG2037
ATOM	2037	CB	GLN	255	138.795	20.621	49.648	1.00168.56		1SG2038
ATOM	2038	CG	GLN	255	137.736	20.182	50.660	1.00168.56		1SG2039
ATOM	2039	CD	GLN	255	136.533	21.104	50.534	1.00168.56		1SG2040
ATOM	2040	OE1	GLN	255	136.584	22.286	50.869	1.00168.56		1SG2041
ATOM	2041	NE2	GLN	255	135.403	20.541	50.031	1.00168.56		1SG2042
ATOM	2042	C	GLN	255	140.812	21.843	49.147	1.00168.56		1SG2043
ATOM	2043	O	GLN	255	141.895	21.353	49.454	1.00168.56		1SG2044
ATOM	2044	N	ILE	256	140.599	22.449	47.963	1.00118.43		1SG2045
ATOM	2045	CA	ILE	256	141.578	22.282	46.927	1.00118.43		1SG2046
ATOM	2046	CB	ILE	256	141.135	22.773	45.580	1.00118.43		1SG2047
ATOM	2047	CG2	ILE	256	139.973	21.887	45.123	1.00118.43		1SG2048
ATOM	2048	CG1	ILE	256	140.825	24.275	45.596	1.00118.43		1SG2049
ATOM	2049	CD1	ILE	256	140.572	24.849	44.203	1.00118.43		1SG2050
ATOM	2050	C	ILE	256	142.908	22.891	47.226	1.00118.43		1SG2051
ATOM	2051	O	ILE	256	143.924	22.212	47.083	1.00118.43		1SG2052
ATOM	2052	N	ASP	257	142.967	24.165	47.659	1.00	90.12	1SG2053
ATOM	2053	CA	ASP	257	144.274	24.728	47.863	1.00	90.12	1SG2054
ATOM	2054	CB	ASP	257	144.277	26.177	48.382	1.00	90.12	1SG2055
ATOM	2055	CG	ASP	257	143.856	27.130	47.276	1.00	90.12	1SG2056
ATOM	2056	OD1	ASP	257	143.539	26.645	46.161	1.00	90.12	1SG2057
ATOM	2057	OD2	ASP	257	143.861	28.364	47.529	1.00	90.12	1SG2058

Supplementary material 1.txt

ATOM	2058	C	ASP	257	144.951	23.944	48.937	1.00	90.12	1SG2059
ATOM	2059	O	ASP	257	146.127	23.601	48.832	1.00	90.12	1SG2060
ATOM	2060	N	SER	258	144.197	23.638	50.004	1.00	91.24	1SG2061
ATOM	2061	CA	SER	258	144.710	22.952	51.153	1.00	91.24	1SG2062
ATOM	2062	CB	SER	258	143.748	23.005	52.351	1.00	91.24	1SG2063
ATOM	2063	OG	SER	258	144.309	22.310	53.455	1.00	91.24	1SG2064
ATOM	2064	C	SER	258	144.965	21.502	50.861	1.00	91.24	1SG2065
ATOM	2065	O	SER	258	145.603	20.820	51.662	1.00	91.24	1SG2066
ATOM	2066	N	GLU	259	144.465	20.976	49.726	1.00	83.72	1SG2067
ATOM	2067	CA	GLU	259	144.609	19.571	49.468	1.00	83.72	1SG2068
ATOM	2068	CB	GLU	259	143.890	19.109	48.188	1.00	83.72	1SG2069
ATOM	2069	CG	GLU	259	143.837	17.588	48.033	1.00	83.72	1SG2070
ATOM	2070	CD	GLU	259	142.793	17.060	49.005	1.00	83.72	1SG2071
ATOM	2071	OE1	GLU	259	141.906	17.857	49.411	1.00	83.72	1SG2072
ATOM	2072	OE2	GLU	259	142.868	15.852	49.356	1.00	83.72	1SG2073
ATOM	2073	C	GLU	259	146.062	19.242	49.340	1.00	83.72	1SG2074
ATOM	2074	O	GLU	259	146.806	19.925	48.637	1.00	83.72	1SG2075
ATOM	2075	N	LEU	260	146.498	18.170	50.037	1.00	57.26	1SG2076
ATOM	2076	CA	LEU	260	147.876	17.779	50.009	1.00	57.26	1SG2077
ATOM	2077	CB	LEU	260	148.183	16.586	50.935	1.00	57.26	1SG2078
ATOM	2078	CG	LEU	260	149.664	16.159	50.918	1.00	57.26	1SG2079
ATOM	2079	CD2	LEU	260	149.877	14.842	51.690	1.00	57.26	1SG2080
ATOM	2080	CD1	LEU	260	150.577	17.287	51.415	1.00	57.26	1SG2081
ATOM	2081	C	LEU	260	148.216	17.369	48.619	1.00	57.26	1SG2082
ATOM	2082	O	LEU	260	149.206	17.831	48.054	1.00	57.26	1SG2083
ATOM	2083	N	LYS	261	147.389	16.497	48.013	1.00	219.81	1SG2084
ATOM	2084	CA	LYS	261	147.707	16.123	46.673	1.00	219.81	1SG2085
ATOM	2085	CB	LYS	261	147.913	14.612	46.468	1.00	219.81	1SG2086
ATOM	2086	CG	LYS	261	148.462	14.278	45.081	1.00	219.81	1SG2087
ATOM	2087	CD	LYS	261	149.010	12.856	44.944	1.00	219.81	1SG2088
ATOM	2088	CE	LYS	261	147.998	11.855	44.385	1.00	219.81	1SG2089
ATOM	2089	NZ	LYS	261	146.929	11.608	45.377	1.00	219.81	1SG2090
ATOM	2090	C	LYS	261	146.570	16.544	45.816	1.00	219.81	1SG2091
ATOM	2091	O	LYS	261	145.650	15.774	45.544	1.00	219.81	1SG2092
ATOM	2092	N	SER	262	146.619	17.801	45.355	1.00	109.28	1SG2093
ATOM	2093	CA	SER	262	145.595	18.283	44.490	1.00	109.28	1SG2094
ATOM	2094	CB	SER	262	144.678	19.342	45.130	1.00	109.28	1SG2095
ATOM	2095	OG	SER	262	143.694	19.765	44.198	1.00	109.28	1SG2096
ATOM	2096	C	SER	262	146.320	18.927	43.369	1.00	109.28	1SG2097
ATOM	2097	O	SER	262	147.542	19.069	43.409	1.00	109.28	1SG2098
ATOM	2098	N	ASN	263	145.594	19.301	42.308	1.00	113.71	1SG2099
ATOM	2099	CA	ASN	263	146.290	19.966	41.255	1.00	113.71	1SG2100
ATOM	2100	CB	ASN	263	145.481	19.970	39.946	1.00	113.71	1SG2101
ATOM	2101	CG	ASN	263	145.534	18.568	39.360	1.00	113.71	1SG2102
ATOM	2102	OD1	ASN	263	146.252	18.322	38.392	1.00	113.71	1SG2103
ATOM	2103	ND2	ASN	263	144.774	17.621	39.971	1.00	113.71	1SG2104
ATOM	2104	C	ASN	263	146.423	21.392	41.699	1.00	113.71	1SG2105
ATOM	2105	O	ASN	263	146.021	22.295	40.970	1.00	113.71	1SG2106
ATOM	2106	N	LEU	264	147.000	21.622	42.906	1.00	94.18	1SG2107
ATOM	2107	CA	LEU	264	147.117	22.950	43.452	1.00	94.18	1SG2108
ATOM	2108	CB	LEU	264	147.860	22.993	44.799	1.00	94.18	1SG2109
ATOM	2109	CG	LEU	264	147.275	22.168	45.955	1.00	94.18	1SG2110
ATOM	2110	CD2	LEU	264	148.049	22.442	47.256	1.00	94.18	1SG2111
ATOM	2111	CD1	LEU	264	147.259	20.671	45.622	1.00	94.18	1SG2112
ATOM	2112	C	LEU	264	148.017	23.742	42.573	1.00	94.18	1SG2113
ATOM	2113	O	LEU	264	147.616	24.725	41.952	1.00	94.18	1SG2114
ATOM	2114	N	SER	265	149.280	23.286	42.497	1.00	87.80	1SG2115
ATOM	2115	CA	SER	265	150.254	23.923	41.674	1.00	87.80	1SG2116
ATOM	2116	CB	SER	265	151.687	23.442	41.949	1.00	87.80	1SG2117
ATOM	2117	OG	SER	265	152.596	24.116	41.091	1.00	87.80	1SG2118
ATOM	2118	C	SER	265	149.888	23.487	40.315	1.00	87.80	1SG2119
ATOM	2119	O	SER	265	150.247	24.104	39.313	1.00	87.80	1SG2120
ATOM	2120	N	LYS	266	149.117	22.389	40.279	1.00	195.24	1SG2121
ATOM	2121	CA	LYS	266	148.757	21.821	39.031	1.00	195.24	1SG2122
ATOM	2122	CB	LYS	266	148.269	20.369	39.103	1.00	195.24	1SG2123
ATOM	2123	CG	LYS	266	149.420	19.387	39.325	1.00	195.24	1SG2124
ATOM	2124	CD	LYS	266	148.978	17.979	39.724	1.00	195.24	1SG2125
ATOM	2125	CE	LYS	266	150.137	16.985	39.829	1.00	195.24	1SG2126
ATOM	2126	NZ	LYS	266	151.026	17.357	40.951	1.00	195.24	1SG2127
ATOM	2127	C	LYS	266	147.754	22.684	38.360	1.00	195.24	1SG2128
ATOM	2128	O	LYS	266	147.306	23.706	38.880	1.00	195.24	1SG2129

Supplementary material 1.txt

ATOM	2129	N	LYS	267	147.406	22.259	37.141	1.00152.66	1SG2130
ATOM	2130	CA	LYS	267	146.617	23.014	36.224	1.00152.66	1SG2131
ATOM	2131	CB	LYS	267	146.417	22.272	34.894	1.00152.66	1SG2132
ATOM	2132	CG	LYS	267	147.736	21.886	34.220	1.00152.66	1SG2133
ATOM	2133	CD	LYS	267	148.645	23.073	33.897	1.00152.66	1SG2134
ATOM	2134	CE	LYS	267	150.029	22.659	33.391	1.00152.66	1SG2135
ATOM	2135	NZ	LYS	267	150.776	21.971	34.469	1.00152.66	1SG2136
ATOM	2136	C	LYS	267	145.256	23.320	36.761	1.00152.66	1SG2137
ATOM	2137	O	LYS	267	144.765	24.431	36.580	1.00152.66	1SG2138
ATOM	2138	N	MET	268	144.602	22.353	37.427	1.00107.32	1SG2139
ATOM	2139	CA	MET	268	143.239	22.551	37.831	1.00107.32	1SG2140
ATOM	2140	CB	MET	268	142.644	21.297	38.487	1.00107.32	1SG2141
ATOM	2141	CG	MET	268	142.654	20.075	37.564	1.00107.32	1SG2142
ATOM	2142	SD	MET	268	141.655	20.248	36.056	1.00107.32	1SG2143
ATOM	2143	CE	MET	268	141.992	18.568	35.453	1.00107.32	1SG2144
ATOM	2144	C	MET	268	143.114	23.679	38.811	1.00107.32	1SG2145
ATOM	2145	O	MET	268	142.224	24.519	38.684	1.00107.32	1SG2146
ATOM	2146	N	LEU	269	144.004	23.731	39.821	1.00 56.95	1SG2147
ATOM	2147	CA	LEU	269	143.902	24.750	40.829	1.00 56.95	1SG2148
ATOM	2148	CB	LEU	269	144.878	24.555	41.999	1.00 56.95	1SG2149
ATOM	2149	CG	LEU	269	144.757	25.655	43.062	1.00 56.95	1SG2150
ATOM	2150	CD2	LEU	269	145.798	25.492	44.179	1.00 56.95	1SG2151
ATOM	2151	CD1	LEU	269	143.322	25.710	43.600	1.00 56.95	1SG2152
ATOM	2152	C	LEU	269	144.170	26.097	40.242	1.00 56.95	1SG2153
ATOM	2153	O	LEU	269	143.476	27.065	40.550	1.00 56.95	1SG2154
ATOM	2154	N	GLU	270	145.196	26.199	39.378	1.00 64.07	1SG2155
ATOM	2155	CA	GLU	270	145.545	27.468	38.813	1.00 64.07	1SG2156
ATOM	2156	CB	GLU	270	146.806	27.412	37.938	1.00 64.07	1SG2157
ATOM	2157	CG	GLU	270	146.675	26.475	36.738	1.00 64.07	1SG2158
ATOM	2158	CD	GLU	270	147.925	26.638	35.890	1.00 64.07	1SG2159
ATOM	2159	OE1	GLU	270	148.534	27.740	35.943	1.00 64.07	1SG2160
ATOM	2160	OE2	GLU	270	148.286	25.664	35.177	1.00 64.07	1SG2161
ATOM	2161	C	GLU	270	144.421	27.940	37.950	1.00 64.07	1SG2162
ATOM	2162	O	GLU	270	144.069	29.118	37.961	1.00 64.07	1SG2163
ATOM	2163	N	LEU	271	143.819	27.015	37.183	1.00 99.76	1SG2164
ATOM	2164	CA	LEU	271	142.775	27.374	36.271	1.00 99.76	1SG2165
ATOM	2165	CB	LEU	271	142.266	26.166	35.459	1.00 99.76	1SG2166
ATOM	2166	CG	LEU	271	141.255	26.506	34.342	1.00 99.76	1SG2167
ATOM	2167	CD2	LEU	271	141.868	27.498	33.342	1.00 99.76	1SG2168
ATOM	2168	CD1	LEU	271	139.894	26.967	34.889	1.00 99.76	1SG2169
ATOM	2169	C	LEU	271	141.628	27.921	37.063	1.00 99.76	1SG2170
ATOM	2170	O	LEU	271	141.051	28.944	36.697	1.00 99.76	1SG2171
ATOM	2171	N	ALA	272	141.281	27.257	38.182	1.00 45.89	1SG2172
ATOM	2172	CA	ALA	272	140.146	27.642	38.970	1.00 45.89	1SG2173
ATOM	2173	CB	ALA	272	139.899	26.694	40.156	1.00 45.89	1SG2174
ATOM	2174	C	ALA	272	140.334	29.021	39.527	1.00 45.89	1SG2175
ATOM	2175	O	ALA	272	139.411	29.833	39.494	1.00 45.89	1SG2176
ATOM	2176	N	LYS	273	141.536	29.325	40.052	1.00 59.36	1SG2177
ATOM	2177	CA	LYS	273	141.782	30.597	40.672	1.00 59.36	1SG2178
ATOM	2178	CB	LYS	273	143.182	30.700	41.298	1.00 59.36	1SG2179
ATOM	2179	CG	LYS	273	143.393	29.798	42.513	1.00 59.36	1SG2180
ATOM	2180	CD	LYS	273	144.859	29.709	42.941	1.00 59.36	1SG2181
ATOM	2181	CE	LYS	273	145.078	28.903	44.221	1.00 59.36	1SG2182
ATOM	2182	NZ	LYS	273	146.518	28.871	44.558	1.00 59.36	1SG2183
ATOM	2183	C	LYS	273	141.692	31.712	39.672	1.00 59.36	1SG2184
ATOM	2184	O	LYS	273	141.069	32.739	39.937	1.00 59.36	1SG2185
ATOM	2185	N	LEU	274	142.318	31.537	38.495	1.00 53.24	1SG2186
ATOM	2186	CA	LEU	274	142.359	32.575	37.502	1.00 53.24	1SG2187
ATOM	2187	CB	LEU	274	143.183	32.180	36.262	1.00 53.24	1SG2188
ATOM	2188	CG	LEU	274	144.684	31.964	36.536	1.00 53.24	1SG2189
ATOM	2189	CD2	LEU	274	145.314	33.178	37.234	1.00 53.24	1SG2190
ATOM	2190	CD1	LEU	274	145.428	31.574	35.249	1.00 53.24	1SG2191
ATOM	2191	C	LEU	274	140.975	32.877	37.019	1.00 53.24	1SG2192
ATOM	2192	O	LEU	274	140.583	34.039	36.917	1.00 53.24	1SG2193
ATOM	2193	N	ASP	275	140.195	31.822	36.726	1.00 69.26	1SG2194
ATOM	2194	CA	ASP	275	138.877	31.956	36.169	1.00 69.26	1SG2195
ATOM	2195	CB	ASP	275	138.267	30.573	35.863	1.00 69.26	1SG2196
ATOM	2196	CG	ASP	275	136.936	30.742	35.149	1.00 69.26	1SG2197
ATOM	2197	OD1	ASP	275	135.942	31.115	35.827	1.00 69.26	1SG2198
ATOM	2198	OD2	ASP	275	136.890	30.484	33.918	1.00 69.26	1SG2199
ATOM	2199	C	ASP	275	137.980	32.682	37.131	1.00 69.26	1SG2200

Supplementary material 1.txt

ATOM	2200	O	ASP	275	137.250	33.595	36.747	1.00	69.26	1SG2201
ATOM	2201	N	PHE	276	138.037	32.322	38.426	1.00	125.71	1SG2202
ATOM	2202	CA	PHE	276	137.171	32.918	39.405	1.00	125.71	1SG2203
ATOM	2203	CB	PHE	276	137.392	32.296	40.803	1.00	125.71	1SG2204
ATOM	2204	CG	PHE	276	136.404	32.824	41.793	1.00	125.71	1SG2205
ATOM	2205	CD1	PHE	276	136.668	33.967	42.514	1.00	125.71	1SG2206
ATOM	2206	CD2	PHE	276	135.213	32.167	42.014	1.00	125.71	1SG2207
ATOM	2207	CE1	PHE	276	135.759	34.448	43.428	1.00	125.71	1SG2208
ATOM	2208	CE2	PHE	276	134.301	32.644	42.927	1.00	125.71	1SG2209
ATOM	2209	CZ	PHE	276	134.574	33.787	43.639	1.00	125.71	1SG2210
ATOM	2210	C	PHE	276	137.466	34.386	39.470	1.00	125.71	1SG2211
ATOM	2211	O	PHE	276	136.552	35.209	39.498	1.00	125.71	1SG2212
ATOM	2212	N	ASN	277	138.764	34.747	39.487	1.00	48.98	1SG2213
ATOM	2213	CA	ASN	277	139.186	36.119	39.588	1.00	48.98	1SG2214
ATOM	2214	CB	ASN	277	140.714	36.267	39.719	1.00	48.98	1SG2215
ATOM	2215	CG	ASN	277	141.135	35.763	41.092	1.00	48.98	1SG2216
ATOM	2216	OD1	ASN	277	140.318	35.675	42.008	1.00	48.98	1SG2217
ATOM	2217	ND2	ASN	277	142.446	35.434	41.248	1.00	48.98	1SG2218
ATOM	2218	C	ASN	277	138.784	36.896	38.368	1.00	48.98	1SG2219
ATOM	2219	O	ASN	277	138.392	38.056	38.479	1.00	48.98	1SG2220
ATOM	2220	N	ILE	278	138.903	36.297	37.166	1.00	82.80	1SG2221
ATOM	2221	CA	ILE	278	138.591	37.016	35.958	1.00	82.80	1SG2222
ATOM	2222	CB	ILE	278	138.972	36.275	34.701	1.00	82.80	1SG2223
ATOM	2223	CG2	ILE	278	138.096	35.021	34.568	1.00	82.80	1SG2224
ATOM	2224	CG1	ILE	278	138.893	37.208	33.481	1.00	82.80	1SG2225
ATOM	2225	CD1	ILE	278	139.550	36.621	32.232	1.00	82.80	1SG2226
ATOM	2226	C	ILE	278	137.127	37.331	35.907	1.00	82.80	1SG2227
ATOM	2227	O	ILE	278	136.738	38.443	35.551	1.00	82.80	1SG2228
ATOM	2228	N	LEU	279	136.272	36.352	36.263	1.00	53.62	1SG2229
ATOM	2229	CA	LEU	279	134.848	36.535	36.244	1.00	53.62	1SG2230
ATOM	2230	CB	LEU	279	134.066	35.265	36.626	1.00	53.62	1SG2231
ATOM	2231	CG	LEU	279	134.197	34.101	35.628	1.00	53.62	1SG2232
ATOM	2232	CD2	LEU	279	133.858	34.543	34.195	1.00	53.62	1SG2233
ATOM	2233	CD1	LEU	279	133.367	32.890	36.082	1.00	53.62	1SG2234
ATOM	2234	C	LEU	279	134.489	37.575	37.257	1.00	53.62	1SG2235
ATOM	2235	O	LEU	279	133.583	38.378	37.047	1.00	53.62	1SG2236
ATOM	2236	N	GLN	280	135.206	37.598	38.392	1.00	101.90	1SG2237
ATOM	2237	CA	GLN	280	134.891	38.523	39.445	1.00	101.90	1SG2238
ATOM	2238	CB	GLN	280	135.879	38.500	40.622	1.00	101.90	1SG2239
ATOM	2239	CG	GLN	280	135.898	37.221	41.450	1.00	101.90	1SG2240
ATOM	2240	CD	GLN	280	136.798	37.513	42.641	1.00	101.90	1SG2241
ATOM	2241	OE1	GLN	280	137.907	36.992	42.750	1.00	101.90	1SG2242
ATOM	2242	NE2	GLN	280	136.313	38.392	43.559	1.00	101.90	1SG2243
ATOM	2243	C	GLN	280	134.988	39.907	38.898	1.00	101.90	1SG2244
ATOM	2244	O	GLN	280	134.212	40.781	39.279	1.00	101.90	1SG2245
ATOM	2245	N	CYS	281	135.961	40.145	38.001	1.00	33.94	1SG2246
ATOM	2246	CA	CYS	281	136.161	41.457	37.461	1.00	33.94	1SG2247
ATOM	2247	CB	CYS	281	137.323	41.521	36.456	1.00	33.94	1SG2248
ATOM	2248	SG	CYS	281	138.934	41.229	37.243	1.00	33.94	1SG2249
ATOM	2249	C	CYS	281	134.925	41.878	36.733	1.00	33.94	1SG2250
ATOM	2250	O	CYS	281	134.513	43.032	36.837	1.00	33.94	1SG2251
ATOM	2251	N	THR	282	134.305	40.960	35.965	1.00	97.09	1SG2252
ATOM	2252	CA	THR	282	133.133	41.329	35.222	1.00	97.09	1SG2253
ATOM	2253	CB	THR	282	132.657	40.290	34.243	1.00	97.09	1SG2254
ATOM	2254	OG1	THR	282	131.746	40.881	33.329	1.00	97.09	1SG2255
ATOM	2255	CG2	THR	282	131.953	39.148	34.991	1.00	97.09	1SG2256
ATOM	2256	C	THR	282	132.016	41.626	36.173	1.00	97.09	1SG2257
ATOM	2257	O	THR	282	131.250	42.565	35.965	1.00	97.09	1SG2258
ATOM	2258	N	HIS	283	131.906	40.836	37.257	1.00	52.05	1SG2259
ATOM	2259	CA	HIS	283	130.864	41.007	38.229	1.00	52.05	1SG2260
ATOM	2260	ND1	HIS	283	131.293	37.521	39.773	1.00	52.05	1SG2261
ATOM	2261	CG	HIS	283	130.932	38.586	38.977	1.00	52.05	1SG2262
ATOM	2262	CB	HIS	283	131.010	40.021	39.403	1.00	52.05	1SG2263
ATOM	2263	NE2	HIS	283	130.604	36.665	37.840	1.00	52.05	1SG2264
ATOM	2264	CD2	HIS	283	130.514	38.045	37.800	1.00	52.05	1SG2265
ATOM	2265	CE1	HIS	283	131.077	36.397	39.044	1.00	52.05	1SG2266
ATOM	2266	C	HIS	283	131.006	42.378	38.805	1.00	52.05	1SG2267
ATOM	2267	O	HIS	283	130.024	43.092	39.000	1.00	52.05	1SG2268
ATOM	2268	N	GLN	284	132.260	42.770	39.085	1.00	77.61	1SG2269
ATOM	2269	CA	GLN	284	132.565	44.037	39.676	1.00	77.61	1SG2270
ATOM	2270	CB	GLN	284	134.071	44.170	39.956	1.00	77.61	1SG2271

Supplementary material 1.txt

ATOM	2271	CG	GLN	284	134.497	45.493	40.590	1.00	77.61	1SG2272
ATOM	2272	CD	GLN	284	136.002	45.402	40.810	1.00	77.61	1SG2273
ATOM	2273	OE1	GLN	284	136.472	44.547	41.560	1.00	77.61	1SG2274
ATOM	2274	NE2	GLN	284	136.781	46.289	40.135	1.00	77.61	1SG2275
ATOM	2275	C	GLN	284	132.145	45.135	38.747	1.00	77.61	1SG2276
ATOM	2276	O	GLN	284	131.594	46.145	39.182	1.00	77.61	1SG2277
ATOM	2277	N	LYS	285	132.396	44.970	37.435	1.00	113.60	1SG2278
ATOM	2278	CA	LYS	285	132.053	46.003	36.501	1.00	113.60	1SG2279
ATOM	2279	CB	LYS	285	132.557	45.717	35.076	1.00	113.60	1SG2280
ATOM	2280	CG	LYS	285	132.658	46.976	34.212	1.00	113.60	1SG2281
ATOM	2281	CD	LYS	285	131.344	47.747	34.086	1.00	113.60	1SG2282
ATOM	2282	CE	LYS	285	131.508	49.120	33.430	1.00	113.60	1SG2283
ATOM	2283	NZ	LYS	285	130.210	49.832	33.418	1.00	113.60	1SG2284
ATOM	2284	C	LYS	285	130.561	46.154	36.447	1.00	113.60	1SG2285
ATOM	2285	O	LYS	285	130.044	47.270	36.458	1.00	113.60	1SG2286
ATOM	2286	N	GLU	286	129.825	45.026	36.400	1.00	125.01	1SG2287
ATOM	2287	CA	GLU	286	128.396	45.083	36.286	1.00	125.01	1SG2288
ATOM	2288	CB	GLU	286	127.766	43.719	35.980	1.00	125.01	1SG2289
ATOM	2289	CG	GLU	286	128.189	42.608	36.925	1.00	125.01	1SG2290
ATOM	2290	CD	GLU	286	127.604	41.342	36.348	1.00	125.01	1SG2291
ATOM	2291	OE1	GLU	286	127.496	41.241	35.097	1.00	125.01	1SG2292
ATOM	2292	OE2	GLU	286	127.258	40.453	37.167	1.00	125.01	1SG2293
ATOM	2293	C	GLU	286	127.785	45.683	37.519	1.00	125.01	1SG2294
ATOM	2294	O	GLU	286	126.835	46.458	37.424	1.00	125.01	1SG2295
ATOM	2295	N	LEU	287	128.313	45.357	38.713	1.00	58.48	1SG2296
ATOM	2296	CA	LEU	287	127.780	45.898	39.933	1.00	58.48	1SG2297
ATOM	2297	CB	LEU	287	128.450	45.305	41.185	1.00	58.48	1SG2298
ATOM	2298	CG	LEU	287	127.911	45.872	42.512	1.00	58.48	1SG2299
ATOM	2299	CD2	LEU	287	128.714	45.329	43.704	1.00	58.48	1SG2300
ATOM	2300	CD1	LEU	287	126.401	45.618	42.660	1.00	58.48	1SG2301
ATOM	2301	C	LEU	287	127.995	47.386	39.935	1.00	58.48	1SG2302
ATOM	2302	O	LEU	287	127.200	48.142	40.487	1.00	58.48	1SG2303
ATOM	2303	N	GLN	288	129.111	47.841	39.343	1.00	60.64	1SG2304
ATOM	2304	CA	GLN	288	129.441	49.239	39.263	1.00	60.64	1SG2305
ATOM	2305	CB	GLN	288	130.771	49.412	38.512	1.00	60.64	1SG2306
ATOM	2306	CG	GLN	288	131.193	50.841	38.172	1.00	60.64	1SG2307
ATOM	2307	CD	GLN	288	132.363	50.698	37.208	1.00	60.64	1SG2308
ATOM	2308	OE1	GLN	288	132.658	49.587	36.772	1.00	60.64	1SG2309
ATOM	2309	NE2	GLN	288	133.053	51.820	36.872	1.00	60.64	1SG2310
ATOM	2310	C	GLN	288	128.398	49.954	38.457	1.00	60.64	1SG2311
ATOM	2311	O	GLN	288	127.898	51.002	38.865	1.00	60.64	1SG2312
ATOM	2312	N	ILE	289	128.028	49.387	37.292	1.00	123.93	1SG2313
ATOM	2313	CA	ILE	289	127.099	50.034	36.408	1.00	123.93	1SG2314
ATOM	2314	CB	ILE	289	126.946	49.355	35.075	1.00	123.93	1SG2315
ATOM	2315	CG2	ILE	289	126.200	48.029	35.273	1.00	123.93	1SG2316
ATOM	2316	CG1	ILE	289	126.247	50.301	34.084	1.00	123.93	1SG2317
ATOM	2317	CD1	ILE	289	127.088	51.520	33.702	1.00	123.93	1SG2318
ATOM	2318	C	ILE	289	125.757	50.116	37.063	1.00	123.93	1SG2319
ATOM	2319	O	ILE	289	125.049	51.111	36.924	1.00	123.93	1SG2320
ATOM	2320	N	ILE	290	125.362	49.044	37.770	1.00	146.65	1SG2321
ATOM	2321	CA	ILE	290	124.095	48.984	38.438	1.00	146.65	1SG2322
ATOM	2322	CB	ILE	290	123.744	47.598	38.929	1.00	146.65	1SG2323
ATOM	2323	CG2	ILE	290	123.623	46.706	37.684	1.00	146.65	1SG2324
ATOM	2324	CG1	ILE	290	124.745	47.050	39.960	1.00	146.65	1SG2325
ATOM	2325	CD1	ILE	290	124.643	47.680	41.347	1.00	146.65	1SG2326
ATOM	2326	C	ILE	290	124.053	49.978	39.559	1.00	146.65	1SG2327
ATOM	2327	O	ILE	290	122.993	50.517	39.871	1.00	146.65	1SG2328
ATOM	2328	N	SER	291	125.195	50.203	40.234	1.00	43.09	1SG2329
ATOM	2329	CA	SER	291	125.267	51.118	41.338	1.00	43.09	1SG2330
ATOM	2330	CB	SER	291	126.628	51.063	42.039	1.00	43.09	1SG2331
ATOM	2331	OG	SER	291	126.810	49.790	42.641	1.00	43.09	1SG2332
ATOM	2332	C	SER	291	125.066	52.524	40.863	1.00	43.09	1SG2333
ATOM	2333	O	SER	291	124.380	53.311	41.513	1.00	43.09	1SG2334
ATOM	2334	N	ARG	292	125.683	52.878	39.721	1.00	60.69	1SG2335
ATOM	2335	CA	ARG	292	125.593	54.207	39.183	1.00	60.69	1SG2336
ATOM	2336	CB	ARG	292	126.491	54.391	37.949	1.00	60.69	1SG2337
ATOM	2337	CG	ARG	292	127.979	54.335	38.301	1.00	60.69	1SG2338
ATOM	2338	CD	ARG	292	128.918	54.433	37.098	1.00	60.69	1SG2339
ATOM	2339	NE	ARG	292	130.307	54.464	37.634	1.00	60.69	1SG2340
ATOM	2340	CZ	ARG	292	131.377	54.411	36.788	1.00	60.69	1SG2341
ATOM	2341	NH1	ARG	292	131.185	54.250	35.447	1.00	60.69	1SG2342

Supplementary material 1.txt

ATOM	2342	NH2	ARG	292	132.639	54.537	37.290	1.00	60.69	1SG2343
ATOM	2343	C	ARG	292	124.177	54.470	38.784	1.00	60.69	1SG2344
ATOM	2344	O	ARG	292	123.638	55.549	39.023	1.00	60.69	1SG2345
ATOM	2345	N	TRP	293	123.537	53.460	38.175	1.00	63.58	1SG2346
ATOM	2346	CA	TRP	293	122.185	53.552	37.710	1.00	63.58	1SG2347
ATOM	2347	CB	TRP	293	121.756	52.225	37.066	1.00	63.58	1SG2348
ATOM	2348	CG	TRP	293	120.330	52.108	36.592	1.00	63.58	1SG2349
ATOM	2349	CD2	TRP	293	119.313	51.411	37.326	1.00	63.58	1SG2350
ATOM	2350	CD1	TRP	293	119.754	52.516	35.424	1.00	63.58	1SG2351
ATOM	2351	NE1	TRP	293	118.445	52.095	35.375	1.00	63.58	1SG2352
ATOM	2352	CE2	TRP	293	118.161	51.414	36.542	1.00	63.58	1SG2353
ATOM	2353	CE3	TRP	293	119.347	50.799	38.546	1.00	63.58	1SG2354
ATOM	2354	CZ2	TRP	293	117.019	50.798	36.968	1.00	63.58	1SG2355
ATOM	2355	CZ3	TRP	293	118.188	50.199	38.984	1.00	63.58	1SG2356
ATOM	2356	CH2	TRP	293	117.047	50.197	38.208	1.00	63.58	1SG2357
ATOM	2357	C	TRP	293	121.320	53.810	38.901	1.00	63.58	1SG2358
ATOM	2358	O	TRP	293	120.400	54.625	38.860	1.00	63.58	1SG2359
ATOM	2359	N	PHE	294	121.614	53.097	39.998	1.00	107.42	1SG2360
ATOM	2360	CA	PHE	294	120.912	53.173	41.245	1.00	107.42	1SG2361
ATOM	2361	CB	PHE	294	121.393	52.098	42.234	1.00	107.42	1SG2362
ATOM	2362	CG	PHE	294	120.613	52.222	43.496	1.00	107.42	1SG2363
ATOM	2363	CD1	PHE	294	119.419	51.555	43.648	1.00	107.42	1SG2364
ATOM	2364	CD2	PHE	294	121.075	53.003	44.530	1.00	107.42	1SG2365
ATOM	2365	CE1	PHE	294	118.698	51.664	44.814	1.00	107.42	1SG2366
ATOM	2366	CE2	PHE	294	120.358	53.117	45.697	1.00	107.42	1SG2367
ATOM	2367	CZ	PHE	294	119.166	52.447	45.841	1.00	107.42	1SG2368
ATOM	2368	C	PHE	294	121.148	54.510	41.886	1.00	107.42	1SG2369
ATOM	2369	O	PHE	294	120.263	55.046	42.552	1.00	107.42	1SG2370
ATOM	2370	N	ALA	295	122.352	55.086	41.701	1.00	62.88	1SG2371
ATOM	2371	CA	ALA	295	122.750	56.264	42.420	1.00	62.88	1SG2372
ATOM	2372	CB	ALA	295	124.168	56.735	42.051	1.00	62.88	1SG2373
ATOM	2373	C	ALA	295	121.829	57.411	42.190	1.00	62.88	1SG2374
ATOM	2374	O	ALA	295	121.427	58.069	43.147	1.00	62.88	1SG2375
ATOM	2375	N	ASP	296	121.446	57.703	40.937	1.00	204.67	1SG2376
ATOM	2376	CA	ASP	296	120.561	58.824	40.836	1.00	204.67	1SG2377
ATOM	2377	CB	ASP	296	120.460	59.423	39.421	1.00	204.67	1SG2378
ATOM	2378	CG	ASP	296	119.618	60.696	39.484	1.00	204.67	1SG2379
ATOM	2379	OD1	ASP	296	118.479	60.647	40.020	1.00	204.67	1SG2380
ATOM	2380	OD2	ASP	296	120.108	61.741	38.979	1.00	204.67	1SG2381
ATOM	2381	C	ASP	296	119.223	58.290	41.198	1.00	204.67	1SG2382
ATOM	2382	O	ASP	296	118.451	57.919	40.314	1.00	204.67	1SG2383
ATOM	2383	N	SER	297	118.891	58.253	42.509	1.00	194.84	1SG2384
ATOM	2384	CA	SER	297	117.650	57.602	42.777	1.00	194.84	1SG2385
ATOM	2385	CB	SER	297	117.725	56.067	42.715	1.00	194.84	1SG2386
ATOM	2386	OG	SER	297	118.024	55.625	41.400	1.00	194.84	1SG2387
ATOM	2387	C	SER	297	117.049	57.902	44.110	1.00	194.84	1SG2388
ATOM	2388	O	SER	297	117.291	58.912	44.767	1.00	194.84	1SG2389
ATOM	2389	N	SER	298	116.198	56.932	44.493	1.00	107.55	1SG2390
ATOM	2390	CA	SER	298	115.276	56.899	45.584	1.00	107.55	1SG2391
ATOM	2391	CB	SER	298	114.199	55.826	45.392	1.00	107.55	1SG2392
ATOM	2392	OG	SER	298	113.427	56.115	44.236	1.00	107.55	1SG2393
ATOM	2393	C	SER	298	115.895	56.729	46.929	1.00	107.55	1SG2394
ATOM	2394	O	SER	298	115.169	56.517	47.901	1.00	107.55	1SG2395
ATOM	2395	N	ILE	299	117.232	56.763	47.046	1.00	102.92	1SG2396
ATOM	2396	CA	ILE	299	117.727	56.653	48.383	1.00	102.92	1SG2397
ATOM	2397	CB	ILE	299	119.234	56.607	48.433	1.00	102.92	1SG2398
ATOM	2398	CG2	ILE	299	119.807	57.860	47.748	1.00	102.92	1SG2399
ATOM	2399	CG1	ILE	299	119.724	56.373	49.871	1.00	102.92	1SG2400
ATOM	2400	CD1	ILE	299	121.198	55.974	49.949	1.00	102.92	1SG2401
ATOM	2401	C	ILE	299	117.214	57.843	49.142	1.00	102.92	1SG2402
ATOM	2402	O	ILE	299	116.649	57.693	50.224	1.00	102.92	1SG2403
ATOM	2403	N	ALA	300	117.407	59.064	48.604	1.00	48.29	1SG2404
ATOM	2404	CA	ALA	300	116.891	60.251	49.225	1.00	48.29	1SG2405
ATOM	2405	CB	ALA	300	117.510	61.535	48.647	1.00	48.29	1SG2406
ATOM	2406	C	ALA	300	115.404	60.376	49.053	1.00	48.29	1SG2407
ATOM	2407	O	ALA	300	114.674	60.620	50.014	1.00	48.29	1SG2408
ATOM	2408	N	SER	301	114.923	60.185	47.806	1.00	51.61	1SG2409
ATOM	2409	CA	SER	301	113.553	60.445	47.451	1.00	51.61	1SG2410
ATOM	2410	CB	SER	301	113.287	60.319	45.940	1.00	51.61	1SG2411
ATOM	2411	OG	SER	301	113.400	58.965	45.528	1.00	51.61	1SG2412
ATOM	2412	C	SER	301	112.605	59.525	48.149	1.00	51.61	1SG2413

Supplementary material 1.txt

ATOM	2413	O	SER	301	111.603	59.971	48.706	1.00	51.61	1SG2414
ATOM	2414	N	LEU	302	112.882	58.207	48.120	1.00	79.09	1SG2415
ATOM	2415	CA	LEU	302	111.986	57.287	48.757	1.00	79.09	1SG2416
ATOM	2416	CB	LEU	302	111.524	56.173	47.808	1.00	79.09	1SG2417
ATOM	2417	CG	LEU	302	110.741	56.726	46.602	1.00	79.09	1SG2418
ATOM	2418	CD2	LEU	302	109.585	57.629	47.060	1.00	79.09	1SG2419
ATOM	2419	CD1	LEU	302	110.281	55.600	45.666	1.00	79.09	1SG2420
ATOM	2420	C	LEU	302	112.724	56.657	49.895	1.00	79.09	1SG2421
ATOM	2421	O	LEU	302	113.286	55.569	49.770	1.00	79.09	1SG2422
ATOM	2422	N	ASN	303	112.682	57.335	51.056	1.00	98.49	1SG2423
ATOM	2423	CA	ASN	303	113.381	56.967	52.253	1.00	98.49	1SG2424
ATOM	2424	CB	ASN	303	113.278	58.038	53.351	1.00	98.49	1SG2425
ATOM	2425	CG	ASN	303	111.814	58.154	53.750	1.00	98.49	1SG2426
ATOM	2426	OD1	ASN	303	110.923	58.091	52.905	1.00	98.49	1SG2427
ATOM	2427	ND2	ASN	303	111.553	58.326	55.074	1.00	98.49	1SG2428
ATOM	2428	C	ASN	303	112.817	55.705	52.820	1.00	98.49	1SG2429
ATOM	2429	O	ASN	303	113.527	54.952	53.482	1.00	98.49	1SG2430
ATOM	2430	N	PHE	304	111.514	55.459	52.589	1.00	89.38	1SG2431
ATOM	2431	CA	PHE	304	110.818	54.351	53.171	1.00	89.38	1SG2432
ATOM	2432	CB	PHE	304	109.286	54.407	52.990	1.00	89.38	1SG2433
ATOM	2433	CG	PHE	304	108.918	54.419	51.548	1.00	89.38	1SG2434
ATOM	2434	CD1	PHE	304	108.926	55.597	50.837	1.00	89.38	1SG2435
ATOM	2435	CD2	PHE	304	108.542	53.259	50.911	1.00	89.38	1SG2436
ATOM	2436	CE1	PHE	304	108.576	55.613	49.508	1.00	89.38	1SG2437
ATOM	2437	CE2	PHE	304	108.191	53.271	49.582	1.00	89.38	1SG2438
ATOM	2438	CZ	PHE	304	108.210	54.449	48.877	1.00	89.38	1SG2439
ATOM	2439	C	PHE	304	111.337	53.032	52.685	1.00	89.38	1SG2440
ATOM	2440	O	PHE	304	111.301	52.056	53.433	1.00	89.38	1SG2441
ATOM	2441	N	TYR	305	111.855	52.929	51.445	1.00	169.12	1SG2442
ATOM	2442	CA	TYR	305	112.187	51.594	51.025	1.00	169.12	1SG2443
ATOM	2443	CB	TYR	305	111.799	51.243	49.573	1.00	169.12	1SG2444
ATOM	2444	CG	TYR	305	112.738	51.848	48.601	1.00	169.12	1SG2445
ATOM	2445	CD1	TYR	305	113.869	51.155	48.258	1.00	169.12	1SG2446
ATOM	2446	CD2	TYR	305	112.496	53.072	48.026	1.00	169.12	1SG2447
ATOM	2447	CE1	TYR	305	114.767	51.665	47.359	1.00	169.12	1SG2448
ATOM	2448	CE2	TYR	305	113.393	53.590	47.122	1.00	169.12	1SG2449
ATOM	2449	CZ	TYR	305	114.529	52.887	46.788	1.00	169.12	1SG2450
ATOM	2450	OH	TYR	305	115.463	53.398	45.863	1.00	169.12	1SG2451
ATOM	2451	C	TYR	305	113.636	51.283	51.279	1.00	169.12	1SG2452
ATOM	2452	O	TYR	305	114.395	52.118	51.769	1.00	169.12	1SG2453
ATOM	2453	N	ARG	306	114.018	50.007	51.046	1.00	106.43	1SG2454
ATOM	2454	CA	ARG	306	115.326	49.502	51.387	1.00	106.43	1SG2455
ATOM	2455	CB	ARG	306	115.308	47.996	51.701	1.00	106.43	1SG2456
ATOM	2456	CG	ARG	306	114.496	47.649	52.950	1.00	106.43	1SG2457
ATOM	2457	CD	ARG	306	114.295	46.147	53.154	1.00	106.43	1SG2458
ATOM	2458	NE	ARG	306	113.407	45.667	52.058	1.00	106.43	1SG2459
ATOM	2459	CZ	ARG	306	112.671	44.531	52.234	1.00	106.43	1SG2460
ATOM	2460	NH1	ARG	306	112.764	43.841	53.408	1.00	106.43	1SG2461
ATOM	2461	NH2	ARG	306	111.841	44.088	51.245	1.00	106.43	1SG2462
ATOM	2462	C	ARG	306	116.325	49.714	50.282	1.00	106.43	1SG2463
ATOM	2463	O	ARG	306	115.991	49.654	49.102	1.00	106.43	1SG2464
ATOM	2464	N	LYS	307	117.607	49.954	50.654	1.00	124.52	1SG2465
ATOM	2465	CA	LYS	307	118.645	50.166	49.674	1.00	124.52	1SG2466
ATOM	2466	CB	LYS	307	119.561	51.343	50.032	1.00	124.52	1SG2467
ATOM	2467	CG	LYS	307	118.846	52.674	50.257	1.00	124.52	1SG2468
ATOM	2468	CD	LYS	307	119.686	53.678	51.055	1.00	124.52	1SG2469
ATOM	2469	CE	LYS	307	119.736	53.360	52.554	1.00	124.52	1SG2470
ATOM	2470	NZ	LYS	307	120.564	54.357	53.266	1.00	124.52	1SG2471
ATOM	2471	C	LYS	307	119.519	48.930	49.618	1.00	124.52	1SG2472
ATOM	2472	O	LYS	307	120.626	48.882	50.146	1.00	124.52	1SG2473
ATOM	2473	N	CYS	308	118.964	47.863	49.035	1.00	190.41	1SG2474
ATOM	2474	CA	CYS	308	119.456	46.533	48.781	1.00	190.41	1SG2475
ATOM	2475	CB	CYS	308	118.356	45.497	49.002	1.00	190.41	1SG2476
ATOM	2476	SG	CYS	308	116.770	46.199	48.488	1.00	190.41	1SG2477
ATOM	2477	C	CYS	308	120.100	46.292	47.437	1.00	190.41	1SG2478
ATOM	2478	O	CYS	308	120.135	45.142	47.006	1.00	190.41	1SG2479
ATOM	2479	N	TYR	309	120.505	47.314	46.665	1.00	125.47	1SG2480
ATOM	2480	CA	TYR	309	120.895	47.063	45.297	1.00	125.47	1SG2481
ATOM	2481	CB	TYR	309	121.333	48.338	44.559	1.00	125.47	1SG2482
ATOM	2482	CG	TYR	309	121.122	48.073	43.107	1.00	125.47	1SG2483
ATOM	2483	CD1	TYR	309	121.939	47.228	42.398	1.00	125.47	1SG2484

Supplementary material 1.txt

ATOM	2484	CD2	TYR	309	120.083	48.690	42.451	1.00125.47	1SG2485
ATOM	2485	CE1	TYR	309	121.722	46.998	41.058	1.00125.47	1SG2486
ATOM	2486	CE2	TYR	309	119.858	48.467	41.115	1.00125.47	1SG2487
ATOM	2487	CZ	TYR	309	120.678	47.619	40.414	1.00125.47	1SG2488
ATOM	2488	OH	TYR	309	120.447	47.389	39.041	1.00125.47	1SG2489
ATOM	2489	C	TYR	309	122.017	46.054	45.199	1.00125.47	1SG2490
ATOM	2490	O	TYR	309	122.031	45.236	44.277	1.00125.47	1SG2491
ATOM	2491	N	VAL	310	123.014	46.099	46.106	1.00 52.63	1SG2492
ATOM	2492	CA	VAL	310	124.107	45.161	46.052	1.00 52.63	1SG2493
ATOM	2493	CB	VAL	310	125.159	45.438	47.088	1.00 52.63	1SG2494
ATOM	2494	CG1	VAL	310	126.264	44.371	46.973	1.00 52.63	1SG2495
ATOM	2495	CG2	VAL	310	125.659	46.880	46.900	1.00 52.63	1SG2496
ATOM	2496	C	VAL	310	123.582	43.775	46.292	1.00 52.63	1SG2497
ATOM	2497	O	VAL	310	123.964	42.820	45.616	1.00 52.63	1SG2498
ATOM	2498	N	GLU	311	122.670	43.648	47.271	1.00 93.72	1SG2499
ATOM	2499	CA	GLU	311	122.082	42.396	47.653	1.00 93.72	1SG2500
ATOM	2500	CB	GLU	311	121.097	42.545	48.829	1.00 93.72	1SG2501
ATOM	2501	CG	GLU	311	121.778	42.831	50.172	1.00 93.72	1SG2502
ATOM	2502	CD	GLU	311	122.215	44.291	50.233	1.00 93.72	1SG2503
ATOM	2503	OE1	GLU	311	121.851	45.068	49.312	1.00 93.72	1SG2504
ATOM	2504	OE2	GLU	311	122.919	44.649	51.214	1.00 93.72	1SG2505
ATOM	2505	C	GLU	311	121.327	41.840	46.482	1.00 93.72	1SG2506
ATOM	2506	O	GLU	311	121.324	40.630	46.260	1.00 93.72	1SG2507
ATOM	2507	N	PHE	312	120.655	42.712	45.704	1.00110.05	1SG2508
ATOM	2508	CA	PHE	312	119.928	42.271	44.545	1.00110.05	1SG2509
ATOM	2509	CB	PHE	312	119.090	43.333	43.814	1.00110.05	1SG2510
ATOM	2510	CG	PHE	312	117.811	43.580	44.538	1.00110.05	1SG2511
ATOM	2511	CD1	PHE	312	116.925	42.551	44.759	1.00110.05	1SG2512
ATOM	2512	CD2	PHE	312	117.507	44.824	45.029	1.00110.05	1SG2513
ATOM	2513	CE1	PHE	312	115.737	42.764	45.416	1.00110.05	1SG2514
ATOM	2514	CE2	PHE	312	116.319	45.043	45.686	1.00110.05	1SG2515
ATOM	2515	CZ	PHE	312	115.426	44.018	45.881	1.00110.05	1SG2516
ATOM	2516	C	PHE	312	120.886	41.737	43.532	1.00110.05	1SG2517
ATOM	2517	O	PHE	312	120.547	40.840	42.762	1.00110.05	1SG2518
ATOM	2518	N	TYR	313	122.088	42.330	43.453	1.00 78.18	1SG2519
ATOM	2519	CA	TYR	313	123.082	41.883	42.522	1.00 78.18	1SG2520
ATOM	2520	CB	TYR	313	124.324	42.792	42.495	1.00 78.18	1SG2521
ATOM	2521	CG	TYR	313	125.349	42.071	41.696	1.00 78.18	1SG2522
ATOM	2522	CD1	TYR	313	125.312	42.077	40.321	1.00 78.18	1SG2523
ATOM	2523	CD2	TYR	313	126.350	41.382	42.338	1.00 78.18	1SG2524
ATOM	2524	CE1	TYR	313	126.264	41.396	39.603	1.00 78.18	1SG2525
ATOM	2525	CE2	TYR	313	127.305	40.699	41.628	1.00 78.18	1SG2526
ATOM	2526	CZ	TYR	313	127.257	40.707	40.257	1.00 78.18	1SG2527
ATOM	2527	OH	TYR	313	128.229	40.008	39.515	1.00 78.18	1SG2528
ATOM	2528	C	TYR	313	123.504	40.488	42.880	1.00 78.18	1SG2529
ATOM	2529	O	TYR	313	123.698	39.647	42.003	1.00 78.18	1SG2530
ATOM	2530	N	PHE	314	123.654	40.203	44.188	1.00 45.78	1SG2531
ATOM	2531	CA	PHE	314	124.050	38.899	44.637	1.00 45.78	1SG2532
ATOM	2532	CB	PHE	314	124.159	38.796	46.167	1.00 45.78	1SG2533
ATOM	2533	CG	PHE	314	124.548	37.392	46.484	1.00 45.78	1SG2534
ATOM	2534	CD1	PHE	314	125.861	36.988	46.397	1.00 45.78	1SG2535
ATOM	2535	CD2	PHE	314	123.595	36.479	46.871	1.00 45.78	1SG2536
ATOM	2536	CE1	PHE	314	126.215	35.692	46.691	1.00 45.78	1SG2537
ATOM	2537	CE2	PHE	314	123.943	35.182	47.166	1.00 45.78	1SG2538
ATOM	2538	CZ	PHE	314	125.256	34.786	47.075	1.00 45.78	1SG2539
ATOM	2539	C	PHE	314	123.013	37.912	44.204	1.00 45.78	1SG2540
ATOM	2540	O	PHE	314	123.338	36.807	43.773	1.00 45.78	1SG2541
ATOM	2541	N	TRP	315	121.728	38.295	44.308	1.00 68.75	1SG2542
ATOM	2542	CA	TRP	315	120.639	37.419	43.987	1.00 68.75	1SG2543
ATOM	2543	CB	TRP	315	119.276	38.088	44.222	1.00 68.75	1SG2544
ATOM	2544	CG	TRP	315	118.139	37.118	44.423	1.00 68.75	1SG2545
ATOM	2545	CD2	TRP	315	117.719	36.712	45.732	1.00 68.75	1SG2546
ATOM	2546	CD1	TRP	315	117.323	36.480	43.535	1.00 68.75	1SG2547
ATOM	2547	NE1	TRP	315	116.423	35.690	44.215	1.00 68.75	1SG2548
ATOM	2548	CE2	TRP	315	116.654	35.827	45.569	1.00 68.75	1SG2549
ATOM	2549	CE3	TRP	315	118.183	37.052	46.971	1.00 68.75	1SG2550
ATOM	2550	CZ2	TRP	315	116.039	35.265	46.652	1.00 68.75	1SG2551
ATOM	2551	CZ3	TRP	315	117.560	36.486	48.060	1.00 68.75	1SG2552
ATOM	2552	CH2	TRP	315	116.507	35.608	47.903	1.00 68.75	1SG2553
ATOM	2553	C	TRP	315	120.740	37.074	42.529	1.00 68.75	1SG2554
ATOM	2554	O	TRP	315	120.519	35.934	42.123	1.00 68.75	1SG2555

Supplementary material 1.txt

ATOM	2555	N	MET	316	121.071	38.082	41.704	1.00168.94	1SG2556
ATOM	2556	CA	MET	316	121.224	37.948	40.285	1.00168.94	1SG2557
ATOM	2557	CB	MET	316	121.725	39.236	39.650	1.00168.94	1SG2558
ATOM	2558	CG	MET	316	122.001	38.967	38.187	1.00168.94	1SG2559
ATOM	2559	SD	MET	316	120.423	38.541	37.462	1.00168.94	1SG2560
ATOM	2560	CE	MET	316	119.971	39.943	38.516	1.00168.94	1SG2561
ATOM	2561	C	MET	316	122.349	37.024	39.976	1.00168.94	1SG2562
ATOM	2562	O	MET	316	122.281	36.235	39.035	1.00168.94	1SG2563
ATOM	2563	N	ALA	317	123.445	37.180	40.735	1.00 42.48	1SG2564
ATOM	2564	CA	ALA	317	124.649	36.430	40.557	1.00 42.48	1SG2565
ATOM	2565	CB	ALA	317	125.770	36.882	41.505	1.00 42.48	1SG2566
ATOM	2566	C	ALA	317	124.369	34.995	40.852	1.00 42.48	1SG2567
ATOM	2567	O	ALA	317	124.948	34.097	40.244	1.00 42.48	1SG2568
ATOM	2568	N	ALA	318	123.499	34.752	41.845	1.00 41.94	1SG2569
ATOM	2569	CA	ALA	318	123.158	33.418	42.243	1.00 41.94	1SG2570
ATOM	2570	CB	ALA	318	122.199	33.386	43.446	1.00 41.94	1SG2571
ATOM	2571	C	ALA	318	122.476	32.720	41.108	1.00 41.94	1SG2572
ATOM	2572	O	ALA	318	122.702	31.529	40.890	1.00 41.94	1SG2573
ATOM	2573	N	ALA	319	121.603	33.446	40.377	1.00 54.22	1SG2574
ATOM	2574	CA	ALA	319	120.842	32.879	39.300	1.00 54.22	1SG2575
ATOM	2575	CB	ALA	319	119.862	33.890	38.680	1.00 54.22	1SG2576
ATOM	2576	C	ALA	319	121.761	32.411	38.211	1.00 54.22	1SG2577
ATOM	2577	O	ALA	319	121.597	31.297	37.712	1.00 54.22	1SG2578
ATOM	2578	N	ILE	320	122.732	33.257	37.795	1.00124.57	1SG2579
ATOM	2579	CA	ILE	320	123.686	32.861	36.792	1.00124.57	1SG2580
ATOM	2580	CB	ILE	320	123.207	33.084	35.390	1.00124.57	1SG2581
ATOM	2581	CG2	ILE	320	124.408	32.849	34.463	1.00124.57	1SG2582
ATOM	2582	CG1	ILE	320	121.993	32.196	35.070	1.00124.57	1SG2583
ATOM	2583	CD1	ILE	320	122.299	30.700	35.128	1.00124.57	1SG2584
ATOM	2584	C	ILE	320	124.929	33.690	36.942	1.00124.57	1SG2585
ATOM	2585	O	ILE	320	124.850	34.904	37.122	1.00124.57	1SG2586
ATOM	2586	N	SER	321	126.107	33.029	36.961	1.00119.54	1SG2587
ATOM	2587	CA	SER	321	127.393	33.673	37.039	1.00119.54	1SG2588
ATOM	2588	CB	SER	321	128.363	32.916	37.962	1.00119.54	1SG2589
ATOM	2589	OG	SER	321	129.616	33.583	38.008	1.00119.54	1SG2590
ATOM	2590	C	SER	321	128.092	33.830	35.709	1.00119.54	1SG2591
ATOM	2591	O	SER	321	128.942	34.708	35.566	1.00119.54	1SG2592
ATOM	2592	N	GLU	322	127.781	32.983	34.701	1.00147.31	1SG2593
ATOM	2593	CA	GLU	322	128.586	32.975	33.504	1.00147.31	1SG2594
ATOM	2594	CB	GLU	322	128.333	31.795	32.544	1.00147.31	1SG2595
ATOM	2595	CG	GLU	322	126.880	31.537	32.167	1.00147.31	1SG2596
ATOM	2596	CD	GLU	322	126.324	30.524	33.159	1.00147.31	1SG2597
ATOM	2597	OE1	GLU	322	126.288	30.847	34.376	1.00147.31	1SG2598
ATOM	2598	OE2	GLU	322	125.934	29.412	32.714	1.00147.31	1SG2599
ATOM	2599	C	GLU	322	128.488	34.261	32.747	1.00147.31	1SG2600
ATOM	2600	O	GLU	322	127.457	34.925	32.704	1.00147.31	1SG2601
ATOM	2601	N	PRO	323	129.597	34.603	32.140	1.00 67.69	1SG2602
ATOM	2602	CA	PRO	323	129.787	35.841	31.428	1.00 67.69	1SG2603
ATOM	2603	CD	PRO	323	130.639	33.632	31.847	1.00 67.69	1SG2604
ATOM	2604	CB	PRO	323	131.219	35.783	30.896	1.00 67.69	1SG2605
ATOM	2605	CG	PRO	323	131.480	34.276	30.733	1.00 67.69	1SG2606
ATOM	2606	C	PRO	323	128.793	36.076	30.327	1.00 67.69	1SG2607
ATOM	2607	O	PRO	323	128.540	37.237	30.010	1.00 67.69	1SG2608
ATOM	2608	N	GLU	324	128.234	35.014	29.717	1.00 95.01	1SG2609
ATOM	2609	CA	GLU	324	127.300	35.160	28.631	1.00 95.01	1SG2610
ATOM	2610	CB	GLU	324	126.831	33.811	28.065	1.00 95.01	1SG2611
ATOM	2611	CG	GLU	324	127.945	33.008	27.395	1.00 95.01	1SG2612
ATOM	2612	CD	GLU	324	128.821	32.394	28.476	1.00 95.01	1SG2613
ATOM	2613	OE1	GLU	324	128.427	31.327	29.021	1.00 95.01	1SG2614
ATOM	2614	OE2	GLU	324	129.894	32.983	28.773	1.00 95.01	1SG2615
ATOM	2615	C	GLU	324	126.073	35.852	29.143	1.00 95.01	1SG2616
ATOM	2616	O	GLU	324	125.401	36.589	28.423	1.00 95.01	1SG2617
ATOM	2617	N	PHE	325	125.759	35.579	30.415	1.00131.48	1SG2618
ATOM	2618	CA	PHE	325	124.635	36.029	31.186	1.00131.48	1SG2619
ATOM	2619	CB	PHE	325	124.288	35.112	32.367	1.00131.48	1SG2620
ATOM	2620	CG	PHE	325	123.618	33.944	31.725	1.00131.48	1SG2621
ATOM	2621	CD1	PHE	325	122.311	34.046	31.314	1.00131.48	1SG2622
ATOM	2622	CD2	PHE	325	124.279	32.756	31.522	1.00131.48	1SG2623
ATOM	2623	CE1	PHE	325	121.675	32.984	30.716	1.00131.48	1SG2624
ATOM	2624	CE2	PHE	325	123.650	31.688	30.924	1.00131.48	1SG2625
ATOM	2625	CZ	PHE	325	122.342	31.800	30.520	1.00131.48	1SG2626

Supplementary material 1.txt

ATOM	2626	C	PHE	325	124.752	37.457	31.635	1.00131.48	1SG2627
ATOM	2627	O	PHE	325	123.896	37.938	32.374	1.00131.48	1SG2628
ATOM	2628	N	SER	326	125.863	38.145	31.325	1.00 62.12	1SG2629
ATOM	2629	CA	SER	326	126.058	39.478	31.831	1.00 62.12	1SG2630
ATOM	2630	CB	SER	326	127.313	40.162	31.261	1.00 62.12	1SG2631
ATOM	2631	OG	SER	326	127.450	41.464	31.813	1.00 62.12	1SG2632
ATOM	2632	C	SER	326	124.876	40.370	31.551	1.00 62.12	1SG2633
ATOM	2633	O	SER	326	124.413	41.063	32.456	1.00 62.12	1SG2634
ATOM	2634	N	GLY	327	124.337	40.387	30.314	1.00 28.56	1SG2635
ATOM	2635	CA	GLY	327	123.226	41.254	30.022	1.00 28.56	1SG2636
ATOM	2636	C	GLY	327	122.058	40.862	30.881	1.00 28.56	1SG2637
ATOM	2637	O	GLY	327	121.319	41.720	31.363	1.00 28.56	1SG2638
ATOM	2638	N	SER	328	121.855	39.543	31.068	1.00 83.55	1SG2639
ATOM	2639	CA	SER	328	120.758	38.997	31.824	1.00 83.55	1SG2640
ATOM	2640	CB	SER	328	120.736	37.460	31.814	1.00 83.55	1SG2641
ATOM	2641	OG	SER	328	119.634	36.986	32.573	1.00 83.55	1SG2642
ATOM	2642	C	SER	328	120.820	39.432	33.238	1.00 83.55	1SG2643
ATOM	2643	O	SER	328	119.815	39.852	33.808	1.00 83.55	1SG2644
ATOM	2644	N	ARG	329	122.013	39.346	33.832	1.00 60.45	1SG2645
ATOM	2645	CA	ARG	329	122.157	39.668	35.214	1.00 60.45	1SG2646
ATOM	2646	CB	ARG	329	123.578	39.419	35.745	1.00 60.45	1SG2647
ATOM	2647	CG	ARG	329	123.910	37.929	35.848	1.00 60.45	1SG2648
ATOM	2648	CD	ARG	329	125.148	37.635	36.693	1.00 60.45	1SG2649
ATOM	2649	NE	ARG	329	126.306	38.269	36.009	1.00 60.45	1SG2650
ATOM	2650	CZ	ARG	329	127.076	37.556	35.141	1.00 60.45	1SG2651
ATOM	2651	NH1	ARG	329	126.780	36.249	34.901	1.00 60.45	1SG2652
ATOM	2652	NH2	ARG	329	128.141	38.150	34.525	1.00 60.45	1SG2653
ATOM	2653	C	ARG	329	121.815	41.101	35.450	1.00 60.45	1SG2654
ATOM	2654	O	ARG	329	121.072	41.419	36.377	1.00 60.45	1SG2655
ATOM	2655	N	VAL	330	122.315	42.003	34.589	1.00 38.19	1SG2656
ATOM	2656	CA	VAL	330	122.112	43.406	34.792	1.00 38.19	1SG2657
ATOM	2657	CB	VAL	330	122.789	44.238	33.744	1.00 38.19	1SG2658
ATOM	2658	CG1	VAL	330	122.455	45.715	34.004	1.00 38.19	1SG2659
ATOM	2659	CG2	VAL	330	124.298	43.937	33.788	1.00 38.19	1SG2660
ATOM	2660	C	VAL	330	120.646	43.713	34.766	1.00 38.19	1SG2661
ATOM	2661	O	VAL	330	120.146	44.443	35.620	1.00 38.19	1SG2662
ATOM	2662	N	ALA	331	119.909	43.154	33.789	1.00 37.35	1SG2663
ATOM	2663	CA	ALA	331	118.506	43.437	33.685	1.00 37.35	1SG2664
ATOM	2664	CB	ALA	331	117.839	42.770	32.474	1.00 37.35	1SG2665
ATOM	2665	C	ALA	331	117.798	42.937	34.906	1.00 37.35	1SG2666
ATOM	2666	O	ALA	331	116.939	43.623	35.456	1.00 37.35	1SG2667
ATOM	2667	N	PHE	332	118.145	41.725	35.376	1.00120.31	1SG2668
ATOM	2668	CA	PHE	332	117.442	41.174	36.497	1.00120.31	1SG2669
ATOM	2669	CB	PHE	332	117.686	39.671	36.717	1.00120.31	1SG2670
ATOM	2670	CG	PHE	332	116.841	39.188	37.854	1.00120.31	1SG2671
ATOM	2671	CD1	PHE	332	117.153	39.443	39.173	1.00120.31	1SG2672
ATOM	2672	CD2	PHE	332	115.717	38.445	37.594	1.00120.31	1SG2673
ATOM	2673	CE1	PHE	332	116.365	38.987	40.204	1.00120.31	1SG2674
ATOM	2674	CE2	PHE	332	114.922	37.984	38.617	1.00120.31	1SG2675
ATOM	2675	CZ	PHE	332	115.239	38.253	39.928	1.00120.31	1SG2676
ATOM	2676	C	PHE	332	117.724	41.961	37.750	1.00120.31	1SG2677
ATOM	2677	O	PHE	332	116.843	42.102	38.593	1.00120.31	1SG2678
ATOM	2678	N	THR	333	118.951	42.491	37.928	1.00 98.38	1SG2679
ATOM	2679	CA	THR	333	119.264	43.189	39.147	1.00 98.38	1SG2680
ATOM	2680	CB	THR	333	120.702	43.629	39.234	1.00 98.38	1SG2681
ATOM	2681	OG1	THR	333	120.992	44.080	40.548	1.00 98.38	1SG2682
ATOM	2682	CG2	THR	333	120.964	44.752	38.218	1.00 98.38	1SG2683
ATOM	2683	C	THR	333	118.382	44.393	39.251	1.00 98.38	1SG2684
ATOM	2684	O	THR	333	117.892	44.728	40.329	1.00 98.38	1SG2685
ATOM	2685	N	LYS	334	118.158	45.075	38.116	1.00 78.36	1SG2686
ATOM	2686	CA	LYS	334	117.339	46.250	38.089	1.00 78.36	1SG2687
ATOM	2687	CB	LYS	334	117.313	46.922	36.707	1.00 78.36	1SG2688
ATOM	2688	CG	LYS	334	118.627	47.630	36.376	1.00 78.36	1SG2689
ATOM	2689	CD	LYS	334	118.775	48.026	34.907	1.00 78.36	1SG2690
ATOM	2690	CE	LYS	334	120.052	48.819	34.617	1.00 78.36	1SG2691
ATOM	2691	NZ	LYS	334	121.231	48.098	35.149	1.00 78.36	1SG2692
ATOM	2692	C	LYS	334	115.927	45.907	38.462	1.00 78.36	1SG2693
ATOM	2693	O	LYS	334	115.259	46.678	39.149	1.00 78.36	1SG2694
ATOM	2694	N	ILE	335	115.414	44.755	37.994	1.00139.62	1SG2695
ATOM	2695	CA	ILE	335	114.049	44.400	38.275	1.00139.62	1SG2696
ATOM	2696	CB	ILE	335	113.545	43.261	37.418	1.00139.62	1SG2697

Supplementary material 1.txt

ATOM	2697	CG2	ILE	335	113.662	43.730	35.958	1.00139.62	1SG2698
ATOM	2698	CG1	ILE	335	114.264	41.925	37.680	1.00139.62	1SG2699
ATOM	2699	CD1	ILE	335	113.740	41.156	38.893	1.00139.62	1SG2700
ATOM	2700	C	ILE	335	113.860	44.096	39.733	1.00139.62	1SG2701
ATOM	2701	O	ILE	335	112.892	44.541	40.346	1.00139.62	1SG2702
ATOM	2702	N	ALA	336	114.789	43.334	40.334	1.00 34.76	1SG2703
ATOM	2703	CA	ALA	336	114.652	42.937	41.705	1.00 34.76	1SG2704
ATOM	2704	CB	ALA	336	115.765	41.966	42.125	1.00 34.76	1SG2705
ATOM	2705	C	ALA	336	114.702	44.154	42.574	1.00 34.76	1SG2706
ATOM	2706	O	ALA	336	113.918	44.291	43.512	1.00 34.76	1SG2707
ATOM	2707	N	ILE	337	115.627	45.084	42.273	1.00123.02	1SG2708
ATOM	2708	CA	ILE	337	115.744	46.267	43.068	1.00123.02	1SG2709
ATOM	2709	CB	ILE	337	116.913	47.139	42.687	1.00123.02	1SG2710
ATOM	2710	CG2	ILE	337	116.697	47.656	41.261	1.00123.02	1SG2711
ATOM	2711	CG1	ILE	337	117.107	48.261	43.722	1.00123.02	1SG2712
ATOM	2712	CD1	ILE	337	117.582	47.769	45.086	1.00123.02	1SG2713
ATOM	2713	C	ILE	337	114.488	47.072	42.936	1.00123.02	1SG2714
ATOM	2714	O	ILE	337	113.988	47.609	43.921	1.00123.02	1SG2715
ATOM	2715	N	LEU	338	113.940	47.193	41.711	1.00 70.21	1SG2716
ATOM	2716	CA	LEU	338	112.781	48.024	41.546	1.00 70.21	1SG2717
ATOM	2717	CB	LEU	338	112.423	48.318	40.079	1.00 70.21	1SG2718
ATOM	2718	CG	LEU	338	111.394	49.459	39.964	1.00 70.21	1SG2719
ATOM	2719	CD2	LEU	338	111.039	49.760	38.501	1.00 70.21	1SG2720
ATOM	2720	CD1	LEU	338	111.908	50.721	40.679	1.00 70.21	1SG2721
ATOM	2721	C	LEU	338	111.591	47.444	42.255	1.00 70.21	1SG2722
ATOM	2722	O	LEU	338	110.850	48.160	42.923	1.00 70.21	1SG2723
ATOM	2723	N	MET	339	111.395	46.118	42.157	1.00119.87	1SG2724
ATOM	2724	CA	MET	339	110.274	45.444	42.750	1.00119.87	1SG2725
ATOM	2725	CB	MET	339	110.245	43.947	42.394	1.00119.87	1SG2726
ATOM	2726	CG	MET	339	110.103	43.687	40.892	1.00119.87	1SG2727
ATOM	2727	SD	MET	339	110.193	41.935	40.412	1.00119.87	1SG2728
ATOM	2728	CE	MET	339	110.104	42.250	38.625	1.00119.87	1SG2729
ATOM	2729	C	MET	339	110.371	45.559	44.238	1.00119.87	1SG2730
ATOM	2730	O	MET	339	109.353	45.563	44.925	1.00119.87	1SG2731
ATOM	2731	N	THR	340	111.596	45.622	44.791	1.00106.88	1SG2732
ATOM	2732	CA	THR	340	111.701	45.683	46.220	1.00106.88	1SG2733
ATOM	2733	CB	THR	340	113.105	45.686	46.760	1.00106.88	1SG2734
ATOM	2734	OG1	THR	340	113.083	45.359	48.142	1.00106.88	1SG2735
ATOM	2735	CG2	THR	340	113.720	47.083	46.591	1.00106.88	1SG2736
ATOM	2736	C	THR	340	111.029	46.935	46.685	1.00106.88	1SG2737
ATOM	2737	O	THR	340	110.414	46.948	47.748	1.00106.88	1SG2738
ATOM	2738	N	MET	341	111.150	48.030	45.910	1.00123.62	1SG2739
ATOM	2739	CA	MET	341	110.558	49.292	46.259	1.00123.62	1SG2740
ATOM	2740	CB	MET	341	110.882	50.371	45.217	1.00123.62	1SG2741
ATOM	2741	CG	MET	341	110.281	51.741	45.526	1.00123.62	1SG2742
ATOM	2742	SD	MET	341	110.456	52.930	44.164	1.00123.62	1SG2743
ATOM	2743	CE	MET	341	112.249	53.133	44.357	1.00123.62	1SG2744
ATOM	2744	C	MET	341	109.067	49.174	46.294	1.00123.62	1SG2745
ATOM	2745	O	MET	341	108.423	49.637	47.234	1.00123.62	1SG2746
ATOM	2746	N	LEU	342	108.474	48.519	45.279	1.00156.54	1SG2747
ATOM	2747	CA	LEU	342	107.045	48.420	45.222	1.00156.54	1SG2748
ATOM	2748	CB	LEU	342	106.513	47.626	44.011	1.00156.54	1SG2749
ATOM	2749	CG	LEU	342	106.712	48.306	42.644	1.00156.54	1SG2750
ATOM	2750	CD2	LEU	342	108.197	48.426	42.275	1.00156.54	1SG2751
ATOM	2751	CD1	LEU	342	105.954	49.641	42.572	1.00156.54	1SG2752
ATOM	2752	C	LEU	342	106.600	47.688	46.440	1.00156.54	1SG2753
ATOM	2753	O	LEU	342	105.575	48.022	47.029	1.00156.54	1SG2754
ATOM	2754	N	ASP	343	107.368	46.657	46.838	1.00 67.66	1SG2755
ATOM	2755	CA	ASP	343	107.035	45.860	47.981	1.00 67.66	1SG2756
ATOM	2756	CB	ASP	343	108.031	44.704	48.193	1.00 67.66	1SG2757
ATOM	2757	CG	ASP	343	107.609	43.906	49.418	1.00 67.66	1SG2758
ATOM	2758	OD1	ASP	343	108.040	44.275	50.543	1.00 67.66	1SG2759
ATOM	2759	OD2	ASP	343	106.865	42.905	49.244	1.00 67.66	1SG2760
ATOM	2760	C	ASP	343	107.067	46.730	49.192	1.00 67.66	1SG2761
ATOM	2761	O	ASP	343	106.175	46.652	50.033	1.00 67.66	1SG2762
ATOM	2762	N	ASP	344	108.091	47.598	49.297	1.00 75.59	1SG2763
ATOM	2763	CA	ASP	344	108.234	48.452	50.438	1.00 75.59	1SG2764
ATOM	2764	CB	ASP	344	109.568	49.224	50.476	1.00 75.59	1SG2765
ATOM	2765	CG	ASP	344	110.669	48.272	50.946	1.00 75.59	1SG2766
ATOM	2766	OD1	ASP	344	111.085	47.385	50.155	1.00 75.59	1SG2767
ATOM	2767	OD2	ASP	344	111.110	48.423	52.115	1.00 75.59	1SG2768

Supplementary material 1.txt

ATOM	2768	C	ASP	344	107.102	49.433	50.483	1.00	75.59	1SG2769
ATOM	2769	O	ASP	344	106.700	49.859	51.562	1.00	75.59	1SG2770
ATOM	2770	N	LEU	345	106.584	49.862	49.317	1.00	53.41	1SG2771
ATOM	2771	CA	LEU	345	105.498	50.805	49.275	1.00	53.41	1SG2772
ATOM	2772	CB	LEU	345	105.169	51.259	47.844	1.00	53.41	1SG2773
ATOM	2773	CG	LEU	345	104.010	52.270	47.784	1.00	53.41	1SG2774
ATOM	2774	CD2	LEU	345	103.552	52.508	46.336	1.00	53.41	1SG2775
ATOM	2775	CD1	LEU	345	104.377	53.571	48.516	1.00	53.41	1SG2776
ATOM	2776	C	LEU	345	104.241	50.202	49.837	1.00	53.41	1SG2777
ATOM	2777	O	LEU	345	103.569	50.808	50.668	1.00	53.41	1SG2778
ATOM	2778	N	TYR	346	103.893	48.977	49.400	1.00143.72		1SG2779
ATOM	2779	CA	TYR	346	102.680	48.332	49.821	1.00143.72		1SG2780
ATOM	2780	CB	TYR	346	102.450	46.969	49.129	1.00143.72		1SG2781
ATOM	2781	CG	TYR	346	102.014	47.152	47.710	1.00143.72		1SG2782
ATOM	2782	CD1	TYR	346	102.880	47.594	46.735	1.00143.72		1SG2783
ATOM	2783	CD2	TYR	346	100.721	46.845	47.348	1.00143.72		1SG2784
ATOM	2784	CE1	TYR	346	102.462	47.744	45.432	1.00143.72		1SG2785
ATOM	2785	CE2	TYR	346	100.297	46.991	46.047	1.00143.72		1SG2786
ATOM	2786	CZ	TYR	346	101.165	47.451	45.088	1.00143.72		1SG2787
ATOM	2787	OH	TYR	346	100.734	47.605	43.753	1.00143.72		1SG2788
ATOM	2788	C	TYR	346	102.726	48.050	51.288	1.00143.72		1SG2789
ATOM	2789	O	TYR	346	101.718	48.206	51.974	1.00143.72		1SG2790
ATOM	2790	N	ASP	347	103.858	47.523	51.799	1.00147.61		1SG2791
ATOM	2791	CA	ASP	347	103.875	47.226	53.201	1.00147.61		1SG2792
ATOM	2792	CB	ASP	347	104.909	46.151	53.605	1.00147.61		1SG2793
ATOM	2793	CG	ASP	347	106.326	46.611	53.298	1.00147.61		1SG2794
ATOM	2794	OD1	ASP	347	106.486	47.485	52.408	1.00147.61		1SG2795
ATOM	2795	OD2	ASP	347	107.272	46.086	53.945	1.00147.61		1SG2796
ATOM	2796	C	ASP	347	104.037	48.426	54.097	1.00147.61		1SG2797
ATOM	2797	O	ASP	347	103.236	48.637	55.007	1.00147.61		1SG2798
ATOM	2798	N	THR	348	105.117	49.210	53.902	1.00195.88		1SG2799
ATOM	2799	CA	THR	348	105.420	50.292	54.799	1.00195.88		1SG2800
ATOM	2800	CB	THR	348	106.893	50.574	54.907	1.00195.88		1SG2801
ATOM	2801	OG1	THR	348	107.392	51.117	53.695	1.00195.88		1SG2802
ATOM	2802	CG2	THR	348	107.614	49.254	55.231	1.00195.88		1SG2803
ATOM	2803	C	THR	348	104.751	51.624	54.556	1.00195.88		1SG2804
ATOM	2804	O	THR	348	104.472	52.316	55.526	1.00195.88		1SG2805
ATOM	2805	N	HIS	349	104.663	52.125	53.302	1.00147.89		1SG2806
ATOM	2806	CA	HIS	349	104.139	53.461	53.096	1.00147.89		1SG2807
ATOM	2807	ND1	HIS	349	104.731	56.703	52.548	1.00147.89		1SG2808
ATOM	2808	CG	HIS	349	104.356	55.611	51.803	1.00147.89		1SG2809
ATOM	2809	CB	HIS	349	104.900	54.226	52.002	1.00147.89		1SG2810
ATOM	2810	NE2	HIS	349	103.211	57.421	51.093	1.00147.89		1SG2811
ATOM	2811	CD2	HIS	349	103.426	56.067	50.916	1.00147.89		1SG2812
ATOM	2812	CE1	HIS	349	104.015	57.761	52.083	1.00147.89		1SG2813
ATOM	2813	C	HIS	349	102.680	53.684	52.789	1.00147.89		1SG2814
ATOM	2814	O	HIS	349	101.966	54.370	53.519	1.00147.89		1SG2815
ATOM	2815	N	GLY	350	102.198	53.060	51.693	1.00	55.65	1SG2816
ATOM	2816	CA	GLY	350	100.961	53.438	51.057	1.00	55.65	1SG2817
ATOM	2817	C	GLY	350	99.738	53.113	51.847	1.00	55.65	1SG2818
ATOM	2818	O	GLY	350	99.704	52.184	52.652	1.00	55.65	1SG2819
ATOM	2819	N	THR	351	98.682	53.912	51.576	1.00106.55		1SG2820
ATOM	2820	CA	THR	351	97.391	53.799	52.180	1.00106.55		1SG2821
ATOM	2821	CB	THR	351	96.722	55.131	52.326	1.00106.55		1SG2822
ATOM	2822	OG1	THR	351	95.517	55.010	53.062	1.00106.55		1SG2823
ATOM	2823	CG2	THR	351	96.429	55.675	50.920	1.00106.55		1SG2824
ATOM	2824	C	THR	351	96.545	52.961	51.274	1.00106.55		1SG2825
ATOM	2825	O	THR	351	96.917	52.684	50.135	1.00106.55		1SG2826
ATOM	2826	N	LEU	352	95.358	52.554	51.759	1.00	42.17	1SG2827
ATOM	2827	CA	LEU	352	94.517	51.682	50.995	1.00	42.17	1SG2828
ATOM	2828	CB	LEU	352	93.218	51.314	51.732	1.00	42.17	1SG2829
ATOM	2829	CG	LEU	352	92.303	50.377	50.927	1.00	42.17	1SG2830
ATOM	2830	CD2	LEU	352	90.908	50.264	51.562	1.00	42.17	1SG2831
ATOM	2831	CD1	LEU	352	92.972	49.011	50.707	1.00	42.17	1SG2832
ATOM	2832	C	LEU	352	94.140	52.360	49.715	1.00	42.17	1SG2833
ATOM	2833	O	LEU	352	94.174	51.739	48.655	1.00	42.17	1SG2834
ATOM	2834	N	ASP	353	93.764	53.652	49.777	1.00	39.89	1SG2835
ATOM	2835	CA	ASP	353	93.358	54.352	48.588	1.00	39.89	1SG2836
ATOM	2836	CB	ASP	353	92.763	55.739	48.879	1.00	39.89	1SG2837
ATOM	2837	CG	ASP	353	91.374	55.534	49.469	1.00	39.89	1SG2838
ATOM	2838	OD1	ASP	353	90.566	54.797	48.840	1.00	39.89	1SG2839

Supplementary material 1.txt

ATOM	2839	OD2	ASP	353	91.097	56.118	50.550	1.00	39.89	1SG2840
ATOM	2840	C	ASP	353	94.514	54.543	47.650	1.00	39.89	1SG2841
ATOM	2841	O	ASP	353	94.385	54.316	46.448	1.00	39.89	1SG2842
ATOM	2842	N	GLN	354	95.682	54.955	48.176	1.00	44.28	1SG2843
ATOM	2843	CA	GLN	354	96.806	55.248	47.334	1.00	44.28	1SG2844
ATOM	2844	CB	GLN	354	98.003	55.810	48.121	1.00	44.28	1SG2845
ATOM	2845	CG	GLN	354	97.715	57.183	48.736	1.00	44.28	1SG2846
ATOM	2846	CD	GLN	354	98.950	57.655	49.489	1.00	44.28	1SG2847
ATOM	2847	OE1	GLN	354	99.323	57.105	50.526	1.00	44.28	1SG2848
ATOM	2848	NE2	GLN	354	99.610	58.716	48.951	1.00	44.28	1SG2849
ATOM	2849	C	GLN	354	97.241	53.997	46.648	1.00	44.28	1SG2850
ATOM	2850	O	GLN	354	97.578	54.003	45.465	1.00	44.28	1SG2851
ATOM	2851	N	LEU	355	97.231	52.879	47.390	1.00	133.55	1SG2852
ATOM	2852	CA	LEU	355	97.673	51.623	46.871	1.00	133.55	1SG2853
ATOM	2853	CB	LEU	355	97.683	50.533	47.953	1.00	133.55	1SG2854
ATOM	2854	CG	LEU	355	98.459	49.287	47.519	1.00	133.55	1SG2855
ATOM	2855	CD2	LEU	355	99.896	49.693	47.157	1.00	133.55	1SG2856
ATOM	2856	CD1	LEU	355	97.750	48.507	46.399	1.00	133.55	1SG2857
ATOM	2857	C	LEU	355	96.744	51.207	45.771	1.00	133.55	1SG2858
ATOM	2858	O	LEU	355	97.174	50.655	44.759	1.00	133.55	1SG2859
ATOM	2859	N	LYS	356	95.433	51.458	45.947	1.00	50.39	1SG2860
ATOM	2860	CA	LYS	356	94.468	51.069	44.959	1.00	50.39	1SG2861
ATOM	2861	CB	LYS	356	93.021	51.386	45.376	1.00	50.39	1SG2862
ATOM	2862	CG	LYS	356	91.987	50.952	44.335	1.00	50.39	1SG2863
ATOM	2863	CD	LYS	356	90.551	50.932	44.859	1.00	50.39	1SG2864
ATOM	2864	CE	LYS	356	89.529	50.497	43.807	1.00	50.39	1SG2865
ATOM	2865	NZ	LYS	356	89.667	49.048	43.534	1.00	50.39	1SG2866
ATOM	2866	C	LYS	356	94.750	51.818	43.695	1.00	50.39	1SG2867
ATOM	2867	O	LYS	356	94.673	51.258	42.603	1.00	50.39	1SG2868
ATOM	2868	N	ILE	357	95.083	53.116	43.818	1.00	29.44	1SG2869
ATOM	2869	CA	ILE	357	95.355	53.950	42.682	1.00	29.44	1SG2870
ATOM	2870	CB	ILE	357	95.604	55.378	43.070	1.00	29.44	1SG2871
ATOM	2871	CG2	ILE	357	96.052	56.143	41.813	1.00	29.44	1SG2872
ATOM	2872	CG1	ILE	357	94.353	55.967	43.743	1.00	29.44	1SG2873
ATOM	2873	CD1	ILE	357	94.606	57.297	44.451	1.00	29.44	1SG2874
ATOM	2874	C	ILE	357	96.584	53.444	41.997	1.00	29.44	1SG2875
ATOM	2875	O	ILE	357	96.654	53.417	40.769	1.00	29.44	1SG2876
ATOM	2876	N	PHE	358	97.594	53.053	42.793	1.00	62.81	1SG2877
ATOM	2877	CA	PHE	358	98.856	52.590	42.293	1.00	62.81	1SG2878
ATOM	2878	CB	PHE	358	99.823	52.271	43.452	1.00	62.81	1SG2879
ATOM	2879	CG	PHE	358	101.211	52.106	42.934	1.00	62.81	1SG2880
ATOM	2880	CD1	PHE	358	101.995	53.213	42.699	1.00	62.81	1SG2881
ATOM	2881	CD2	PHE	358	101.738	50.857	42.701	1.00	62.81	1SG2882
ATOM	2882	CE1	PHE	358	103.279	53.081	42.226	1.00	62.81	1SG2883
ATOM	2883	CE2	PHE	358	103.022	50.718	42.228	1.00	62.81	1SG2884
ATOM	2884	CZ	PHE	358	103.795	51.829	41.989	1.00	62.81	1SG2885
ATOM	2885	C	PHE	358	98.635	51.334	41.505	1.00	62.81	1SG2886
ATOM	2886	O	PHE	358	99.121	51.203	40.382	1.00	62.81	1SG2887
ATOM	2887	N	THR	359	97.859	50.388	42.071	1.00	47.66	1SG2888
ATOM	2888	CA	THR	359	97.617	49.117	41.450	1.00	47.66	1SG2889
ATOM	2889	CB	THR	359	96.739	48.231	42.286	1.00	47.66	1SG2890
ATOM	2890	OG1	THR	359	97.324	48.028	43.566	1.00	47.66	1SG2891
ATOM	2891	CG2	THR	359	96.577	46.883	41.564	1.00	47.66	1SG2892
ATOM	2892	C	THR	359	96.929	49.341	40.136	1.00	47.66	1SG2893
ATOM	2893	O	THR	359	97.277	48.729	39.128	1.00	47.66	1SG2894
ATOM	2894	N	GLU	360	95.932	50.239	40.100	1.00	42.62	1SG2895
ATOM	2895	CA	GLU	360	95.226	50.478	38.872	1.00	42.62	1SG2896
ATOM	2896	CB	GLU	360	94.114	51.534	38.987	1.00	42.62	1SG2897
ATOM	2897	CG	GLU	360	92.840	51.045	39.669	1.00	42.62	1SG2898
ATOM	2898	CD	GLU	360	91.860	52.209	39.697	1.00	42.62	1SG2899
ATOM	2899	OE1	GLU	360	92.330	53.378	39.702	1.00	42.62	1SG2900
ATOM	2900	OE2	GLU	360	90.628	51.944	39.716	1.00	42.62	1SG2901
ATOM	2901	C	GLU	360	96.183	51.022	37.867	1.00	42.62	1SG2902
ATOM	2902	O	GLU	360	96.151	50.640	36.699	1.00	42.62	1SG2903
ATOM	2903	N	GLY	361	97.074	51.928	38.304	1.00	25.56	1SG2904
ATOM	2904	CA	GLY	361	97.964	52.557	37.378	1.00	25.56	1SG2905
ATOM	2905	C	GLY	361	98.835	51.523	36.730	1.00	25.56	1SG2906
ATOM	2906	O	GLY	361	99.059	51.574	35.522	1.00	25.56	1SG2907
ATOM	2907	N	VAL	362	99.355	50.551	37.509	1.00	104.37	1SG2908
ATOM	2908	CA	VAL	362	100.249	49.586	36.931	1.00	104.37	1SG2909
ATOM	2909	CB	VAL	362	100.866	48.642	37.926	1.00	104.37	1SG2910

Supplementary material 1.txt

ATOM	2910	CG1	VAL	362	101.683	49.464	38.937	1.00104.37	1SG2911
ATOM	2911	CG2	VAL	362	99.773	47.761	38.547	1.00104.37	1SG2912
ATOM	2912	C	VAL	362	99.531	48.763	35.910	1.00104.37	1SG2913
ATOM	2913	O	VAL	362	100.081	48.461	34.853	1.00104.37	1SG2914
ATOM	2914	N	ARG	363	98.275	48.375	36.188	1.00 43.75	1SG2915
ATOM	2915	CA	ARG	363	97.574	47.535	35.260	1.00 43.75	1SG2916
ATOM	2916	CB	ARG	363	96.181	47.124	35.765	1.00 43.75	1SG2917
ATOM	2917	CG	ARG	363	96.263	46.193	36.978	1.00 43.75	1SG2918
ATOM	2918	CD	ARG	363	94.930	45.568	37.389	1.00 43.75	1SG2919
ATOM	2919	NE	ARG	363	95.209	44.662	38.539	1.00 43.75	1SG2920
ATOM	2920	CZ	ARG	363	95.611	43.377	38.313	1.00 43.75	1SG2921
ATOM	2921	NH1	ARG	363	95.760	42.922	37.035	1.00 43.75	1SG2922
ATOM	2922	NH2	ARG	363	95.865	42.545	39.366	1.00 43.75	1SG2923
ATOM	2923	C	ARG	363	97.430	48.239	33.946	1.00 43.75	1SG2924
ATOM	2924	O	ARG	363	97.612	47.631	32.892	1.00 43.75	1SG2925
ATOM	2925	N	ARG	364	97.106	49.543	33.975	1.00124.02	1SG2926
ATOM	2926	CA	ARG	364	96.892	50.307	32.779	1.00124.02	1SG2927
ATOM	2927	CB	ARG	364	96.350	51.701	33.095	1.00124.02	1SG2928
ATOM	2928	CG	ARG	364	95.081	51.631	33.953	1.00124.02	1SG2929
ATOM	2929	CD	ARG	364	93.903	50.925	33.283	1.00124.02	1SG2930
ATOM	2930	NE	ARG	364	92.771	50.925	34.253	1.00124.02	1SG2931
ATOM	2931	CZ	ARG	364	91.940	52.005	34.338	1.00124.02	1SG2932
ATOM	2932	NH1	ARG	364	92.152	53.095	33.545	1.00124.02	1SG2933
ATOM	2933	NH2	ARG	364	90.896	51.993	35.217	1.00124.02	1SG2934
ATOM	2934	C	ARG	364	98.178	50.429	32.017	1.00124.02	1SG2935
ATOM	2935	O	ARG	364	98.186	50.341	30.790	1.00124.02	1SG2936
ATOM	2936	N	TRP	365	99.309	50.600	32.731	1.00 96.65	1SG2937
ATOM	2937	CA	TRP	365	100.599	50.689	32.098	1.00 96.65	1SG2938
ATOM	2938	CB	TRP	365	100.908	49.423	31.272	1.00 96.65	1SG2939
ATOM	2939	CG	TRP	365	102.291	49.325	30.670	1.00 96.65	1SG2940
ATOM	2940	CD2	TRP	365	103.423	48.842	31.404	1.00 96.65	1SG2941
ATOM	2941	CD1	TRP	365	102.738	49.618	29.414	1.00 96.65	1SG2942
ATOM	2942	NE1	TRP	365	104.081	49.342	29.319	1.00 96.65	1SG2943
ATOM	2943	CE2	TRP	365	104.517	48.865	30.538	1.00 96.65	1SG2944
ATOM	2944	CE3	TRP	365	103.541	48.411	32.693	1.00 96.65	1SG2945
ATOM	2945	CZ2	TRP	365	105.751	48.454	30.953	1.00 96.65	1SG2946
ATOM	2946	CZ3	TRP	365	104.787	48.001	33.111	1.00 96.65	1SG2947
ATOM	2947	CH2	TRP	365	105.870	48.024	32.257	1.00 96.65	1SG2948
ATOM	2948	C	TRP	365	100.688	51.884	31.186	1.00 96.65	1SG2949
ATOM	2949	O	TRP	365	101.197	51.781	30.072	1.00 96.65	1SG2950
ATOM	2950	N	ASP	366	100.178	53.059	31.616	1.00 75.78	1SG2951
ATOM	2951	CA	ASP	366	100.328	54.233	30.797	1.00 75.78	1SG2952
ATOM	2952	CB	ASP	366	99.016	54.723	30.167	1.00 75.78	1SG2953
ATOM	2953	CG	ASP	366	99.371	55.781	29.132	1.00 75.78	1SG2954
ATOM	2954	OD1	ASP	366	100.201	55.480	28.233	1.00 75.78	1SG2955
ATOM	2955	OD2	ASP	366	98.806	56.903	29.222	1.00 75.78	1SG2956
ATOM	2956	C	ASP	366	100.845	55.346	31.666	1.00 75.78	1SG2957
ATOM	2957	O	ASP	366	100.463	55.473	32.827	1.00 75.78	1SG2958
ATOM	2958	N	VAL	367	101.739	56.188	31.112	1.00109.41	1SG2959
ATOM	2959	CA	VAL	367	102.346	57.279	31.824	1.00109.41	1SG2960
ATOM	2960	CB	VAL	367	103.479	57.917	31.077	1.00109.41	1SG2961
ATOM	2961	CG1	VAL	367	104.622	56.890	31.011	1.00109.41	1SG2962
ATOM	2962	CG2	VAL	367	102.977	58.385	29.699	1.00109.41	1SG2963
ATOM	2963	C	VAL	367	101.332	58.328	32.176	1.00109.41	1SG2964
ATOM	2964	O	VAL	367	101.499	59.045	33.160	1.00109.41	1SG2965
ATOM	2965	N	SER	368	100.261	58.466	31.374	1.00 80.71	1SG2966
ATOM	2966	CA	SER	368	99.280	59.492	31.605	1.00 80.71	1SG2967
ATOM	2967	CB	SER	368	98.152	59.484	30.561	1.00 80.71	1SG2968
ATOM	2968	OG	SER	368	97.222	60.520	30.845	1.00 80.71	1SG2969
ATOM	2969	C	SER	368	98.640	59.310	32.950	1.00 80.71	1SG2970
ATOM	2970	O	SER	368	98.194	60.275	33.566	1.00 80.71	1SG2971
ATOM	2971	N	LEU	369	98.588	58.063	33.440	1.00113.73	1SG2972
ATOM	2972	CA	LEU	369	97.958	57.704	34.680	1.00113.73	1SG2973
ATOM	2973	CB	LEU	369	97.755	56.198	34.857	1.00113.73	1SG2974
ATOM	2974	CG	LEU	369	96.736	55.670	33.838	1.00113.73	1SG2975
ATOM	2975	CD2	LEU	369	96.106	54.364	34.320	1.00113.73	1SG2976
ATOM	2976	CD1	LEU	369	97.323	55.618	32.417	1.00113.73	1SG2977
ATOM	2977	C	LEU	369	98.698	58.252	35.863	1.00113.73	1SG2978
ATOM	2978	O	LEU	369	98.187	58.217	36.982	1.00113.73	1SG2979
ATOM	2979	N	VAL	370	99.939	58.724	35.658	1.00106.05	1SG2980
ATOM	2980	CA	VAL	370	100.789	59.195	36.719	1.00106.05	1SG2981

Supplementary material 1.txt

ATOM	2981	CB	VAL	370	102.102	59.741	36.226	1.00106.05	1SG2982
ATOM	2982	CG1	VAL	370	101.835	60.960	35.327	1.00106.05	1SG2983
ATOM	2983	CG2	VAL	370	102.982	60.059	37.447	1.00106.05	1SG2984
ATOM	2984	C	VAL	370	100.130	60.283	37.523	1.00106.05	1SG2985
ATOM	2985	O	VAL	370	100.332	60.359	38.734	1.00106.05	1SG2986
ATOM	2986	N	GLU	371	99.320	61.151	36.893	1.0073.80	1SG2987
ATOM	2987	CA	GLU	371	98.735	62.268	37.590	1.0073.80	1SG2988
ATOM	2988	CB	GLU	371	97.838	63.127	36.684	1.0073.80	1SG2989
ATOM	2989	CG	GLU	371	98.615	63.966	35.666	1.0073.80	1SG2990
ATOM	2990	CD	GLU	371	99.012	65.271	36.343	1.0073.80	1SG2991
ATOM	2991	OE1	GLU	371	98.326	65.658	37.327	1.0073.80	1SG2992
ATOM	2992	OE2	GLU	371	100.002	65.901	35.884	1.0073.80	1SG2993
ATOM	2993	C	GLU	371	97.899	61.797	38.746	1.0073.80	1SG2994
ATOM	2994	O	GLU	371	97.835	62.469	39.774	1.0073.80	1SG2995
ATOM	2995	N	GLY	372	97.220	60.644	38.605	1.0035.50	1SG2996
ATOM	2996	CA	GLY	372	96.361	60.118	39.632	1.0035.50	1SG2997
ATOM	2997	C	GLY	372	97.161	59.802	40.864	1.0035.50	1SG2998
ATOM	2998	O	GLY	372	96.647	59.870	41.981	1.0035.50	1SG2999
ATOM	2999	N	LEU	373	98.428	59.390	40.682	1.0069.54	1SG3000
ATOM	3000	CA	LEU	373	99.286	58.983	41.763	1.0069.54	1SG3001
ATOM	3001	CB	LEU	373	100.492	58.167	41.262	1.0069.54	1SG3002
ATOM	3002	CG	LEU	373	100.113	56.888	40.491	1.0069.54	1SG3003
ATOM	3003	CD2	LEU	373	99.152	56.006	41.300	1.0069.54	1SG3004
ATOM	3004	CD1	LEU	373	101.363	56.127	40.022	1.0069.54	1SG3005
ATOM	3005	C	LEU	373	99.855	60.188	42.455	1.0069.54	1SG3006
ATOM	3006	O	LEU	373	100.050	61.245	41.857	1.0069.54	1SG3007
ATOM	3007	N	PRO	374	100.132	60.033	43.726	1.0083.12	1SG3008
ATOM	3008	CA	PRO	374	100.738	61.073	44.514	1.0083.12	1SG3009
ATOM	3009	CD	PRO	374	99.445	59.052	44.545	1.0083.12	1SG3010
ATOM	3010	CB	PRO	374	100.543	60.666	45.976	1.0083.12	1SG3011
ATOM	3011	CG	PRO	374	100.123	59.185	45.916	1.0083.12	1SG3012
ATOM	3012	C	PRO	374	102.167	61.181	44.078	1.0083.12	1SG3013
ATOM	3013	O	PRO	374	102.663	60.250	43.449	1.0083.12	1SG3014
ATOM	3014	N	ASP	375	102.854	62.286	44.423	1.0048.05	1SG3015
ATOM	3015	CA	ASP	375	104.168	62.561	43.911	1.0048.05	1SG3016
ATOM	3016	CB	ASP	375	104.742	63.903	44.398	1.0048.05	1SG3017
ATOM	3017	CG	ASP	375	104.040	65.023	43.635	1.0048.05	1SG3018
ATOM	3018	OD1	ASP	375	103.351	64.713	42.627	1.0048.05	1SG3019
ATOM	3019	OD2	ASP	375	104.195	66.206	44.041	1.0048.05	1SG3020
ATOM	3020	C	ASP	375	105.156	61.483	44.250	1.0048.05	1SG3021
ATOM	3021	O	ASP	375	105.998	61.149	43.419	1.0048.05	1SG3022
ATOM	3022	N	PHE	376	105.117	60.896	45.459	1.0064.62	1SG3023
ATOM	3023	CA	PHE	376	106.135	59.920	45.733	1.0064.62	1SG3024
ATOM	3024	CB	PHE	376	106.167	59.418	47.193	1.0064.62	1SG3025
ATOM	3025	CG	PHE	376	104.979	58.573	47.495	1.0064.62	1SG3026
ATOM	3026	CD1	PHE	376	103.764	59.137	47.810	1.0064.62	1SG3027
ATOM	3027	CD2	PHE	376	105.095	57.202	47.488	1.0064.62	1SG3028
ATOM	3028	CE1	PHE	376	102.677	58.343	48.095	1.0064.62	1SG3029
ATOM	3029	CE2	PHE	376	104.013	56.403	47.772	1.0064.62	1SG3030
ATOM	3030	CZ	PHE	376	102.800	56.974	48.076	1.0064.62	1SG3031
ATOM	3031	C	PHE	376	105.962	58.743	44.817	1.0064.62	1SG3032
ATOM	3032	O	PHE	376	106.937	58.178	44.325	1.0064.62	1SG3033
ATOM	3033	N	MET	377	104.704	58.336	44.577	1.0066.59	1SG3034
ATOM	3034	CA	MET	377	104.391	57.208	43.745	1.0066.59	1SG3035
ATOM	3035	CB	MET	377	102.909	56.797	43.796	1.0066.59	1SG3036
ATOM	3036	CG	MET	377	102.517	56.091	45.096	1.0066.59	1SG3037
ATOM	3037	SD	MET	377	100.776	55.574	45.177	1.0066.59	1SG3038
ATOM	3038	CE	MET	377	101.028	54.341	46.487	1.0066.59	1SG3039
ATOM	3039	C	MET	377	104.746	57.485	42.317	1.0066.59	1SG3040
ATOM	3040	O	MET	377	105.041	56.559	41.564	1.0066.59	1SG3041
ATOM	3041	N	LYS	378	104.677	58.756	41.881	1.00152.66	1SG3042
ATOM	3042	CA	LYS	378	104.960	59.034	40.502	1.00152.66	1SG3043
ATOM	3043	CB	LYS	378	104.730	60.495	40.077	1.00152.66	1SG3044
ATOM	3044	CG	LYS	378	105.691	61.492	40.717	1.00152.66	1SG3045
ATOM	3045	CD	LYS	378	105.747	62.844	40.001	1.00152.66	1SG3046
ATOM	3046	CE	LYS	378	104.455	63.210	39.266	1.00152.66	1SG3047
ATOM	3047	NZ	LYS	378	104.415	62.547	37.942	1.00152.66	1SG3048
ATOM	3048	C	LYS	378	106.382	58.686	40.199	1.00152.66	1SG3049
ATOM	3049	O	LYS	378	106.692	58.247	39.093	1.00152.66	1SG3050
ATOM	3050	N	ILE	379	107.293	58.883	41.169	1.0039.93	1SG3051
ATOM	3051	CA	ILE	379	108.678	58.615	40.920	1.0039.93	1SG3052

Supplementary material 1.txt

ATOM	3052	CB	ILE	379	109.541	58.936	42.108	1.00	39.93	1SG3053
ATOM	3053	CG2	ILE	379	110.996	58.587	41.752	1.00	39.93	1SG3054
ATOM	3054	CG1	ILE	379	109.355	60.406	42.518	1.00	39.93	1SG3055
ATOM	3055	CD1	ILE	379	109.958	60.739	43.881	1.00	39.93	1SG3056
ATOM	3056	C	ILE	379	108.840	57.152	40.626	1.00	39.93	1SG3057
ATOM	3057	O	ILE	379	109.511	56.773	39.667	1.00	39.93	1SG3058
ATOM	3058	N	ALA	380	108.213	56.288	41.448	1.00	38.16	1SG3059
ATOM	3059	CA	ALA	380	108.330	54.863	41.296	1.00	38.16	1SG3060
ATOM	3060	CB	ALA	380	107.597	54.089	42.405	1.00	38.16	1SG3061
ATOM	3061	C	ALA	380	107.736	54.423	39.992	1.00	38.16	1SG3062
ATOM	3062	O	ALA	380	108.325	53.622	39.267	1.00	38.16	1SG3063
ATOM	3063	N	PHE	381	106.555	54.964	39.651	1.00	50.62	1SG3064
ATOM	3064	CA	PHE	381	105.815	54.554	38.491	1.00	50.62	1SG3065
ATOM	3065	CB	PHE	381	104.472	55.302	38.396	1.00	50.62	1SG3066
ATOM	3066	CG	PHE	381	103.701	54.793	37.229	1.00	50.62	1SG3067
ATOM	3067	CD1	PHE	381	102.890	53.688	37.351	1.00	50.62	1SG3068
ATOM	3068	CD2	PHE	381	103.785	55.427	36.011	1.00	50.62	1SG3069
ATOM	3069	CE1	PHE	381	102.176	53.223	36.271	1.00	50.62	1SG3070
ATOM	3070	CE2	PHE	381	103.074	54.966	34.929	1.00	50.62	1SG3071
ATOM	3071	CZ	PHE	381	102.268	53.861	35.058	1.00	50.62	1SG3072
ATOM	3072	C	PHE	381	106.590	54.833	37.238	1.00	50.62	1SG3073
ATOM	3073	O	PHE	381	106.664	53.985	36.349	1.00	50.62	1SG3074
ATOM	3074	N	GLU	382	107.181	56.037	37.130	1.00	38.04	1SG3075
ATOM	3075	CA	GLU	382	107.891	56.431	35.943	1.00	38.04	1SG3076
ATOM	3076	CB	GLU	382	108.375	57.887	36.024	1.00	38.04	1SG3077
ATOM	3077	CG	GLU	382	109.061	58.389	34.754	1.00	38.04	1SG3078
ATOM	3078	CD	GLU	382	109.480	59.830	35.003	1.00	38.04	1SG3079
ATOM	3079	OE1	GLU	382	110.121	60.082	36.057	1.00	38.04	1SG3080
ATOM	3080	OE2	GLU	382	109.162	60.698	34.146	1.00	38.04	1SG3081
ATOM	3081	C	GLU	382	109.102	55.574	35.768	1.00	38.04	1SG3082
ATOM	3082	O	GLU	382	109.404	55.110	34.670	1.00	38.04	1SG3083
ATOM	3083	N	PHE	383	109.814	55.310	36.873	1.00	83.08	1SG3084
ATOM	3084	CA	PHE	383	111.058	54.604	36.828	1.00	83.08	1SG3085
ATOM	3085	CB	PHE	383	111.598	54.400	38.254	1.00	83.08	1SG3086
ATOM	3086	CG	PHE	383	113.010	53.934	38.221	1.00	83.08	1SG3087
ATOM	3087	CD1	PHE	383	114.034	54.849	38.129	1.00	83.08	1SG3088
ATOM	3088	CD2	PHE	383	113.313	52.595	38.301	1.00	83.08	1SG3089
ATOM	3089	CE1	PHE	383	115.344	54.435	38.108	1.00	83.08	1SG3090
ATOM	3090	CE2	PHE	383	114.622	52.175	38.280	1.00	83.08	1SG3091
ATOM	3091	CZ	PHE	383	115.637	53.096	38.184	1.00	83.08	1SG3092
ATOM	3092	C	PHE	383	110.810	53.258	36.225	1.00	83.08	1SG3093
ATOM	3093	O	PHE	383	111.556	52.803	35.358	1.00	83.08	1SG3094
ATOM	3094	N	TRP	384	109.744	52.578	36.680	1.00	158.48	1SG3095
ATOM	3095	CA	TRP	384	109.461	51.256	36.207	1.00	158.48	1SG3096
ATOM	3096	CB	TRP	384	108.301	50.574	36.960	1.00	158.48	1SG3097
ATOM	3097	CG	TRP	384	107.820	49.276	36.341	1.00	158.48	1SG3098
ATOM	3098	CD2	TRP	384	108.394	47.978	36.568	1.00	158.48	1SG3099
ATOM	3099	CD1	TRP	384	106.784	49.088	35.473	1.00	158.48	1SG3100
ATOM	3100	NE1	TRP	384	106.674	47.756	35.148	1.00	158.48	1SG3101
ATOM	3101	CE2	TRP	384	107.659	47.062	35.815	1.00	158.48	1SG3102
ATOM	3102	CE3	TRP	384	109.445	47.578	37.339	1.00	158.48	1SG3103
ATOM	3103	CZ2	TRP	384	107.969	45.731	35.823	1.00	158.48	1SG3104
ATOM	3104	CZ3	TRP	384	109.755	46.236	37.347	1.00	158.48	1SG3105
ATOM	3105	CH2	TRP	384	109.031	45.330	36.603	1.00	158.48	1SG3106
ATOM	3106	C	TRP	384	109.109	51.206	34.755	1.00	158.48	1SG3107
ATOM	3107	O	TRP	384	109.705	50.452	33.989	1.00	158.48	1SG3108
ATOM	3108	N	LEU	385	108.128	52.020	34.341	1.00	165.31	1SG3109
ATOM	3109	CA	LEU	385	107.534	51.837	33.048	1.00	165.31	1SG3110
ATOM	3110	CB	LEU	385	106.280	52.729	32.908	1.00	165.31	1SG3111
ATOM	3111	CG	LEU	385	105.260	52.363	31.802	1.00	165.31	1SG3112
ATOM	3112	CD2	LEU	385	105.896	51.927	30.474	1.00	165.31	1SG3113
ATOM	3113	CD1	LEU	385	104.219	53.484	31.637	1.00	165.31	1SG3114
ATOM	3114	C	LEU	385	108.447	52.137	31.915	1.00	165.31	1SG3115
ATOM	3115	O	LEU	385	108.736	51.273	31.094	1.00	165.31	1SG3116
ATOM	3116	N	LYS	386	109.002	53.348	31.873	1.00	283.15	1SG3117
ATOM	3117	CA	LYS	386	109.679	53.710	30.670	1.00	283.15	1SG3118
ATOM	3118	CB	LYS	386	111.017	53.008	30.366	1.00	283.15	1SG3119
ATOM	3119	CG	LYS	386	111.671	53.604	29.107	1.00	283.15	1SG3120
ATOM	3120	CD	LYS	386	113.126	53.223	28.832	1.00	283.15	1SG3121
ATOM	3121	CE	LYS	386	114.059	54.400	28.540	1.00	283.15	1SG3122
ATOM	3122	NZ	LYS	386	113.727	54.994	27.226	1.00	283.15	1SG3123

Supplementary material 1.txt

ATOM	3123	C	LYS	386	108.778	53.490	29.491	1.00283.15	1SG3124
ATOM	3124	O	LYS	386	109.138	52.776	28.559	1.00283.15	1SG3125
ATOM	3125	N	THR	387	107.536	54.013	29.501	1.00147.05	1SG3126
ATOM	3126	CA	THR	387	106.907	53.922	28.217	1.00147.05	1SG3127
ATOM	3127	CB	THR	387	105.453	54.336	28.168	1.00147.05	1SG3128
ATOM	3128	OG1	THR	387	104.886	53.936	26.929	1.00147.05	1SG3129
ATOM	3129	CG2	THR	387	105.292	55.854	28.340	1.00147.05	1SG3130
ATOM	3130	C	THR	387	107.765	54.852	27.426	1.00147.05	1SG3131
ATOM	3131	O	THR	387	108.165	54.581	26.295	1.00147.05	1SG3132
ATOM	3132	N	SER	388	108.086	55.980	28.086	1.00113.77	1SG3133
ATOM	3133	CA	SER	388	109.045	56.955	27.676	1.00113.77	1SG3134
ATOM	3134	CB	SER	388	108.403	58.206	27.052	1.00113.77	1SG3135
ATOM	3135	OG	SER	388	107.563	58.850	27.999	1.00113.77	1SG3136
ATOM	3136	C	SER	388	109.646	57.353	28.984	1.00113.77	1SG3137
ATOM	3137	O	SER	388	109.759	58.533	29.313	1.00113.77	1SG3138
ATOM	3138	N	ASN	389	110.078	56.338	29.754	1.00163.78	1SG3139
ATOM	3139	CA	ASN	389	110.544	56.549	31.092	1.00163.78	1SG3140
ATOM	3140	CB	ASN	389	109.504	56.224	32.176	1.00163.78	1SG3141
ATOM	3141	CG	ASN	389	108.362	57.224	32.079	1.00163.78	1SG3142
ATOM	3142	OD1	ASN	389	108.501	58.305	31.509	1.00163.78	1SG3143
ATOM	3143	ND2	ASN	389	107.192	56.854	32.664	1.00163.78	1SG3144
ATOM	3144	C	ASN	389	111.749	55.696	31.323	1.00163.78	1SG3145
ATOM	3145	O	ASN	389	112.665	55.697	30.507	1.00163.78	1SG3146
ATOM	3146	N	GLU	390	111.875	55.082	32.520	1.00187.68	1SG3147
ATOM	3147	CA	GLU	390	113.086	54.331	32.712	1.00187.68	1SG3148
ATOM	3148	CB	GLU	390	113.600	54.408	34.162	1.00187.68	1SG3149
ATOM	3149	CG	GLU	390	114.292	55.732	34.496	1.00187.68	1SG3150
ATOM	3150	CD	GLU	390	113.236	56.810	34.693	1.00187.68	1SG3151
ATOM	3151	OE1	GLU	390	112.030	56.453	34.761	1.00187.68	1SG3152
ATOM	3152	OE2	GLU	390	113.622	58.006	34.776	1.00187.68	1SG3153
ATOM	3153	C	GLU	390	113.233	52.876	32.297	1.00187.68	1SG3154
ATOM	3154	O	GLU	390	113.950	52.555	31.351	1.00187.68	1SG3155
ATOM	3155	N	LEU	391	112.542	51.959	33.014	1.00104.73	1SG3156
ATOM	3156	CA	LEU	391	112.923	50.560	32.967	1.00104.73	1SG3157
ATOM	3157	CB	LEU	391	112.519	49.812	34.251	1.00104.73	1SG3158
ATOM	3158	CG	LEU	391	113.016	48.354	34.296	1.00104.73	1SG3159
ATOM	3159	CD2	LEU	391	112.463	47.618	35.527	1.00104.73	1SG3160
ATOM	3160	CD1	LEU	391	114.552	48.282	34.215	1.00104.73	1SG3161
ATOM	3161	C	LEU	391	112.540	49.673	31.813	1.00104.73	1SG3162
ATOM	3162	O	LEU	391	113.414	49.097	31.166	1.00104.73	1SG3163
ATOM	3163	N	ILE	392	111.230	49.519	31.521	1.00151.15	1SG3164
ATOM	3164	CA	ILE	392	110.862	48.480	30.591	1.00151.15	1SG3165
ATOM	3165	CB	ILE	392	109.406	48.083	30.561	1.00151.15	1SG3166
ATOM	3166	CG2	ILE	392	108.640	49.001	29.598	1.00151.15	1SG3167
ATOM	3167	CG1	ILE	392	109.296	46.623	30.086	1.00151.15	1SG3168
ATOM	3168	CD1	ILE	392	109.852	45.608	31.084	1.00151.15	1SG3169
ATOM	3169	C	ILE	392	111.276	48.815	29.200	1.00151.15	1SG3170
ATOM	3170	O	ILE	392	111.715	47.932	28.468	1.00151.15	1SG3171
ATOM	3171	N	ALA	393	111.108	50.084	28.774	1.00 63.68	1SG3172
ATOM	3172	CA	ALA	393	111.485	50.413	27.431	1.00 63.68	1SG3173
ATOM	3173	CB	ALA	393	111.074	51.791	26.898	1.00 63.68	1SG3174
ATOM	3174	C	ALA	393	112.960	50.278	27.307	1.00 63.68	1SG3175
ATOM	3175	O	ALA	393	113.478	50.027	26.223	1.00 63.68	1SG3176
ATOM	3176	N	GLU	394	113.700	50.504	28.402	1.00 69.06	1SG3177
ATOM	3177	CA	GLU	394	115.114	50.355	28.276	1.00 69.06	1SG3178
ATOM	3178	CB	GLU	394	115.874	50.656	29.577	1.00 69.06	1SG3179
ATOM	3179	CG	GLU	394	117.391	50.668	29.387	1.00 69.06	1SG3180
ATOM	3180	CD	GLU	394	118.015	51.312	30.616	1.00 69.06	1SG3181
ATOM	3181	OE1	GLU	394	117.244	51.696	31.536	1.00 69.06	1SG3182
ATOM	3182	OE2	GLU	394	119.269	51.433	30.652	1.00 69.06	1SG3183
ATOM	3183	C	GLU	394	115.343	48.927	27.902	1.00 69.06	1SG3184
ATOM	3184	O	GLU	394	116.173	48.619	27.047	1.00 69.06	1SG3185
ATOM	3185	N	ALA	395	114.576	48.016	28.529	1.00 32.85	1SG3186
ATOM	3186	CA	ALA	395	114.687	46.619	28.242	1.00 32.85	1SG3187
ATOM	3187	CB	ALA	395	113.763	45.756	29.120	1.00 32.85	1SG3188
ATOM	3188	C	ALA	395	114.302	46.387	26.812	1.00 32.85	1SG3189
ATOM	3189	O	ALA	395	114.976	45.650	26.094	1.00 32.85	1SG3190
ATOM	3190	N	VAL	396	113.213	47.027	26.343	1.00105.46	1SG3191
ATOM	3191	CA	VAL	396	112.801	46.785	24.991	1.00105.46	1SG3192
ATOM	3192	CB	VAL	396	111.498	47.429	24.584	1.00105.46	1SG3193
ATOM	3193	CG1	VAL	396	110.392	46.927	25.527	1.00105.46	1SG3194

Supplementary material 1.txt

ATOM	3194	CG2	VAL	396	111.648	48.953	24.505	1.00105.46	1SG3195
ATOM	3195	C	VAL	396	113.882	47.277	24.082	1.00105.46	1SG3196
ATOM	3196	O	VAL	396	114.153	46.671	23.048	1.00105.46	1SG3197
ATOM	3197	N	LYS	397	114.526	48.402	24.450	1.00133.59	1SG3198
ATOM	3198	CA	LYS	397	115.559	48.996	23.646	1.00133.59	1SG3199
ATOM	3199	CB	LYS	397	116.059	50.342	24.198	1.00133.59	1SG3200
ATOM	3200	CG	LYS	397	115.098	51.500	23.929	1.00133.59	1SG3201
ATOM	3201	CD	LYS	397	114.847	51.729	22.436	1.00133.59	1SG3202
ATOM	3202	CE	LYS	397	114.007	52.969	22.131	1.00133.59	1SG3203
ATOM	3203	NZ	LYS	397	114.839	54.186	22.268	1.00133.59	1SG3204
ATOM	3204	C	LYS	397	116.750	48.090	23.533	1.00133.59	1SG3205
ATOM	3205	O	LYS	397	117.327	47.958	22.455	1.00133.59	1SG3206
ATOM	3206	N	ALA	398	117.158	47.443	24.641	1.00 37.53	1SG3207
ATOM	3207	CA	ALA	398	118.324	46.600	24.623	1.00 37.53	1SG3208
ATOM	3208	CB	ALA	398	118.648	46.010	26.005	1.00 37.53	1SG3209
ATOM	3209	C	ALA	398	118.085	45.449	23.693	1.00 37.53	1SG3210
ATOM	3210	O	ALA	398	118.978	45.019	22.963	1.00 37.53	1SG3211
ATOM	3211	N	GLN	399	116.856	44.916	23.742	1.00 77.81	1SG3212
ATOM	3212	CA	GLN	399	116.349	43.796	23.003	1.00 77.81	1SG3213
ATOM	3213	CB	GLN	399	114.995	43.331	23.556	1.00 77.81	1SG3214
ATOM	3214	CG	GLN	399	115.086	42.852	25.005	1.00 77.81	1SG3215
ATOM	3215	CD	GLN	399	113.671	42.623	25.507	1.00 77.81	1SG3216
ATOM	3216	OE1	GLN	399	113.318	41.523	25.929	1.00 77.81	1SG3217
ATOM	3217	NE2	GLN	399	112.835	43.694	25.469	1.00 77.81	1SG3218
ATOM	3218	C	GLN	399	116.145	44.118	21.552	1.00 77.81	1SG3219
ATOM	3219	O	GLN	399	116.099	43.215	20.717	1.00 77.81	1SG3220
ATOM	3220	N	GLY	400	115.986	45.410	21.218	1.00 42.56	1SG3221
ATOM	3221	CA	GLY	400	115.573	45.839	19.910	1.00 42.56	1SG3222
ATOM	3222	C	GLY	400	116.455	45.298	18.824	1.00 42.56	1SG3223
ATOM	3223	O	GLY	400	115.965	44.983	17.742	1.00 42.56	1SG3224
ATOM	3224	N	GLN	401	117.778	45.200	19.039	1.00 78.09	1SG3225
ATOM	3225	CA	GLN	401	118.596	44.748	17.947	1.00 78.09	1SG3226
ATOM	3226	CB	GLN	401	120.101	44.814	18.255	1.00 78.09	1SG3227
ATOM	3227	CG	GLN	401	120.976	44.395	17.071	1.00 78.09	1SG3228
ATOM	3228	CD	GLN	401	122.431	44.656	17.436	1.00 78.09	1SG3229
ATOM	3229	OE1	GLN	401	122.732	45.170	18.512	1.00 78.09	1SG3230
ATOM	3230	NE2	GLN	401	123.363	44.300	16.511	1.00 78.09	1SG3231
ATOM	3231	C	GLN	401	118.256	43.330	17.577	1.00 78.09	1SG3232
ATOM	3232	O	GLN	401	118.114	43.005	16.399	1.00 78.09	1SG3233
ATOM	3233	N	ASP	402	118.104	42.458	18.589	1.00 74.61	1SG3234
ATOM	3234	CA	ASP	402	117.831	41.050	18.459	1.00 74.61	1SG3235
ATOM	3235	CB	ASP	402	118.031	40.280	19.774	1.00 74.61	1SG3236
ATOM	3236	CG	ASP	402	119.519	40.270	20.095	1.00 74.61	1SG3237
ATOM	3237	OD1	ASP	402	120.332	40.117	19.144	1.00 74.61	1SG3238
ATOM	3238	OD2	ASP	402	119.862	40.406	21.300	1.00 74.61	1SG3239
ATOM	3239	C	ASP	402	116.418	40.804	17.995	1.00 74.61	1SG3240
ATOM	3240	O	ASP	402	116.124	39.722	17.489	1.00 74.61	1SG3241
ATOM	3241	N	MET	403	115.533	41.825	18.075	1.00136.58	1SG3242
ATOM	3242	CA	MET	403	114.107	41.694	17.870	1.00136.58	1SG3243
ATOM	3243	CB	MET	403	113.738	41.151	16.478	1.00136.58	1SG3244
ATOM	3244	CG	MET	403	113.992	42.143	15.341	1.00136.58	1SG3245
ATOM	3245	SD	MET	403	112.834	43.545	15.288	1.00136.58	1SG3246
ATOM	3246	CE	MET	403	113.462	44.360	16.784	1.00136.58	1SG3247
ATOM	3247	C	MET	403	113.494	40.784	18.897	1.00136.58	1SG3248
ATOM	3248	O	MET	403	112.508	40.089	18.645	1.00136.58	1SG3249
ATOM	3249	N	ALA	404	114.135	40.767	20.078	1.00107.19	1SG3250
ATOM	3250	CA	ALA	404	113.805	40.181	21.349	1.00107.19	1SG3251
ATOM	3251	CB	ALA	404	115.009	40.087	22.302	1.00107.19	1SG3252
ATOM	3252	C	ALA	404	112.735	40.970	22.064	1.00107.19	1SG3253
ATOM	3253	O	ALA	404	112.241	40.522	23.091	1.00107.19	1SG3254
ATOM	3254	N	ALA	405	112.435	42.209	21.630	1.00 68.16	1SG3255
ATOM	3255	CA	ALA	405	111.585	43.158	22.319	1.00 68.16	1SG3256
ATOM	3256	CB	ALA	405	111.398	44.459	21.518	1.00 68.16	1SG3257
ATOM	3257	C	ALA	405	110.209	42.623	22.612	1.00 68.16	1SG3258
ATOM	3258	O	ALA	405	109.617	42.968	23.634	1.00 68.16	1SG3259
ATOM	3259	N	TYR	406	109.655	41.768	21.740	1.00131.84	1SG3260
ATOM	3260	CA	TYR	406	108.309	41.282	21.879	1.00131.84	1SG3261
ATOM	3261	CB	TYR	406	107.878	40.361	20.720	1.00131.84	1SG3262
ATOM	3262	CG	TYR	406	108.813	39.204	20.644	1.00131.84	1SG3263
ATOM	3263	CD1	TYR	406	108.622	38.099	21.440	1.00131.84	1SG3264
ATOM	3264	CD2	TYR	406	109.875	39.224	19.767	1.00131.84	1SG3265

Supplementary material 1.txt

ATOM	3265	CE1	TYR	406	109.485	37.031	21.367	1.00131.84	1SG3266
ATOM	3266	CE2	TYR	406	110.741	38.158	19.691	1.00131.84	1SG3267
ATOM	3267	CZ	TYR	406	110.545	37.060	20.494	1.00131.84	1SG3268
ATOM	3268	OH	TYR	406	111.431	35.964	20.420	1.00131.84	1SG3269
ATOM	3269	C	TYR	406	108.113	40.566	23.192	1.00131.84	1SG3270
ATOM	3270	O	TYR	406	106.995	40.526	23.701	1.00131.84	1SG3271
ATOM	3271	N	ILE	407	109.173	39.934	23.733	1.00103.00	1SG3272
ATOM	3272	CA	ILE	407	109.206	39.142	24.944	1.00103.00	1SG3273
ATOM	3273	CB	ILE	407	110.501	38.412	25.185	1.00103.00	1SG3274
ATOM	3274	CG2	ILE	407	110.782	37.516	23.970	1.00103.00	1SG3275
ATOM	3275	CG1	ILE	407	111.637	39.395	25.504	1.00103.00	1SG3276
ATOM	3276	CD1	ILE	407	112.901	38.724	26.040	1.00103.00	1SG3277
ATOM	3277	C	ILE	407	108.968	39.920	26.216	1.00103.00	1SG3278
ATOM	3278	O	ILE	407	108.573	39.326	27.216	1.00103.00	1SG3279
ATOM	3279	N	ARG	408	109.271	41.233	26.265	1.00149.10	1SG3280
ATOM	3280	CA	ARG	408	109.236	41.991	27.495	1.00149.10	1SG3281
ATOM	3281	CB	ARG	408	109.651	43.470	27.332	1.00149.10	1SG3282
ATOM	3282	CG	ARG	408	108.778	44.321	26.402	1.00149.10	1SG3283
ATOM	3283	CD	ARG	408	107.368	44.569	26.942	1.00149.10	1SG3284
ATOM	3284	NE	ARG	408	106.739	45.656	26.143	1.00149.10	1SG3285
ATOM	3285	CZ	ARG	408	106.652	46.910	26.672	1.00149.10	1SG3286
ATOM	3286	NH1	ARG	408	107.141	47.155	27.923	1.00149.10	1SG3287
ATOM	3287	NH2	ARG	408	106.060	47.916	25.962	1.00149.10	1SG3288
ATOM	3288	C	ARG	408	107.884	41.944	28.147	1.00149.10	1SG3289
ATOM	3289	O	ARG	408	107.781	42.053	29.368	1.00149.10	1SG3290
ATOM	3290	N	LYS	409	106.808	41.795	27.359	1.00118.20	1SG3291
ATOM	3291	CA	LYS	409	105.461	41.828	27.860	1.00118.20	1SG3292
ATOM	3292	CB	LYS	409	104.435	41.486	26.769	1.00118.20	1SG3293
ATOM	3293	CG	LYS	409	103.000	41.382	27.283	1.00118.20	1SG3294
ATOM	3294	CD	LYS	409	101.956	41.317	26.169	1.00118.20	1SG3295
ATOM	3295	CE	LYS	409	100.549	40.997	26.676	1.00118.20	1SG3296
ATOM	3296	NZ	LYS	409	100.512	39.619	27.215	1.00118.20	1SG3297
ATOM	3297	C	LYS	409	105.261	40.821	28.956	1.00118.20	1SG3298
ATOM	3298	O	LYS	409	104.577	41.103	29.940	1.00118.20	1SG3299
ATOM	3299	N	ASN	410	105.856	39.624	28.825	1.00 47.12	1SG3300
ATOM	3300	CA	ASN	410	105.641	38.572	29.779	1.00 47.12	1SG3301
ATOM	3301	CB	ASN	410	106.413	37.291	29.424	1.00 47.12	1SG3302
ATOM	3302	CG	ASN	410	105.735	36.681	28.205	1.00 47.12	1SG3303
ATOM	3303	OD1	ASN	410	104.706	36.018	28.324	1.00 47.12	1SG3304
ATOM	3304	ND2	ASN	410	106.313	36.920	26.997	1.00 47.12	1SG3305
ATOM	3305	C	ASN	410	106.077	39.011	31.142	1.00 47.12	1SG3306
ATOM	3306	O	ASN	410	105.396	38.746	32.132	1.00 47.12	1SG3307
ATOM	3307	N	ALA	411	107.230	39.693	31.234	1.00 37.79	1SG3308
ATOM	3308	CA	ALA	411	107.719	40.136	32.504	1.00 37.79	1SG3309
ATOM	3309	CB	ALA	411	109.080	40.845	32.405	1.00 37.79	1SG3310
ATOM	3310	C	ALA	411	106.749	41.111	33.097	1.00 37.79	1SG3311
ATOM	3311	O	ALA	411	106.508	41.084	34.304	1.00 37.79	1SG3312
ATOM	3312	N	TRP	412	106.172	42.015	32.276	1.00179.14	1SG3313
ATOM	3313	CA	TRP	412	105.304	43.006	32.853	1.00179.14	1SG3314
ATOM	3314	CB	TRP	412	104.907	44.205	31.963	1.00179.14	1SG3315
ATOM	3315	CG	TRP	412	103.968	43.972	30.807	1.00179.14	1SG3316
ATOM	3316	CD2	TRP	412	102.556	43.753	30.948	1.00179.14	1SG3317
ATOM	3317	CD1	TRP	412	104.229	43.948	29.472	1.00179.14	1SG3318
ATOM	3318	NE1	TRP	412	103.067	43.736	28.768	1.00179.14	1SG3319
ATOM	3319	CE2	TRP	412	102.029	43.611	29.666	1.00179.14	1SG3320
ATOM	3320	CE3	TRP	412	101.762	43.677	32.055	1.00179.14	1SG3321
ATOM	3321	CZ2	TRP	412	100.696	43.392	29.469	1.00179.14	1SG3322
ATOM	3322	CZ3	TRP	412	100.418	43.454	31.855	1.00179.14	1SG3323
ATOM	3323	CH2	TRP	412	99.894	43.315	30.587	1.00179.14	1SG3324
ATOM	3324	C	TRP	412	104.051	42.392	33.394	1.00179.14	1SG3325
ATOM	3325	O	TRP	412	103.603	42.751	34.481	1.00179.14	1SG3326
ATOM	3326	N	GLU	413	103.461	41.427	32.669	1.00120.66	1SG3327
ATOM	3327	CA	GLU	413	102.217	40.860	33.103	1.00120.66	1SG3328
ATOM	3328	CB	GLU	413	101.721	39.743	32.175	1.00120.66	1SG3329
ATOM	3329	CG	GLU	413	100.323	39.249	32.535	1.00120.66	1SG3330
ATOM	3330	CD	GLU	413	99.370	40.415	32.323	1.00120.66	1SG3331
ATOM	3331	OE1	GLU	413	99.300	41.295	33.222	1.00120.66	1SG3332
ATOM	3332	OE2	GLU	413	98.705	40.446	31.254	1.00120.66	1SG3333
ATOM	3333	C	GLU	413	102.424	40.269	34.460	1.00120.66	1SG3334
ATOM	3334	O	GLU	413	101.556	40.353	35.328	1.00120.66	1SG3335
ATOM	3335	N	ARG	414	103.592	39.644	34.672	1.00 77.09	1SG3336

Supplementary material 1.txt

ATOM	3336	CA	ARG	414	103.923	39.045	35.929	1.00	77.09	1SG3337
ATOM	3337	CB	ARG	414	105.257	38.284	35.877	1.00	77.09	1SG3338
ATOM	3338	CG	ARG	414	105.176	37.039	34.994	1.00	77.09	1SG3339
ATOM	3339	CD	ARG	414	105.047	35.742	35.792	1.00	77.09	1SG3340
ATOM	3340	NE	ARG	414	104.684	34.665	34.829	1.00	77.09	1SG3341
ATOM	3341	CZ	ARG	414	103.405	34.192	34.798	1.00	77.09	1SG3342
ATOM	3342	NH1	ARG	414	102.488	34.645	35.703	1.00	77.09	1SG3343
ATOM	3343	NH2	ARG	414	103.044	33.255	33.874	1.00	77.09	1SG3344
ATOM	3344	C	ARG	414	104.033	40.125	36.961	1.00	77.09	1SG3345
ATOM	3345	O	ARG	414	103.688	39.922	38.123	1.00	77.09	1SG3346
ATOM	3346	N	TYR	415	104.540	41.307	36.567	1.00	97.74	1SG3347
ATOM	3347	CA	TYR	415	104.695	42.398	37.487	1.00	97.74	1SG3348
ATOM	3348	CB	TYR	415	105.341	43.645	36.851	1.00	97.74	1SG3349
ATOM	3349	CG	TYR	415	105.223	44.758	37.839	1.00	97.74	1SG3350
ATOM	3350	CD1	TYR	415	106.129	44.896	38.866	1.00	97.74	1SG3351
ATOM	3351	CD2	TYR	415	104.198	45.671	37.735	1.00	97.74	1SG3352
ATOM	3352	CE1	TYR	415	106.012	45.925	39.772	1.00	97.74	1SG3353
ATOM	3353	CE2	TYR	415	104.075	46.702	38.638	1.00	97.74	1SG3354
ATOM	3354	CZ	TYR	415	104.982	46.829	39.662	1.00	97.74	1SG3355
ATOM	3355	OH	TYR	415	104.860	47.885	40.590	1.00	97.74	1SG3356
ATOM	3356	C	TYR	415	103.356	42.832	38.001	1.00	97.74	1SG3357
ATOM	3357	O	TYR	415	103.189	43.070	39.196	1.00	97.74	1SG3358
ATOM	3358	N	LEU	416	102.350	42.924	37.115	1.00	102.08	1SG3359
ATOM	3359	CA	LEU	416	101.062	43.417	37.511	1.00	102.08	1SG3360
ATOM	3360	CB	LEU	416	100.060	43.529	36.348	1.00	102.08	1SG3361
ATOM	3361	CG	LEU	416	100.313	44.741	35.430	1.00	102.08	1SG3362
ATOM	3362	CD2	LEU	416	99.208	44.874	34.370	1.00	102.08	1SG3363
ATOM	3363	CD1	LEU	416	101.718	44.710	34.818	1.00	102.08	1SG3364
ATOM	3364	C	LEU	416	100.460	42.539	38.569	1.00	102.08	1SG3365
ATOM	3365	O	LEU	416	99.795	43.028	39.478	1.00	102.08	1SG3366
ATOM	3366	N	GLU	417	100.699	41.220	38.501	1.00	117.75	1SG3367
ATOM	3367	CA	GLU	417	100.061	40.263	39.372	1.00	117.75	1SG3368
ATOM	3368	CB	GLU	417	100.323	38.798	38.977	1.00	117.75	1SG3369
ATOM	3369	CG	GLU	417	101.754	38.319	39.204	1.00	117.75	1SG3370
ATOM	3370	CD	GLU	417	101.889	36.957	38.542	1.00	117.75	1SG3371
ATOM	3371	OE1	GLU	417	100.912	36.530	37.871	1.00	117.75	1SG3372
ATOM	3372	OE2	GLU	417	102.969	36.326	38.694	1.00	117.75	1SG3373
ATOM	3373	C	GLU	417	100.412	40.419	40.844	1.00	117.75	1SG3374
ATOM	3374	O	GLU	417	99.626	40.022	41.699	1.00	117.75	1SG3375
ATOM	3375	N	ALA	418	101.568	41.019	41.188	1.00	197.09	1SG3376
ATOM	3376	CA	ALA	418	102.193	41.021	42.504	1.00	197.09	1SG3377
ATOM	3377	CB	ALA	418	103.567	41.715	42.460	1.00	197.09	1SG3378
ATOM	3378	C	ALA	418	101.508	41.552	43.851	1.00	197.09	1SG3379
ATOM	3379	O	ALA	418	101.821	40.946	44.855	1.00	197.09	1SG3380
ATOM	3380	N	TYR	419	100.661	42.613	44.122	1.00	273.32	1SG3381
ATOM	3381	CA	TYR	419	100.530	42.882	45.597	1.00	273.32	1SG3382
ATOM	3382	CB	TYR	419	101.653	43.799	46.116	1.00	273.32	1SG3383
ATOM	3383	CG	TYR	419	102.987	43.137	46.060	1.00	273.32	1SG3384
ATOM	3384	CD1	TYR	419	103.363	42.231	47.026	1.00	273.32	1SG3385
ATOM	3385	CD2	TYR	419	103.878	43.449	45.057	1.00	273.32	1SG3386
ATOM	3386	CE1	TYR	419	104.600	41.632	46.983	1.00	273.32	1SG3387
ATOM	3387	CE2	TYR	419	105.117	42.853	45.008	1.00	273.32	1SG3388
ATOM	3388	CZ	TYR	419	105.479	41.944	45.973	1.00	273.32	1SG3389
ATOM	3389	OH	TYR	419	106.750	41.332	45.928	1.00	273.32	1SG3390
ATOM	3390	C	TYR	419	99.282	43.518	46.249	1.00	273.32	1SG3391
ATOM	3391	O	TYR	419	99.271	43.661	47.475	1.00	273.32	1SG3392
ATOM	3392	N	LEU	420	98.221	43.955	45.548	1.00	185.54	1SG3393
ATOM	3393	CA	LEU	420	97.144	44.681	46.213	1.00	185.54	1SG3394
ATOM	3394	CB	LEU	420	96.161	45.290	45.182	1.00	185.54	1SG3395
ATOM	3395	CG	LEU	420	95.077	46.277	45.692	1.00	185.54	1SG3396
ATOM	3396	CD2	LEU	420	94.150	45.693	46.772	1.00	185.54	1SG3397
ATOM	3397	CD1	LEU	420	94.256	46.811	44.507	1.00	185.54	1SG3398
ATOM	3398	C	LEU	420	96.364	43.821	47.176	1.00	185.54	1SG3399
ATOM	3399	O	LEU	420	96.003	44.270	48.265	1.00	185.54	1SG3400
ATOM	3400	N	GLN	421	96.085	42.559	46.811	1.00	130.11	1SG3401
ATOM	3401	CA	GLN	421	95.198	41.720	47.577	1.00	130.11	1SG3402
ATOM	3402	CB	GLN	421	95.013	40.328	46.947	1.00	130.11	1SG3403
ATOM	3403	CG	GLN	421	94.076	39.410	47.734	1.00	130.11	1SG3404
ATOM	3404	CD	GLN	421	92.669	39.985	47.666	1.00	130.11	1SG3405
ATOM	3405	OE1	GLN	421	92.369	40.993	48.304	1.00	130.11	1SG3406
ATOM	3406	NE2	GLN	421	91.778	39.326	46.878	1.00	130.11	1SG3407

Supplementary material 1.txt

ATOM	3407	C	GLN	421	95.717	41.518	48.967	1.00130.11	1SG3408
ATOM	3408	O	GLN	421	94.941	41.466	49.921	1.00130.11	1SG3409
ATOM	3409	N	ASP	422	97.043	41.401	49.123	1.00 46.20	1SG3410
ATOM	3410	CA	ASP	422	97.606	41.123	50.412	1.00 46.20	1SG3411
ATOM	3411	CB	ASP	422	99.145	41.088	50.389	1.00 46.20	1SG3412
ATOM	3412	CG	ASP	422	99.605	39.894	49.565	1.00 46.20	1SG3413
ATOM	3413	OD1	ASP	422	99.094	38.768	49.808	1.00 46.20	1SG3414
ATOM	3414	OD2	ASP	422	100.488	40.091	48.688	1.00 46.20	1SG3415
ATOM	3415	C	ASP	422	97.221	42.218	51.350	1.00 46.20	1SG3416
ATOM	3416	O	ASP	422	96.868	41.961	52.499	1.00 46.20	1SG3417
ATOM	3417	N	ALA	423	97.289	43.474	50.880	1.00 36.58	1SG3418
ATOM	3418	CA	ALA	423	96.990	44.597	51.718	1.00 36.58	1SG3419
ATOM	3419	CB	ALA	423	97.226	45.941	51.008	1.00 36.58	1SG3420
ATOM	3420	C	ALA	423	95.556	44.564	52.136	1.00 36.58	1SG3421
ATOM	3421	O	ALA	423	95.240	44.813	53.298	1.00 36.58	1SG3422
ATOM	3422	N	GLU	424	94.644	44.237	51.203	1.00 69.61	1SG3423
ATOM	3423	CA	GLU	424	93.251	44.289	51.541	1.00 69.61	1SG3424
ATOM	3424	CB	GLU	424	92.310	43.974	50.365	1.00 69.61	1SG3425
ATOM	3425	CG	GLU	424	90.830	44.119	50.738	1.00 69.61	1SG3426
ATOM	3426	CD	GLU	424	89.985	43.861	49.499	1.00 69.61	1SG3427
ATOM	3427	OE1	GLU	424	90.549	43.921	48.374	1.00 69.61	1SG3428
ATOM	3428	OE2	GLU	424	88.762	43.603	49.661	1.00 69.61	1SG3429
ATOM	3429	C	GLU	424	92.974	43.301	52.625	1.00 69.61	1SG3430
ATOM	3430	O	GLU	424	92.216	43.585	53.550	1.00 69.61	1SG3431
ATOM	3431	N	TRP	425	93.593	42.111	52.547	1.00 53.91	1SG3432
ATOM	3432	CA	TRP	425	93.344	41.096	53.529	1.00 53.91	1SG3433
ATOM	3433	CB	TRP	425	94.042	39.768	53.206	1.00 53.91	1SG3434
ATOM	3434	CG	TRP	425	93.411	39.044	52.042	1.00 53.91	1SG3435
ATOM	3435	CD2	TRP	425	93.948	37.854	51.449	1.00 53.91	1SG3436
ATOM	3436	CD1	TRP	425	92.269	39.337	51.356	1.00 53.91	1SG3437
ATOM	3437	NE1	TRP	425	92.056	38.397	50.376	1.00 53.91	1SG3438
ATOM	3438	CE2	TRP	425	93.083	37.478	50.420	1.00 53.91	1SG3439
ATOM	3439	CE3	TRP	425	95.069	37.131	51.740	1.00 53.91	1SG3440
ATOM	3440	CZ2	TRP	425	93.327	36.367	49.665	1.00 53.91	1SG3441
ATOM	3441	CZ3	TRP	425	95.315	36.014	50.973	1.00 53.91	1SG3442
ATOM	3442	CH2	TRP	425	94.460	35.641	49.957	1.00 53.91	1SG3443
ATOM	3443	C	TRP	425	93.812	41.576	54.863	1.00 53.91	1SG3444
ATOM	3444	O	TRP	425	93.175	41.312	55.882	1.00 53.91	1SG3445
ATOM	3445	N	ILE	426	94.952	42.289	54.890	1.00 81.95	1SG3446
ATOM	3446	CA	ILE	426	95.484	42.767	56.131	1.00 81.95	1SG3447
ATOM	3447	CB	ILE	426	96.786	43.493	55.962	1.00 81.95	1SG3448
ATOM	3448	CG2	ILE	426	97.171	44.093	57.325	1.00 81.95	1SG3449
ATOM	3449	CG1	ILE	426	97.854	42.551	55.382	1.00 81.95	1SG3450
ATOM	3450	CD1	ILE	426	98.147	41.344	56.271	1.00 81.95	1SG3451
ATOM	3451	C	ILE	426	94.513	43.729	56.747	1.00 81.95	1SG3452
ATOM	3452	O	ILE	426	94.250	43.668	57.947	1.00 81.95	1SG3453
ATOM	3453	N	ALA	427	93.953	44.651	55.940	1.00 33.18	1SG3454
ATOM	3454	CA	ALA	427	93.056	45.646	56.463	1.00 33.18	1SG3455
ATOM	3455	CB	ALA	427	92.605	46.659	55.398	1.00 33.18	1SG3456
ATOM	3456	C	ALA	427	91.822	45.000	57.012	1.00 33.18	1SG3457
ATOM	3457	O	ALA	427	91.375	45.330	58.109	1.00 33.18	1SG3458
ATOM	3458	N	THR	428	91.248	44.044	56.260	1.00 99.33	1SG3459
ATOM	3459	CA	THR	428	90.043	43.380	56.664	1.00 99.33	1SG3460
ATOM	3460	CB	THR	428	89.523	42.420	55.633	1.00 99.33	1SG3461
ATOM	3461	OG1	THR	428	90.465	41.381	55.415	1.00 99.33	1SG3462
ATOM	3462	CG2	THR	428	89.260	43.186	54.325	1.00 99.33	1SG3463
ATOM	3463	C	THR	428	90.342	42.590	57.893	1.00 99.33	1SG3464
ATOM	3464	O	THR	428	89.504	42.468	58.785	1.00 99.33	1SG3465
ATOM	3465	N	GLY	429	91.565	42.036	57.976	1.00 23.50	1SG3466
ATOM	3466	CA	GLY	429	91.899	41.212	59.096	1.00 23.50	1SG3467
ATOM	3467	C	GLY	429	91.477	39.830	58.734	1.00 23.50	1SG3468
ATOM	3468	O	GLY	429	91.233	38.990	59.599	1.00 23.50	1SG3469
ATOM	3469	N	HIS	430	91.363	39.572	57.418	1.00 81.55	1SG3470
ATOM	3470	CA	HIS	430	90.913	38.295	56.958	1.00 81.55	1SG3471
ATOM	3471	ND1	HIS	430	88.656	36.482	55.394	1.00 81.55	1SG3472
ATOM	3472	CG	HIS	430	89.875	37.004	55.021	1.00 81.55	1SG3473
ATOM	3473	CB	HIS	430	90.415	38.321	55.500	1.00 81.55	1SG3474
ATOM	3474	NE2	HIS	430	89.576	35.015	53.999	1.00 81.55	1SG3475
ATOM	3475	CD2	HIS	430	90.423	36.096	54.168	1.00 81.55	1SG3476
ATOM	3476	CE1	HIS	430	88.529	35.290	54.754	1.00 81.55	1SG3477
ATOM	3477	C	HIS	430	92.014	37.289	57.061	1.00 81.55	1SG3478

Supplementary material 1.txt

ATOM	3478	O	HIS	430	93.174	37.575	56.763	1.00	81.55	1SG3479
ATOM	3479	N	VAL	431	91.659	36.076	57.533	1.00	126.81	1SG3480
ATOM	3480	CA	VAL	431	92.569	34.972	57.555	1.00	126.81	1SG3481
ATOM	3481	CB	VAL	431	92.851	34.448	58.938	1.00	126.81	1SG3482
ATOM	3482	CG1	VAL	431	91.530	34.114	59.654	1.00	126.81	1SG3483
ATOM	3483	CG2	VAL	431	93.808	33.252	58.807	1.00	126.81	1SG3484
ATOM	3484	C	VAL	431	91.938	33.897	56.719	1.00	126.81	1SG3485
ATOM	3485	O	VAL	431	91.018	33.189	57.131	1.00	126.81	1SG3486
ATOM	3486	N	PRO	432	92.441	33.765	55.528	1.00	81.51	1SG3487
ATOM	3487	CA	PRO	432	91.907	32.818	54.586	1.00	81.51	1SG3488
ATOM	3488	CD	PRO	432	93.143	34.856	54.874	1.00	81.51	1SG3489
ATOM	3489	CB	PRO	432	92.307	33.329	53.201	1.00	81.51	1SG3490
ATOM	3490	CG	PRO	432	93.454	34.317	53.470	1.00	81.51	1SG3491
ATOM	3491	C	PRO	432	92.390	31.432	54.849	1.00	81.51	1SG3492
ATOM	3492	O	PRO	432	93.346	31.251	55.600	1.00	81.51	1SG3493
ATOM	3493	N	THR	433	91.726	30.437	54.236	1.00	110.80	1SG3494
ATOM	3494	CA	THR	433	92.153	29.082	54.369	1.00	110.80	1SG3495
ATOM	3495	CB	THR	433	91.154	28.117	53.811	1.00	110.80	1SG3496
ATOM	3496	OG1	THR	433	91.609	26.782	53.959	1.00	110.80	1SG3497
ATOM	3497	CG2	THR	433	90.903	28.463	52.338	1.00	110.80	1SG3498
ATOM	3498	C	THR	433	93.441	28.959	53.622	1.00	110.80	1SG3499
ATOM	3499	O	THR	433	93.773	29.801	52.789	1.00	110.80	1SG3500
ATOM	3500	N	PHE	434	94.194	27.882	53.905	1.00	89.99	1SG3501
ATOM	3501	CA	PHE	434	95.519	27.707	53.382	1.00	89.99	1SG3502
ATOM	3502	CB	PHE	434	96.156	26.390	53.865	1.00	89.99	1SG3503
ATOM	3503	CG	PHE	434	97.620	26.441	53.599	1.00	89.99	1SG3504
ATOM	3504	CD1	PHE	434	98.443	27.153	54.440	1.00	89.99	1SG3505
ATOM	3505	CD2	PHE	434	98.174	25.767	52.536	1.00	89.99	1SG3506
ATOM	3506	CE1	PHE	434	99.797	27.211	54.216	1.00	89.99	1SG3507
ATOM	3507	CE2	PHE	434	99.530	25.823	52.311	1.00	89.99	1SG3508
ATOM	3508	CZ	PHE	434	100.346	26.545	53.148	1.00	89.99	1SG3509
ATOM	3509	C	PHE	434	95.466	27.689	51.886	1.00	89.99	1SG3510
ATOM	3510	O	PHE	434	96.287	28.326	51.225	1.00	89.99	1SG3511
ATOM	3511	N	ASP	435	94.490	26.971	51.300	1.00	79.63	1SG3512
ATOM	3512	CA	ASP	435	94.455	26.893	49.870	1.00	79.63	1SG3513
ATOM	3513	CB	ASP	435	93.388	25.922	49.328	1.00	79.63	1SG3514
ATOM	3514	CG	ASP	435	92.037	26.298	49.906	1.00	79.63	1SG3515
ATOM	3515	OD1	ASP	435	91.906	26.209	51.156	1.00	79.63	1SG3516
ATOM	3516	OD2	ASP	435	91.123	26.672	49.123	1.00	79.63	1SG3517
ATOM	3517	C	ASP	435	94.259	28.254	49.268	1.00	79.63	1SG3518
ATOM	3518	O	ASP	435	94.913	28.584	48.280	1.00	79.63	1SG3519
ATOM	3519	N	GLU	436	93.371	29.090	49.841	1.00	32.34	1SG3520
ATOM	3520	CA	GLU	436	93.125	30.393	49.280	1.00	32.34	1SG3521
ATOM	3521	CB	GLU	436	91.974	31.146	49.971	1.00	32.34	1SG3522
ATOM	3522	CG	GLU	436	91.643	32.481	49.298	1.00	32.34	1SG3523
ATOM	3523	CD	GLU	436	90.498	33.135	50.059	1.00	32.34	1SG3524
ATOM	3524	OE1	GLU	436	89.945	32.475	50.979	1.00	32.34	1SG3525
ATOM	3525	OE2	GLU	436	90.164	34.305	49.732	1.00	32.34	1SG3526
ATOM	3526	C	GLU	436	94.353	31.247	49.411	1.00	32.34	1SG3527
ATOM	3527	O	GLU	436	94.701	31.996	48.499	1.00	32.34	1SG3528
ATOM	3528	N	TYR	437	95.051	31.137	50.555	1.00	70.56	1SG3529
ATOM	3529	CA	TYR	437	96.199	31.951	50.851	1.00	70.56	1SG3530
ATOM	3530	CB	TYR	437	96.785	31.603	52.236	1.00	70.56	1SG3531
ATOM	3531	CG	TYR	437	98.138	32.210	52.409	1.00	70.56	1SG3532
ATOM	3532	CD1	TYR	437	98.301	33.540	52.725	1.00	70.56	1SG3533
ATOM	3533	CD2	TYR	437	99.258	31.422	52.275	1.00	70.56	1SG3534
ATOM	3534	CE1	TYR	437	99.562	34.070	52.888	1.00	70.56	1SG3535
ATOM	3535	CE2	TYR	437	100.519	31.946	52.437	1.00	70.56	1SG3536
ATOM	3536	CZ	TYR	437	100.676	33.275	52.743	1.00	70.56	1SG3537
ATOM	3537	OH	TYR	437	101.972	33.812	52.910	1.00	70.56	1SG3538
ATOM	3538	C	TYR	437	97.264	31.728	49.823	1.00	70.56	1SG3539
ATOM	3539	O	TYR	437	97.836	32.684	49.296	1.00	70.56	1SG3540
ATOM	3540	N	LEU	438	97.525	30.451	49.489	1.00	49.49	1SG3541
ATOM	3541	CA	LEU	438	98.577	30.082	48.585	1.00	49.49	1SG3542
ATOM	3542	CB	LEU	438	98.721	28.561	48.409	1.00	49.49	1SG3543
ATOM	3543	CG	LEU	438	99.163	27.823	49.684	1.00	49.49	1SG3544
ATOM	3544	CD2	LEU	438	100.411	28.472	50.306	1.00	49.49	1SG3545
ATOM	3545	CD1	LEU	438	99.339	26.320	49.414	1.00	49.49	1SG3546
ATOM	3546	C	LEU	438	98.311	30.643	47.230	1.00	49.49	1SG3547
ATOM	3547	O	LEU	438	99.243	31.058	46.541	1.00	49.49	1SG3548
ATOM	3548	N	ASN	439	97.031	30.676	46.813	1.00	88.76	1SG3549

Supplementary material 1.txt

ATOM	3549	CA	ASN	439	96.713	31.119	45.488	1.00	88.76	1SG3550
ATOM	3550	CB	ASN	439	95.194	31.202	45.247	1.00	88.76	1SG3551
ATOM	3551	CG	ASN	439	94.934	31.413	43.761	1.00	88.76	1SG3552
ATOM	3552	OD1	ASN	439	93.788	31.535	43.330	1.00	88.76	1SG3553
ATOM	3553	ND2	ASN	439	96.023	31.452	42.949	1.00	88.76	1SG3554
ATOM	3554	C	ASN	439	97.273	32.496	45.320	1.00	88.76	1SG3555
ATOM	3555	O	ASN	439	97.880	32.801	44.296	1.00	88.76	1SG3556
ATOM	3556	N	ASN	440	97.046	33.372	46.315	1.00	75.96	1SG3557
ATOM	3557	CA	ASN	440	97.554	34.719	46.287	1.00	75.96	1SG3558
ATOM	3558	CB	ASN	440	96.773	35.649	47.230	1.00	75.96	1SG3559
ATOM	3559	CG	ASN	440	97.255	37.074	47.002	1.00	75.96	1SG3560
ATOM	3560	OD1	ASN	440	97.829	37.394	45.962	1.00	75.96	1SG3561
ATOM	3561	ND2	ASN	440	97.030	37.955	48.013	1.00	75.96	1SG3562
ATOM	3562	C	ASN	440	99.008	34.831	46.677	1.00	75.96	1SG3563
ATOM	3563	O	ASN	440	99.781	35.548	46.041	1.00	75.96	1SG3564
ATOM	3564	N	GLY	441	99.403	34.116	47.751	1.00	65.35	1SG3565
ATOM	3565	CA	GLY	441	100.689	34.221	48.392	1.00	65.35	1SG3566
ATOM	3566	C	GLY	441	101.823	33.769	47.532	1.00	65.35	1SG3567
ATOM	3567	O	GLY	441	102.949	34.229	47.706	1.00	65.35	1SG3568
ATOM	3568	N	THR	442	101.601	32.797	46.636	1.00	138.02	1SG3569
ATOM	3569	CA	THR	442	102.722	32.331	45.883	1.00	138.02	1SG3570
ATOM	3570	CB	THR	442	102.486	31.045	45.116	1.00	138.02	1SG3571
ATOM	3571	OG1	THR	442	101.415	31.144	44.192	1.00	138.02	1SG3572
ATOM	3572	CG2	THR	442	102.186	29.935	46.136	1.00	138.02	1SG3573
ATOM	3573	C	THR	442	103.287	33.411	45.000	1.00	138.02	1SG3574
ATOM	3574	O	THR	442	104.505	33.457	44.864	1.00	138.02	1SG3575
ATOM	3575	N	PRO	443	102.533	34.276	44.369	1.00	155.15	1SG3576
ATOM	3576	CA	PRO	443	103.131	35.297	43.541	1.00	155.15	1SG3577
ATOM	3577	CD	PRO	443	101.177	33.966	43.944	1.00	155.15	1SG3578
ATOM	3578	CB	PRO	443	102.003	35.856	42.675	1.00	155.15	1SG3579
ATOM	3579	CG	PRO	443	100.978	34.712	42.616	1.00	155.15	1SG3580
ATOM	3580	C	PRO	443	103.847	36.378	44.297	1.00	155.15	1SG3581
ATOM	3581	O	PRO	443	104.740	37.004	43.728	1.00	155.15	1SG3582
ATOM	3582	N	ASN	444	103.482	36.615	45.571	1.00	131.61	1SG3583
ATOM	3583	CA	ASN	444	104.030	37.703	46.337	1.00	131.61	1SG3584
ATOM	3584	CB	ASN	444	103.348	37.949	47.704	1.00	131.61	1SG3585
ATOM	3585	CG	ASN	444	103.491	36.746	48.622	1.00	131.61	1SG3586
ATOM	3586	OD1	ASN	444	104.542	36.117	48.724	1.00	131.61	1SG3587
ATOM	3587	ND2	ASN	444	102.374	36.402	49.319	1.00	131.61	1SG3588
ATOM	3588	C	ASN	444	105.487	37.471	46.539	1.00	131.61	1SG3589
ATOM	3589	O	ASN	444	106.233	38.400	46.844	1.00	131.61	1SG3590
ATOM	3590	N	THR	445	105.918	36.203	46.433	1.00	145.09	1SG3591
ATOM	3591	CA	THR	445	107.305	35.895	46.557	1.00	145.09	1SG3592
ATOM	3592	CB	THR	445	107.628	34.434	46.540	1.00	145.09	1SG3593
ATOM	3593	OG1	THR	445	109.026	34.275	46.669	1.00	145.09	1SG3594
ATOM	3594	CG2	THR	445	107.183	33.802	45.224	1.00	145.09	1SG3595
ATOM	3595	C	THR	445	108.025	36.555	45.423	1.00	145.09	1SG3596
ATOM	3596	O	THR	445	109.209	36.860	45.542	1.00	145.09	1SG3597
ATOM	3597	N	GLY	446	107.345	36.730	44.270	1.00	37.55	1SG3598
ATOM	3598	CA	GLY	446	107.909	37.427	43.147	1.00	37.55	1SG3599
ATOM	3599	C	GLY	446	108.693	36.468	42.314	1.00	37.55	1SG3600
ATOM	3600	O	GLY	446	109.318	36.855	41.329	1.00	37.55	1SG3601
ATOM	3601	N	MET	447	108.656	35.180	42.691	1.00	130.88	1SG3602
ATOM	3602	CA	MET	447	109.422	34.147	42.059	1.00	130.88	1SG3603
ATOM	3603	CB	MET	447	109.302	32.825	42.839	1.00	130.88	1SG3604
ATOM	3604	CG	MET	447	110.420	31.828	42.551	1.00	130.88	1SG3605
ATOM	3605	SD	MET	447	112.049	32.325	43.195	1.00	130.88	1SG3606
ATOM	3606	CE	MET	447	111.615	32.139	44.944	1.00	130.88	1SG3607
ATOM	3607	C	MET	447	108.981	33.925	40.644	1.00	130.88	1SG3608
ATOM	3608	O	MET	447	109.804	33.639	39.774	1.00	130.88	1SG3609
ATOM	3609	N	CYS	448	107.664	34.000	40.378	1.00	94.57	1SG3610
ATOM	3610	CA	CYS	448	107.217	33.793	39.034	1.00	94.57	1SG3611
ATOM	3611	CB	CYS	448	105.686	33.775	38.909	1.00	94.57	1SG3612
ATOM	3612	SG	CYS	448	105.158	33.080	37.321	1.00	94.57	1SG3613
ATOM	3613	C	CYS	448	107.749	34.926	38.217	1.00	94.57	1SG3614
ATOM	3614	O	CYS	448	108.228	34.737	37.103	1.00	94.57	1SG3615
ATOM	3615	N	VAL	449	107.686	36.148	38.776	1.00	51.77	1SG3616
ATOM	3616	CA	VAL	449	108.123	37.331	38.093	1.00	51.77	1SG3617
ATOM	3617	CB	VAL	449	107.881	38.573	38.899	1.00	51.77	1SG3618
ATOM	3618	CG1	VAL	449	108.423	39.780	38.113	1.00	51.77	1SG3619
ATOM	3619	CG2	VAL	449	106.381	38.654	39.228	1.00	51.77	1SG3620

Supplementary material 1.txt

ATOM	3620	C	VAL	449	109.596	37.266	37.817	1.00	51.77	1SG3621
ATOM	3621	O	VAL	449	110.041	37.480	36.690	1.00	51.77	1SG3622
ATOM	3622	N	LEU	450	110.391	36.937	38.848	1.00	77.30	1SG3623
ATOM	3623	CA	LEU	450	111.823	36.914	38.774	1.00	77.30	1SG3624
ATOM	3624	CB	LEU	450	112.471	36.603	40.131	1.00	77.30	1SG3625
ATOM	3625	CG	LEU	450	112.142	37.655	41.209	1.00	77.30	1SG3626
ATOM	3626	CD2	LEU	450	112.470	39.077	40.727	1.00	77.30	1SG3627
ATOM	3627	CD1	LEU	450	112.810	37.310	42.549	1.00	77.30	1SG3628
ATOM	3628	C	LEU	450	112.261	35.864	37.810	1.00	77.30	1SG3629
ATOM	3629	O	LEU	450	113.299	36.038	37.187	1.00	77.30	1SG3630
ATOM	3630	N	ASN	451	111.537	34.727	37.727	1.00156.20		1SG3631
ATOM	3631	CA	ASN	451	111.784	33.605	36.849	1.00156.20		1SG3632
ATOM	3632	CB	ASN	451	110.844	32.422	37.137	1.00156.20		1SG3633
ATOM	3633	CG	ASN	451	111.026	31.388	36.032	1.00156.20		1SG3634
ATOM	3634	OD1	ASN	451	112.047	30.715	35.912	1.00156.20		1SG3635
ATOM	3635	ND2	ASN	451	109.979	31.262	35.174	1.00156.20		1SG3636
ATOM	3636	C	ASN	451	111.509	33.952	35.423	1.00156.20		1SG3637
ATOM	3637	O	ASN	451	112.141	33.397	34.523	1.00156.20		1SG3638
ATOM	3638	N	LEU	452	110.493	34.790	35.158	1.00	79.14	1SG3639
ATOM	3639	CA	LEU	452	110.271	35.249	33.818	1.00	79.14	1SG3640
ATOM	3640	CB	LEU	452	108.896	35.897	33.571	1.00	79.14	1SG3641
ATOM	3641	CG	LEU	452	107.760	34.879	33.338	1.00	79.14	1SG3642
ATOM	3642	CD2	LEU	452	106.498	35.570	32.801	1.00	79.14	1SG3643
ATOM	3643	CD1	LEU	452	107.494	34.006	34.570	1.00	79.14	1SG3644
ATOM	3644	C	LEU	452	111.330	36.231	33.425	1.00	79.14	1SG3645
ATOM	3645	O	LEU	452	111.792	36.236	32.287	1.00	79.14	1SG3646
ATOM	3646	N	ILE	453	111.736	37.110	34.357	1.00178.86		1SG3647
ATOM	3647	CA	ILE	453	112.713	38.122	34.047	1.00178.86		1SG3648
ATOM	3648	CB	ILE	453	112.744	39.241	35.069	1.00178.86		1SG3649
ATOM	3649	CG2	ILE	453	113.019	38.654	36.452	1.00178.86		1SG3650
ATOM	3650	CG1	ILE	453	113.664	40.412	34.654	1.00178.86		1SG3651
ATOM	3651	CD1	ILE	453	115.167	40.124	34.687	1.00178.86		1SG3652
ATOM	3652	C	ILE	453	114.095	37.570	33.714	1.00178.86		1SG3653
ATOM	3653	O	ILE	453	114.699	38.098	32.782	1.00178.86		1SG3654
ATOM	3654	N	PRO	454	114.683	36.582	34.357	1.00170.06		1SG3655
ATOM	3655	CA	PRO	454	116.007	36.190	33.998	1.00170.06		1SG3656
ATOM	3656	CD	PRO	454	114.004	35.374	34.630	1.00170.06		1SG3657
ATOM	3657	CB	PRO	454	116.367	35.044	34.922	1.00170.06		1SG3658
ATOM	3658	CG	PRO	454	115.035	34.309	35.040	1.00170.06		1SG3659
ATOM	3659	C	PRO	454	116.082	35.729	32.567	1.00170.06		1SG3660
ATOM	3660	O	PRO	454	117.195	35.650	32.056	1.00170.06		1SG3661
ATOM	3661	N	LEU	455	114.952	35.342	31.934	1.00151.61		1SG3662
ATOM	3662	CA	LEU	455	114.899	34.881	30.580	1.00151.61		1SG3663
ATOM	3663	CB	LEU	455	113.517	34.356	30.162	1.00151.61		1SG3664
ATOM	3664	CG	LEU	455	113.509	33.813	28.721	1.00151.61		1SG3665
ATOM	3665	CD2	LEU	455	112.092	33.754	28.128	1.00151.61		1SG3666
ATOM	3666	CD1	LEU	455	114.273	32.481	28.644	1.00151.61		1SG3667
ATOM	3667	C	LEU	455	115.187	36.027	29.661	1.00151.61		1SG3668
ATOM	3668	O	LEU	455	115.684	35.829	28.555	1.00151.61		1SG3669
ATOM	3669	N	LEU	456	114.867	37.260	30.095	1.00	80.16	1SG3670
ATOM	3670	CA	LEU	456	114.932	38.399	29.220	1.00	80.16	1SG3671
ATOM	3671	CB	LEU	456	114.626	39.722	29.949	1.00	80.16	1SG3672
ATOM	3672	CG	LEU	456	113.206	39.804	30.548	1.00	80.16	1SG3673
ATOM	3673	CD2	LEU	456	112.123	39.497	29.502	1.00	80.16	1SG3674
ATOM	3674	CD1	LEU	456	112.977	41.151	31.254	1.00	80.16	1SG3675
ATOM	3675	C	LEU	456	116.279	38.558	28.572	1.00	80.16	1SG3676
ATOM	3676	O	LEU	456	116.360	38.680	27.350	1.00	80.16	1SG3677
ATOM	3677	N	LEU	457	117.386	38.597	29.330	1.00159.21		1SG3678
ATOM	3678	CA	LEU	457	118.627	38.756	28.617	1.00159.21		1SG3679
ATOM	3679	CB	LEU	457	119.720	39.623	29.220	1.00159.21		1SG3680
ATOM	3680	CG	LEU	457	119.362	41.118	29.238	1.00159.21		1SG3681
ATOM	3681	CD2	LEU	457	117.998	41.337	29.907	1.00159.21		1SG3682
ATOM	3682	CD1	LEU	457	119.413	41.727	27.828	1.00159.21		1SG3683
ATOM	3683	C	LEU	457	119.150	37.503	27.992	1.00159.21		1SG3684
ATOM	3684	O	LEU	457	120.080	37.571	27.191	1.00159.21		1SG3685
ATOM	3685	N	MET	458	118.638	36.320	28.390	1.00	70.12	1SG3686
ATOM	3686	CA	MET	458	119.128	35.096	27.813	1.00	70.12	1SG3687
ATOM	3687	CB	MET	458	118.461	33.849	28.419	1.00	70.12	1SG3688
ATOM	3688	CG	MET	458	118.746	33.654	29.909	1.00	70.12	1SG3689
ATOM	3689	SD	MET	458	117.870	32.249	30.663	1.00	70.12	1SG3690
ATOM	3690	CE	MET	458	118.787	30.967	29.760	1.00	70.12	1SG3691

Supplementary material 1.txt

ATOM	3691	C	MET	458	118.810	35.101	26.344	1.00	70.12	1SG3692
ATOM	3692	O	MET	458	117.657	34.979	25.940	1.00	70.12	1SG3693
ATOM	3693	N	GLY	459	119.856	35.169	25.500	1.00	38.14	1SG3694
ATOM	3694	CA	GLY	459	119.721	35.287	24.073	1.00	38.14	1SG3695
ATOM	3695	C	GLY	459	118.995	34.105	23.508	1.00	38.14	1SG3696
ATOM	3696	O	GLY	459	118.277	34.230	22.517	1.00	38.14	1SG3697
ATOM	3697	N	GLU	460	119.202	32.920	24.107	1.00	118.79	1SG3698
ATOM	3698	CA	GLU	460	118.624	31.690	23.643	1.00	118.79	1SG3699
ATOM	3699	CB	GLU	460	119.175	30.455	24.377	1.00	118.79	1SG3700
ATOM	3700	CG	GLU	460	119.100	30.564	25.899	1.00	118.79	1SG3701
ATOM	3701	CD	GLU	460	120.364	31.270	26.372	1.00	118.79	1SG3702
ATOM	3702	OE1	GLU	460	121.355	31.291	25.593	1.00	118.79	1SG3703
ATOM	3703	OE2	GLU	460	120.359	31.793	27.518	1.00	118.79	1SG3704
ATOM	3704	C	GLU	460	117.128	31.694	23.775	1.00	118.79	1SG3705
ATOM	3705	O	GLU	460	116.446	31.038	22.991	1.00	118.79	1SG3706
ATOM	3706	N	HIS	461	116.579	32.429	24.762	1.00	113.36	1SG3707
ATOM	3707	CA	HIS	461	115.170	32.439	25.071	1.00	113.36	1SG3708
ATOM	3708	ND1	HIS	461	115.459	35.671	24.622	1.00	113.36	1SG3709
ATOM	3709	CG	HIS	461	114.495	34.907	25.243	1.00	113.36	1SG3710
ATOM	3710	CB	HIS	461	114.765	33.622	25.983	1.00	113.36	1SG3711
ATOM	3711	NE2	HIS	461	113.512	36.660	24.215	1.00	113.36	1SG3712
ATOM	3712	CD2	HIS	461	113.312	35.528	24.986	1.00	113.36	1SG3713
ATOM	3713	CE1	HIS	461	114.817	36.705	24.024	1.00	113.36	1SG3714
ATOM	3714	C	HIS	461	114.335	32.573	23.828	1.00	113.36	1SG3715
ATOM	3715	O	HIS	461	114.612	33.387	22.946	1.00	113.36	1SG3716
ATOM	3716	N	LEU	462	113.274	31.739	23.746	1.00	112.56	1SG3717
ATOM	3717	CA	LEU	462	112.346	31.757	22.650	1.00	112.56	1SG3718
ATOM	3718	CB	LEU	462	112.154	30.397	21.953	1.00	112.56	1SG3719
ATOM	3719	CG	LEU	462	113.437	29.775	21.373	1.00	112.56	1SG3720
ATOM	3720	CD2	LEU	462	114.385	29.307	22.487	1.00	112.56	1SG3721
ATOM	3721	CD1	LEU	462	114.098	30.694	20.332	1.00	112.56	1SG3722
ATOM	3722	C	LEU	462	111.009	32.082	23.239	1.00	112.56	1SG3723
ATOM	3723	O	LEU	462	110.843	32.123	24.456	1.00	112.56	1SG3724
ATOM	3724	N	PRO	463	110.058	32.371	22.396	1.00	102.60	1SG3725
ATOM	3725	CA	PRO	463	108.732	32.633	22.878	1.00	102.60	1SG3726
ATOM	3726	CD	PRO	463	110.342	33.077	21.158	1.00	102.60	1SG3727
ATOM	3727	CB	PRO	463	107.969	33.211	21.689	1.00	102.60	1SG3728
ATOM	3728	CG	PRO	463	109.072	33.889	20.852	1.00	102.60	1SG3729
ATOM	3729	C	PRO	463	108.114	31.410	23.478	1.00	102.60	1SG3730
ATOM	3730	O	PRO	463	107.329	31.532	24.417	1.00	102.60	1SG3731
ATOM	3731	N	ILE	464	108.448	30.228	22.934	1.00	97.46	1SG3732
ATOM	3732	CA	ILE	464	107.910	28.980	23.388	1.00	97.46	1SG3733
ATOM	3733	CB	ILE	464	108.293	27.827	22.501	1.00	97.46	1SG3734
ATOM	3734	CG2	ILE	464	107.708	28.087	21.103	1.00	97.46	1SG3735
ATOM	3735	CG1	ILE	464	109.818	27.620	22.504	1.00	97.46	1SG3736
ATOM	3736	CD1	ILE	464	110.254	26.287	21.893	1.00	97.46	1SG3737
ATOM	3737	C	ILE	464	108.422	28.681	24.761	1.00	97.46	1SG3738
ATOM	3738	O	ILE	464	107.682	28.215	25.626	1.00	97.46	1SG3739
ATOM	3739	N	ASP	465	109.716	28.973	24.984	1.00	161.68	1SG3740
ATOM	3740	CA	ASP	465	110.434	28.581	26.160	1.00	161.68	1SG3741
ATOM	3741	CB	ASP	465	111.920	28.960	26.093	1.00	161.68	1SG3742
ATOM	3742	CG	ASP	465	112.653	28.085	27.095	1.00	161.68	1SG3743
ATOM	3743	OD1	ASP	465	112.177	27.978	28.256	1.00	161.68	1SG3744
ATOM	3744	OD2	ASP	465	113.691	27.490	26.700	1.00	161.68	1SG3745
ATOM	3745	C	ASP	465	109.855	29.164	27.396	1.00	161.68	1SG3746
ATOM	3746	O	ASP	465	108.764	28.812	27.841	1.00	161.68	1SG3747
ATOM	3747	N	ILE	466	110.611	30.071	28.017	1.00	135.68	1SG3748
ATOM	3748	CA	ILE	466	110.140	30.615	29.242	1.00	135.68	1SG3749
ATOM	3749	CB	ILE	466	111.065	31.611	29.868	1.00	135.68	1SG3750
ATOM	3750	CG2	ILE	466	110.324	32.254	31.052	1.00	135.68	1SG3751
ATOM	3751	CG1	ILE	466	112.379	30.927	30.274	1.00	135.68	1SG3752
ATOM	3752	CD1	ILE	466	112.193	29.809	31.297	1.00	135.68	1SG3753
ATOM	3753	C	ILE	466	108.851	31.292	28.963	1.00	135.68	1SG3754
ATOM	3754	O	ILE	466	107.972	31.305	29.814	1.00	135.68	1SG3755
ATOM	3755	N	LEU	467	108.686	31.894	27.775	1.00	105.51	1SG3756
ATOM	3756	CA	LEU	467	107.474	32.637	27.685	1.00	105.51	1SG3757
ATOM	3757	CB	LEU	467	107.381	33.467	26.392	1.00	105.51	1SG3758
ATOM	3758	CG	LEU	467	108.476	34.546	26.277	1.00	105.51	1SG3759
ATOM	3759	CD2	LEU	467	108.634	35.340	27.586	1.00	105.51	1SG3760
ATOM	3760	CD1	LEU	467	108.251	35.439	25.046	1.00	105.51	1SG3761
ATOM	3761	C	LEU	467	106.259	31.765	27.751	1.00	105.51	1SG3762

Supplementary material 1.txt

ATOM	3762	O	LEU	467	105.485	31.851	28.705	1.00105.51	1SG3763
ATOM	3763	N	GLU	468	106.103	30.849	26.778	1.00 73.64	1SG3764
ATOM	3764	CA	GLU	468	104.894	30.080	26.734	1.00 73.64	1SG3765
ATOM	3765	CB	GLU	468	104.718	29.299	25.421	1.00 73.64	1SG3766
ATOM	3766	CG	GLU	468	104.461	30.195	24.209	1.00 73.64	1SG3767
ATOM	3767	CD	GLU	468	104.152	29.299	23.020	1.00 73.64	1SG3768
ATOM	3768	OE1	GLU	468	103.983	28.069	23.238	1.00 73.64	1SG3769
ATOM	3769	OE2	GLU	468	104.075	29.831	21.881	1.00 73.64	1SG3770
ATOM	3770	C	GLU	468	104.827	29.088	27.848	1.00 73.64	1SG3771
ATOM	3771	O	GLU	468	103.832	29.011	28.565	1.00 73.64	1SG3772
ATOM	3772	N	GLN	469	105.905	28.312	28.041	1.00143.43	1SG3773
ATOM	3773	CA	GLN	469	105.847	27.254	29.006	1.00143.43	1SG3774
ATOM	3774	CB	GLN	469	107.073	26.329	28.961	1.00143.43	1SG3775
ATOM	3775	CG	GLN	469	106.928	25.113	29.876	1.00143.43	1SG3776
ATOM	3776	CD	GLN	469	105.843	24.216	29.290	1.00143.43	1SG3777
ATOM	3777	OE1	GLN	469	106.898	24.704	28.885	1.00143.43	1SG3778
ATOM	3778	NE2	GLN	469	105.102	24.222	30.429	1.00143.43	1SG3779
ATOM	3779	C	GLN	469	105.730	27.796	30.400	1.00143.43	1SG3780
ATOM	3780	O	GLN	469	104.958	27.277	31.205	1.00143.43	1SG3781
ATOM	3781	N	ILE	470	106.490	28.861	30.721	1.00117.99	1SG3782
ATOM	3782	CA	ILE	470	106.520	29.389	32.063	1.00117.99	1SG3783
ATOM	3783	CB	ILE	470	107.584	30.414	32.342	1.00117.99	1SG3784
ATOM	3784	CG2	ILE	470	107.371	30.961	33.764	1.00117.99	1SG3785
ATOM	3785	CG1	ILE	470	108.983	29.818	32.120	1.00117.99	1SG3786
ATOM	3786	CD1	ILE	470	109.302	28.646	33.047	1.00117.99	1SG3787
ATOM	3787	C	ILE	470	105.204	29.996	32.460	1.00117.99	1SG3788
ATOM	3788	O	ILE	470	104.826	29.946	33.630	1.00117.99	1SG3789
ATOM	3789	N	PHE	471	104.485	30.594	31.491	1.00121.36	1SG3790
ATOM	3790	CA	PHE	471	103.254	31.319	31.683	1.00121.36	1SG3791
ATOM	3791	CB	PHE	471	102.664	31.813	30.349	1.00121.36	1SG3792
ATOM	3792	CG	PHE	471	101.392	32.539	30.627	1.00121.36	1SG3793
ATOM	3793	CD1	PHE	471	101.398	33.874	30.960	1.00121.36	1SG3794
ATOM	3794	CD2	PHE	471	100.189	31.877	30.549	1.00121.36	1SG3795
ATOM	3795	CE1	PHE	471	100.218	34.535	31.210	1.00121.36	1SG3796
ATOM	3796	CE2	PHE	471	99.007	32.533	30.799	1.00121.36	1SG3797
ATOM	3797	CZ	PHE	471	99.021	33.866	31.132	1.00121.36	1SG3798
ATOM	3798	C	PHE	471	102.227	30.430	32.319	1.00121.36	1SG3799
ATOM	3799	O	PHE	471	101.330	30.914	33.007	1.00121.36	1SG3800
ATOM	3800	N	LEU	472	102.293	29.132	31.978	1.00162.97	1SG3801
ATOM	3801	CA	LEU	472	101.558	27.969	32.412	1.00162.97	1SG3802
ATOM	3802	CB	LEU	472	101.615	26.799	31.414	1.00162.97	1SG3803
ATOM	3803	CG	LEU	472	100.795	27.051	30.135	1.00162.97	1SG3804
ATOM	3804	CD2	LEU	472	100.717	25.786	29.265	1.00162.97	1SG3805
ATOM	3805	CD1	LEU	472	101.311	28.273	29.363	1.00162.97	1SG3806
ATOM	3806	C	LEU	472	102.036	27.462	33.752	1.00162.97	1SG3807
ATOM	3807	O	LEU	472	101.606	26.376	34.137	1.00162.97	1SG3808
ATOM	3808	N	PRO	473	102.831	28.211	34.492	1.00147.48	1SG3809
ATOM	3809	CA	PRO	473	103.763	27.667	35.459	1.00147.48	1SG3810
ATOM	3810	CD	PRO	473	102.116	29.308	35.133	1.00147.48	1SG3811
ATOM	3811	CB	PRO	473	103.733	28.548	36.708	1.00147.48	1SG3812
ATOM	3812	CG	PRO	473	102.364	29.214	36.640	1.00147.48	1SG3813
ATOM	3813	C	PRO	473	103.748	26.227	35.800	1.00147.48	1SG3814
ATOM	3814	O	PRO	473	102.819	25.715	36.422	1.00147.48	1SG3815
ATOM	3815	N	SER	474	104.860	25.592	35.392	1.00 85.40	1SG3816
ATOM	3816	CA	SER	474	105.102	24.196	35.532	1.00 85.40	1SG3817
ATOM	3817	CB	SER	474	106.281	23.700	34.679	1.00 85.40	1SG3818
ATOM	3818	OG	SER	474	106.468	22.304	34.856	1.00 85.40	1SG3819
ATOM	3819	C	SER	474	105.409	23.898	36.958	1.00 85.40	1SG3820
ATOM	3820	O	SER	474	105.634	24.792	37.770	1.00 85.40	1SG3821
ATOM	3821	N	ARG	475	105.423	22.594	37.290	1.00113.63	1SG3822
ATOM	3822	CA	ARG	475	105.673	22.182	38.636	1.00113.63	1SG3823
ATOM	3823	CB	ARG	475	105.511	20.674	38.899	1.00113.63	1SG3824
ATOM	3824	CG	ARG	475	104.094	20.316	39.353	1.00113.63	1SG3825
ATOM	3825	CD	ARG	475	103.871	18.830	39.639	1.00113.63	1SG3826
ATOM	3826	NE	ARG	475	103.443	18.182	38.368	1.00113.63	1SG3827
ATOM	3827	CZ	ARG	475	102.109	18.017	38.126	1.00113.63	1SG3828
ATOM	3828	NH1	ARG	475	101.197	18.411	39.062	1.00113.63	1SG3829
ATOM	3829	NH2	ARG	475	101.686	17.457	36.955	1.00113.63	1SG3830
ATOM	3830	C	ARG	475	107.037	22.603	39.075	1.00113.63	1SG3831
ATOM	3831	O	ARG	475	107.215	22.986	40.223	1.00113.63	1SG3832
ATOM	3832	N	PHE	476	108.049	22.569	38.197	1.00 49.28	1SG3833

Supplementary material 1.txt

ATOM	3833	CA	PHE	476	109.369	22.927	38.646	1.00	49.28	1SG3834
ATOM	3834	CB	PHE	476	110.393	22.848	37.500	1.00	49.28	1SG3835
ATOM	3835	CG	PHE	476	111.730	23.227	38.031	1.00	49.28	1SG3836
ATOM	3836	CD1	PHE	476	112.505	22.303	38.692	1.00	49.28	1SG3837
ATOM	3837	CD2	PHE	476	112.213	24.504	37.856	1.00	49.28	1SG3838
ATOM	3838	CE1	PHE	476	113.742	22.650	39.181	1.00	49.28	1SG3839
ATOM	3839	CE2	PHE	476	113.448	24.857	38.341	1.00	49.28	1SG3840
ATOM	3840	CZ	PHE	476	114.213	23.929	39.007	1.00	49.28	1SG3841
ATOM	3841	C	PHE	476	109.337	24.342	39.149	1.00	49.28	1SG3842
ATOM	3842	O	PHE	476	109.892	24.651	40.204	1.00	49.28	1SG3843
ATOM	3843	N	HIS	477	108.688	25.243	38.389	1.00	82.78	1SG3844
ATOM	3844	CA	HIS	477	108.550	26.622	38.766	1.00	82.78	1SG3845
ATOM	3845	ND1	HIS	477	106.667	29.397	38.721	1.00	82.78	1SG3846
ATOM	3846	CG	HIS	477	107.695	28.892	37.966	1.00	82.78	1SG3847
ATOM	3847	CB	HIS	477	107.872	27.437	37.651	1.00	82.78	1SG3848
ATOM	3848	NE2	HIS	477	107.906	31.132	38.095	1.00	82.78	1SG3849
ATOM	3849	CD2	HIS	477	108.447	29.967	37.589	1.00	82.78	1SG3850
ATOM	3850	CE1	HIS	477	106.838	30.746	38.768	1.00	82.78	1SG3851
ATOM	3851	C	HIS	477	107.673	26.692	39.981	1.00	82.78	1SG3852
ATOM	3852	O	HIS	477	107.928	27.446	40.916	1.00	82.78	1SG3853
ATOM	3853	N	HIS	478	106.600	25.888	40.005	1.00	67.41	1SG3854
ATOM	3854	CA	HIS	478	105.690	25.956	41.107	1.00	67.41	1SG3855
ATOM	3855	ND1	HIS	478	102.497	26.093	42.075	1.00	67.41	1SG3856
ATOM	3856	CG	HIS	478	103.476	25.124	42.039	1.00	67.41	1SG3857
ATOM	3857	CB	HIS	478	104.495	24.998	40.944	1.00	67.41	1SG3858
ATOM	3858	NE2	HIS	478	102.227	24.849	43.899	1.00	67.41	1SG3859
ATOM	3859	CD2	HIS	478	103.296	24.373	43.160	1.00	67.41	1SG3860
ATOM	3860	CE1	HIS	478	101.779	25.882	43.208	1.00	67.41	1SG3861
ATOM	3861	C	HIS	478	106.410	25.590	42.369	1.00	67.41	1SG3862
ATOM	3862	O	HIS	478	106.249	26.248	43.395	1.00	67.41	1SG3863
ATOM	3863	N	LEU	479	107.230	24.525	42.328	1.00	106.92	1SG3864
ATOM	3864	CA	LEU	479	107.920	24.075	43.500	1.00	106.92	1SG3865
ATOM	3865	CB	LEU	479	108.548	22.674	43.383	1.00	106.92	1SG3866
ATOM	3866	CG	LEU	479	107.518	21.521	43.516	1.00	106.92	1SG3867
ATOM	3867	CD2	LEU	479	106.558	21.398	42.331	1.00	106.92	1SG3868
ATOM	3868	CD1	LEU	479	106.757	21.587	44.845	1.00	106.92	1SG3869
ATOM	3869	C	LEU	479	108.934	25.079	43.964	1.00	106.92	1SG3870
ATOM	3870	O	LEU	479	109.114	25.254	45.168	1.00	106.92	1SG3871
ATOM	3871	N	ILE	480	109.625	25.775	43.040	1.00	139.56	1SG3872
ATOM	3872	CA	ILE	480	110.619	26.730	43.451	1.00	139.56	1SG3873
ATOM	3873	CB	ILE	480	111.390	27.310	42.296	1.00	139.56	1SG3874
ATOM	3874	CG2	ILE	480	110.453	28.240	41.527	1.00	139.56	1SG3875
ATOM	3875	CG1	ILE	480	112.684	27.999	42.763	1.00	139.56	1SG3876
ATOM	3876	CD1	ILE	480	112.464	29.236	43.632	1.00	139.56	1SG3877
ATOM	3877	C	ILE	480	109.938	27.828	44.223	1.00	139.56	1SG3878
ATOM	3878	O	ILE	480	110.450	28.298	45.237	1.00	139.56	1SG3879
ATOM	3879	N	GLU	481	108.749	28.257	43.758	1.00	81.41	1SG3880
ATOM	3880	CA	GLU	481	107.987	29.319	44.348	1.00	81.41	1SG3881
ATOM	3881	CB	GLU	481	106.721	29.592	43.517	1.00	81.41	1SG3882
ATOM	3882	CG	GLU	481	105.877	30.786	43.958	1.00	81.41	1SG3883
ATOM	3883	CD	GLU	481	104.695	30.854	42.997	1.00	81.41	1SG3884
ATOM	3884	OE1	GLU	481	104.351	29.790	42.414	1.00	81.41	1SG3885
ATOM	3885	OE2	GLU	481	104.126	31.964	42.824	1.00	81.41	1SG3886
ATOM	3886	C	GLU	481	107.564	28.920	45.734	1.00	81.41	1SG3887
ATOM	3887	O	GLU	481	107.585	29.733	46.657	1.00	81.41	1SG3888
ATOM	3888	N	LEU	482	107.170	27.647	45.916	1.00	122.45	1SG3889
ATOM	3889	CA	LEU	482	106.682	27.177	47.184	1.00	122.45	1SG3890
ATOM	3890	CB	LEU	482	106.190	25.718	47.108	1.00	122.45	1SG3891
ATOM	3891	CG	LEU	482	105.525	25.145	48.382	1.00	122.45	1SG3892
ATOM	3892	CD2	LEU	482	104.274	25.951	48.761	1.00	122.45	1SG3893
ATOM	3893	CD1	LEU	482	106.509	24.973	49.552	1.00	122.45	1SG3894
ATOM	3894	C	LEU	482	107.780	27.255	48.201	1.00	122.45	1SG3895
ATOM	3895	O	LEU	482	107.554	27.666	49.338	1.00	122.45	1SG3896
ATOM	3896	N	ALA	483	109.008	26.866	47.817	1.00	29.74	1SG3897
ATOM	3897	CA	ALA	483	110.095	26.841	48.755	1.00	29.74	1SG3898
ATOM	3898	CB	ALA	483	111.406	26.343	48.123	1.00	29.74	1SG3899
ATOM	3899	C	ALA	483	110.329	28.228	49.263	1.00	29.74	1SG3900
ATOM	3900	O	ALA	483	110.536	28.436	50.458	1.00	29.74	1SG3901
ATOM	3901	N	SER	484	110.287	29.225	48.364	1.00	75.54	1SG3902
ATOM	3902	CA	SER	484	110.547	30.571	48.776	1.00	75.54	1SG3903
ATOM	3903	CB	SER	484	110.505	31.569	47.611	1.00	75.54	1SG3904

Supplementary material 1.txt

ATOM	3904	OG	SER	484	110.768	32.884	48.081	1.00	75.54	1SG3905
ATOM	3905	C	SER	484	109.497	31.003	49.751	1.00	75.54	1SG3906
ATOM	3906	O	SER	484	109.806	31.639	50.756	1.00	75.54	1SG3907
ATOM	3907	N	ARG	485	108.222	30.685	49.467	1.00154.52		1SG3908
ATOM	3908	CA	ARG	485	107.141	31.120	50.306	1.00154.52		1SG3909
ATOM	3909	CB	ARG	485	105.769	30.805	49.683	1.00154.52		1SG3910
ATOM	3910	CG	ARG	485	104.575	31.176	50.564	1.00154.52		1SG3911
ATOM	3911	CD	ARG	485	104.590	32.627	51.046	1.00154.52		1SG3912
ATOM	3912	NE	ARG	485	105.420	33.421	50.103	1.00154.52		1SG3913
ATOM	3913	CZ	ARG	485	106.093	34.519	50.556	1.00154.52		1SG3914
ATOM	3914	NH1	ARG	485	106.003	34.882	51.867	1.00154.52		1SG3915
ATOM	3915	NH2	ARG	485	106.862	35.254	49.700	1.00154.52		1SG3916
ATOM	3916	C	ARG	485	107.206	30.500	51.669	1.00154.52		1SG3917
ATOM	3917	O	ARG	485	107.128	31.188	52.687	1.00154.52		1SG3918
ATOM	3918	N	LEU	486	107.386	29.171	51.728	1.00113.01		1SG3919
ATOM	3919	CA	LEU	486	107.377	28.499	52.992	1.00113.01		1SG3920
ATOM	3920	CB	LEU	486	107.347	26.983	52.848	1.00113.01		1SG3921
ATOM	3921	CG	LEU	486	105.917	26.544	52.515	1.00113.01		1SG3922
ATOM	3922	CD2	LEU	486	105.776	25.025	52.586	1.00113.01		1SG3923
ATOM	3923	CD1	LEU	486	105.432	27.162	51.195	1.00113.01		1SG3924
ATOM	3924	C	LEU	486	108.519	28.922	53.847	1.00113.01		1SG3925
ATOM	3925	O	LEU	486	108.340	29.125	55.047	1.00113.01		1SG3926
ATOM	3926	N	VAL	487	109.717	29.071	53.251	1.00	98.15	1SG3927
ATOM	3927	CA	VAL	487	110.875	29.441	54.008	1.00	98.15	1SG3928
ATOM	3928	CB	VAL	487	112.131	29.437	53.181	1.00	98.15	1SG3929
ATOM	3929	CG1	VAL	487	112.387	27.995	52.713	1.00	98.15	1SG3930
ATOM	3930	CG2	VAL	487	111.979	30.438	52.023	1.00	98.15	1SG3931
ATOM	3931	C	VAL	487	110.681	30.815	54.577	1.00	98.15	1SG3932
ATOM	3932	O	VAL	487	110.944	31.049	55.754	1.00	98.15	1SG3933
ATOM	3933	N	ASP	488	110.189	31.763	53.759	1.00	54.53	1SG3934
ATOM	3934	CA	ASP	488	110.034	33.120	54.198	1.00	54.53	1SG3935
ATOM	3935	CB	ASP	488	109.567	34.035	53.048	1.00	54.53	1SG3936
ATOM	3936	CG	ASP	488	109.473	35.473	53.539	1.00	54.53	1SG3937
ATOM	3937	OD1	ASP	488	108.618	35.741	54.424	1.00	54.53	1SG3938
ATOM	3938	OD2	ASP	488	110.255	36.324	53.035	1.00	54.53	1SG3939
ATOM	3939	C	ASP	488	109.029	33.176	55.310	1.00	54.53	1SG3940
ATOM	3940	O	ASP	488	109.230	33.859	56.314	1.00	54.53	1SG3941
ATOM	3941	N	ASP	489	107.923	32.431	55.162	1.00	68.93	1SG3942
ATOM	3942	CA	ASP	489	106.843	32.443	56.108	1.00	68.93	1SG3943
ATOM	3943	CB	ASP	489	105.636	31.618	55.619	1.00	68.93	1SG3944
ATOM	3944	CG	ASP	489	105.030	32.333	54.414	1.00	68.93	1SG3945
ATOM	3945	OD1	ASP	489	105.456	33.484	54.129	1.00	68.93	1SG3946
ATOM	3946	OD2	ASP	489	104.131	31.737	53.762	1.00	68.93	1SG3947
ATOM	3947	C	ASP	489	107.296	31.900	57.429	1.00	68.93	1SG3948
ATOM	3948	O	ASP	489	106.843	32.363	58.475	1.00	68.93	1SG3949
ATOM	3949	N	ALA	490	108.167	30.872	57.420	1.00	45.48	1SG3950
ATOM	3950	CA	ALA	490	108.629	30.298	58.651	1.00	45.48	1SG3951
ATOM	3951	CB	ALA	490	109.511	29.057	58.429	1.00	45.48	1SG3952
ATOM	3952	C	ALA	490	109.455	31.302	59.397	1.00	45.48	1SG3953
ATOM	3953	O	ALA	490	109.283	31.476	60.602	1.00	45.48	1SG3954
ATOM	3954	N	ARG	491	110.388	31.978	58.692	1.00163.78		1SG3955
ATOM	3955	CA	ARG	491	111.288	32.923	59.300	1.00163.78		1SG3956
ATOM	3956	CB	ARG	491	112.376	33.390	58.313	1.00163.78		1SG3957
ATOM	3957	CG	ARG	491	113.395	34.382	58.888	1.00163.78		1SG3958
ATOM	3958	CD	ARG	491	113.024	35.861	58.719	1.00163.78		1SG3959
ATOM	3959	NE	ARG	491	112.525	36.354	60.035	1.00163.78		1SG3960
ATOM	3960	CZ	ARG	491	112.351	37.690	60.251	1.00163.78		1SG3961
ATOM	3961	NH1	ARG	491	112.581	38.583	59.244	1.00163.78		1SG3962
ATOM	3962	NH2	ARG	491	111.955	38.137	61.480	1.00163.78		1SG3963
ATOM	3963	C	ARG	491	110.575	34.156	59.783	1.00163.78		1SG3964
ATOM	3964	O	ARG	491	110.752	34.580	60.924	1.00163.78		1SG3965
ATOM	3965	N	ASP	492	109.751	34.748	58.897	1.00149.56		1SG3966
ATOM	3966	CA	ASP	492	109.044	35.999	59.046	1.00149.56		1SG3967
ATOM	3967	CB	ASP	492	108.586	36.595	57.702	1.00149.56		1SG3968
ATOM	3968	CG	ASP	492	109.813	37.172	57.010	1.00149.56		1SG3969
ATOM	3969	OD1	ASP	492	110.886	37.230	57.666	1.00149.56		1SG3970
ATOM	3970	OD2	ASP	492	109.692	37.572	55.821	1.00149.56		1SG3971
ATOM	3971	C	ASP	492	107.844	35.953	59.951	1.00149.56		1SG3972
ATOM	3972	O	ASP	492	107.328	37.006	60.316	1.00149.56		1SG3973
ATOM	3973	N	PHE	493	107.333	34.768	60.325	1.00	90.85	1SG3974
ATOM	3974	CA	PHE	493	106.052	34.707	60.983	1.00	90.85	1SG3975

Supplementary material 1.txt

ATOM	3975	CB	PHE	493	105.663	33.280	61.401	1.00	90.85	1SG3976
ATOM	3976	CG	PHE	493	104.337	33.373	62.071	1.00	90.85	1SG3977
ATOM	3977	CD1	PHE	493	103.221	33.711	61.343	1.00	90.85	1SG3978
ATOM	3978	CD2	PHE	493	104.202	33.102	63.413	1.00	90.85	1SG3979
ATOM	3979	CE1	PHE	493	101.990	33.799	61.946	1.00	90.85	1SG3980
ATOM	3980	CE2	PHE	493	102.972	33.187	64.022	1.00	90.85	1SG3981
ATOM	3981	CZ	PHE	493	101.864	33.539	63.289	1.00	90.85	1SG3982
ATOM	3982	C	PHE	493	105.941	35.576	62.208	1.00	90.85	1SG3983
ATOM	3983	O	PHE	493	105.013	36.377	62.303	1.00	90.85	1SG3984
ATOM	3984	N	GLN	494	106.872	35.485	63.173	1.00	78.16	1SG3985
ATOM	3985	CA	GLN	494	106.688	36.223	64.395	1.00	78.16	1SG3986
ATOM	3986	CB	GLN	494	107.790	35.961	65.437	1.00	78.16	1SG3987
ATOM	3987	CG	GLN	494	107.765	34.555	66.046	1.00	78.16	1SG3988
ATOM	3988	CD	GLN	494	108.608	33.618	65.190	1.00	78.16	1SG3989
ATOM	3989	OE1	GLN	494	108.528	33.612	63.962	1.00	78.16	1SG3990
ATOM	3990	NE2	GLN	494	109.457	32.797	65.863	1.00	78.16	1SG3991
ATOM	3991	C	GLN	494	106.664	37.704	64.150	1.00	78.16	1SG3992
ATOM	3992	O	GLN	494	105.829	38.415	64.708	1.00	78.16	1SG3993
ATOM	3993	N	ALA	495	107.577	38.216	63.307	1.00	27.89	1SG3994
ATOM	3994	CA	ALA	495	107.660	39.633	63.085	1.00	27.89	1SG3995
ATOM	3995	CB	ALA	495	108.819	40.026	62.155	1.00	27.89	1SG3996
ATOM	3996	C	ALA	495	106.397	40.131	62.455	1.00	27.89	1SG3997
ATOM	3997	O	ALA	495	105.878	41.183	62.822	1.00	27.89	1SG3998
ATOM	3998	N	GLU	496	105.865	39.375	61.485	1.00	51.31	1SG3999
ATOM	3999	CA	GLU	496	104.694	39.762	60.756	1.00	51.31	1SG4000
ATOM	4000	CB	GLU	496	104.383	38.753	59.640	1.00	51.31	1SG4001
ATOM	4001	CG	GLU	496	105.476	38.703	58.569	1.00	51.31	1SG4002
ATOM	4002	CD	GLU	496	105.267	37.460	57.714	1.00	51.31	1SG4003
ATOM	4003	OE1	GLU	496	105.031	36.370	58.301	1.00	51.31	1SG4004
ATOM	4004	OE2	GLU	496	105.349	37.582	56.462	1.00	51.31	1SG4005
ATOM	4005	C	GLU	496	103.525	39.807	61.694	1.00	51.31	1SG4006
ATOM	4006	O	GLU	496	102.654	40.667	61.578	1.00	51.31	1SG4007
ATOM	4007	N	LYS	497	103.478	38.870	62.656	1.00	58.77	1SG4008
ATOM	4008	CA	LYS	497	102.378	38.783	63.570	1.00	58.77	1SG4009
ATOM	4009	CB	LYS	497	102.521	37.597	64.542	1.00	58.77	1SG4010
ATOM	4010	CG	LYS	497	101.327	37.405	65.479	1.00	58.77	1SG4011
ATOM	4011	CD	LYS	497	101.328	36.049	66.192	1.00	58.77	1SG4012
ATOM	4012	CE	LYS	497	100.157	35.848	67.158	1.00	58.77	1SG4013
ATOM	4013	NZ	LYS	497	98.930	35.490	66.411	1.00	58.77	1SG4014
ATOM	4014	C	LYS	497	102.295	40.039	64.383	1.00	58.77	1SG4015
ATOM	4015	O	LYS	497	101.201	40.543	64.631	1.00	58.77	1SG4016
ATOM	4016	N	ASP	498	103.447	40.590	64.815	1.00	97.40	1SG4017
ATOM	4017	CA	ASP	498	103.409	41.760	65.650	1.00	97.40	1SG4018
ATOM	4018	CB	ASP	498	104.775	42.164	66.250	1.00	97.40	1SG4019
ATOM	4019	CG	ASP	498	105.764	42.585	65.174	1.00	97.40	1SG4020
ATOM	4020	OD1	ASP	498	105.472	43.560	64.432	1.00	97.40	1SG4021
ATOM	4021	OD2	ASP	498	106.850	41.949	65.103	1.00	97.40	1SG4022
ATOM	4022	C	ASP	498	102.822	42.907	64.883	1.00	97.40	1SG4023
ATOM	4023	O	ASP	498	102.130	43.750	65.453	1.00	97.40	1SG4024
ATOM	4024	N	HIS	499	103.079	42.968	63.564	1.00	52.87	1SG4025
ATOM	4025	CA	HIS	499	102.538	44.010	62.739	1.00	52.87	1SG4026
ATOM	4026	ND1	HIS	499	104.290	46.126	60.806	1.00	52.87	1SG4027
ATOM	4027	CG	HIS	499	104.283	44.773	61.060	1.00	52.87	1SG4028
ATOM	4028	CB	HIS	499	103.023	43.991	61.278	1.00	52.87	1SG4029
ATOM	4029	NE2	HIS	499	106.413	45.470	60.806	1.00	52.87	1SG4030
ATOM	4030	CD2	HIS	499	105.587	44.386	61.057	1.00	52.87	1SG4031
ATOM	4031	CE1	HIS	499	105.588	46.491	60.662	1.00	52.87	1SG4032
ATOM	4032	C	HIS	499	101.054	43.881	62.718	1.00	52.87	1SG4033
ATOM	4033	O	HIS	499	100.342	44.873	62.574	1.00	52.87	1SG4034
ATOM	4034	N	GLY	500	100.536	42.650	62.862	1.00	32.46	1SG4035
ATOM	4035	CA	GLY	500	99.116	42.502	62.822	1.00	32.46	1SG4036
ATOM	4036	C	GLY	500	98.742	41.845	61.539	1.00	32.46	1SG4037
ATOM	4037	O	GLY	500	97.557	41.711	61.237	1.00	32.46	1SG4038
ATOM	4038	N	ASP	501	99.729	41.425	60.725	1.00	121.30	1SG4039
ATOM	4039	CA	ASP	501	99.308	40.738	59.544	1.00	121.30	1SG4040
ATOM	4040	CB	ASP	501	100.260	40.858	58.335	1.00	121.30	1SG4041
ATOM	4041	CG	ASP	501	101.649	40.364	58.689	1.00	121.30	1SG4042
ATOM	4042	OD1	ASP	501	101.902	39.141	58.537	1.00	121.30	1SG4043
ATOM	4043	OD2	ASP	501	102.481	41.211	59.110	1.00	121.30	1SG4044
ATOM	4044	C	ASP	501	99.042	39.301	59.892	1.00	121.30	1SG4045
ATOM	4045	O	ASP	501	99.948	38.478	60.015	1.00	121.30	1SG4046

Supplementary material 1.txt

ATOM	4046	N	LEU	502	97.743	39.002	60.093	1.00121.95	1SG4047
ATOM	4047	CA	LEU	502	97.159	37.727	60.424	1.00121.95	1SG4048
ATOM	4048	CB	LEU	502	95.665	37.785	60.806	1.00121.95	1SG4049
ATOM	4049	CG	LEU	502	95.335	38.486	62.135	1.00121.95	1SG4050
ATOM	4050	CD2	LEU	502	93.911	38.137	62.600	1.00121.95	1SG4051
ATOM	4051	CD1	LEU	502	95.583	39.998	62.059	1.00121.95	1SG4052
ATOM	4052	C	LEU	502	97.219	36.798	59.249	1.00121.95	1SG4053
ATOM	4053	O	LEU	502	97.055	35.589	59.391	1.00121.95	1SG4054
ATOM	4054	N	SER	503	97.366	37.348	58.037	1.00129.59	1SG4055
ATOM	4055	CA	SER	503	97.264	36.580	56.828	1.00129.59	1SG4056
ATOM	4056	CB	SER	503	97.143	37.469	55.578	1.00129.59	1SG4057
ATOM	4057	OG	SER	503	95.940	38.222	55.632	1.00129.59	1SG4058
ATOM	4058	C	SER	503	98.420	35.621	56.593	1.00129.59	1SG4059
ATOM	4059	O	SER	503	98.504	35.079	55.492	1.00129.59	1SG4060
ATOM	4060	N	CYS	504	99.335	35.371	57.569	1.00105.33	1SG4061
ATOM	4061	CA	CYS	504	100.501	34.529	57.319	1.00105.33	1SG4062
ATOM	4062	CB	CYS	504	101.774	35.029	58.010	1.00105.33	1SG4063
ATOM	4063	SG	CYS	504	102.346	36.596	57.308	1.00105.33	1SG4064
ATOM	4064	C	CYS	504	100.329	33.081	57.769	1.00105.33	1SG4065
ATOM	4065	O	CYS	504	99.280	32.492	57.547	1.00105.33	1SG4066
ATOM	4066	N	ILE	505	101.361	32.478	58.439	1.00132.30	1SG4067
ATOM	4067	CA	ILE	505	101.440	31.099	58.900	1.00132.30	1SG4068
ATOM	4068	CB	ILE	505	102.609	30.835	59.805	1.00132.30	1SG4069
ATOM	4069	CG2	ILE	505	102.404	29.469	60.472	1.00132.30	1SG4070
ATOM	4070	CG1	ILE	505	103.933	30.952	59.038	1.00132.30	1SG4071
ATOM	4071	CD1	ILE	505	105.154	30.772	59.937	1.00132.30	1SG4072
ATOM	4072	C	ILE	505	100.211	30.821	59.685	1.00132.30	1SG4073
ATOM	4073	O	ILE	505	99.754	29.682	59.782	1.00132.30	1SG4074
ATOM	4074	N	GLU	506	99.655	31.877	60.281	1.00113.02	1SG4075
ATOM	4075	CA	GLU	506	98.472	31.737	61.064	1.00113.02	1SG4076
ATOM	4076	CB	GLU	506	97.871	33.082	61.489	1.00113.02	1SG4077
ATOM	4077	CG	GLU	506	98.723	33.881	62.468	1.00113.02	1SG4078
ATOM	4078	CD	GLU	506	97.954	35.158	62.754	1.00113.02	1SG4079
ATOM	4079	OE1	GLU	506	96.695	35.090	62.765	1.00113.02	1SG4080
ATOM	4080	OE2	GLU	506	98.606	36.215	62.963	1.00113.02	1SG4081
ATOM	4081	C	GLU	506	97.413	31.062	60.237	1.00113.02	1SG4082
ATOM	4082	O	GLU	506	96.603	30.307	60.772	1.00113.02	1SG4083
ATOM	4083	N	CYS	507	97.385	31.301	58.911	1.00 41.77	1SG4084
ATOM	4084	CA	CYS	507	96.355	30.726	58.087	1.00 41.77	1SG4085
ATOM	4085	CB	CYS	507	96.550	31.016	56.587	1.00 41.77	1SG4086
ATOM	4086	SG	CYS	507	96.432	32.785	56.187	1.00 41.77	1SG4087
ATOM	4087	C	CYS	507	96.399	29.240	58.252	1.00 41.77	1SG4088
ATOM	4088	O	CYS	507	95.363	28.585	58.363	1.00 41.77	1SG4089
ATOM	4089	N	TYR	508	97.614	28.671	58.280	1.00 48.49	1SG4090
ATOM	4090	CA	TYR	508	97.770	27.250	58.399	1.00 48.49	1SG4091
ATOM	4091	CB	TYR	508	99.242	26.817	58.296	1.00 48.49	1SG4092
ATOM	4092	CG	TYR	508	99.269	25.330	58.314	1.00 48.49	1SG4093
ATOM	4093	CD1	TYR	508	99.018	24.625	57.160	1.00 48.49	1SG4094
ATOM	4094	CD2	TYR	508	99.546	24.643	59.472	1.00 48.49	1SG4095
ATOM	4095	CE1	TYR	508	99.042	23.251	57.160	1.00 48.49	1SG4096
ATOM	4096	CE2	TYR	508	99.571	23.269	59.478	1.00 48.49	1SG4097
ATOM	4097	CZ	TYR	508	99.318	22.571	58.321	1.00 48.49	1SG4098
ATOM	4098	OH	TYR	508	99.345	21.160	58.329	1.00 48.49	1SG4099
ATOM	4099	C	TYR	508	97.249	26.788	59.729	1.00 48.49	1SG4100
ATOM	4100	O	TYR	508	96.558	25.772	59.812	1.00 48.49	1SG4101
ATOM	4101	N	LEU	509	97.558	27.523	60.816	1.00 93.27	1SG4102
ATOM	4102	CA	LEU	509	97.156	27.052	62.113	1.00 93.27	1SG4103
ATOM	4103	CB	LEU	509	97.578	27.987	63.263	1.00 93.27	1SG4104
ATOM	4104	CG	LEU	509	99.094	28.057	63.518	1.00 93.27	1SG4105
ATOM	4105	CD2	LEU	509	99.393	28.799	64.831	1.00 93.27	1SG4106
ATOM	4106	CD1	LEU	509	99.847	28.649	62.319	1.00 93.27	1SG4107
ATOM	4107	C	LEU	509	95.665	26.960	62.198	1.00 93.27	1SG4108
ATOM	4108	O	LEU	509	95.119	25.930	62.594	1.00 93.27	1SG4109
ATOM	4109	N	LYS	510	94.969	28.041	61.809	1.00 52.69	1SG4110
ATOM	4110	CA	LYS	510	93.543	28.097	61.937	1.00 52.69	1SG4111
ATOM	4111	CB	LYS	510	92.993	29.497	61.616	1.00 52.69	1SG4112
ATOM	4112	CG	LYS	510	93.501	30.558	62.597	1.00 52.69	1SG4113
ATOM	4113	CD	LYS	510	93.292	32.000	62.132	1.00 52.69	1SG4114
ATOM	4114	CE	LYS	510	93.811	33.036	63.131	1.00 52.69	1SG4115
ATOM	4115	NZ	LYS	510	93.579	34.402	62.614	1.00 52.69	1SG4116
ATOM	4116	C	LYS	510	92.893	27.104	61.023	1.00 52.69	1SG4117

Supplementary material 1.txt

ATOM	4117	O	LYS	510	91.918	26.454	61.398	1.00	52.69	1SG4118
ATOM	4118	N	ASP	511	93.420	26.955	59.794	1.00	59.29	1SG4119
ATOM	4119	CA	ASP	511	92.793	26.102	58.824	1.00	59.29	1SG4120
ATOM	4120	CB	ASP	511	93.532	26.112	57.474	1.00	59.29	1SG4121
ATOM	4121	CG	ASP	511	92.676	25.393	56.442	1.00	59.29	1SG4122
ATOM	4122	OD1	ASP	511	91.530	24.993	56.780	1.00	59.29	1SG4123
ATOM	4123	OD2	ASP	511	93.172	25.225	55.296	1.00	59.29	1SG4124
ATOM	4124	C	ASP	511	92.761	24.688	59.309	1.00	59.29	1SG4125
ATOM	4125	O	ASP	511	91.702	24.063	59.322	1.00	59.29	1SG4126
ATOM	4126	N	HIS	512	93.919	24.141	59.732	1.00164.34		1SG4127
ATOM	4127	CA	HIS	512	93.931	22.788	60.210	1.00164.34		1SG4128
ATOM	4128	ND1	HIS	512	93.862	20.853	57.420	1.00164.34		1SG4129
ATOM	4129	CG	HIS	512	94.694	21.785	57.999	1.00164.34		1SG4130
ATOM	4130	CB	HIS	512	94.944	21.895	59.474	1.00164.34		1SG4131
ATOM	4131	NE2	HIS	512	94.698	22.075	55.761	1.00164.34		1SG4132
ATOM	4132	CD2	HIS	512	95.196	22.523	56.971	1.00164.34		1SG4133
ATOM	4133	CE1	HIS	512	93.901	21.071	56.082	1.00164.34		1SG4134
ATOM	4134	C	HIS	512	94.417	22.875	61.607	1.00164.34		1SG4135
ATOM	4135	O	HIS	512	95.566	22.531	61.871	1.00164.34		1SG4136
ATOM	4136	N	PRO	513	93.509	23.212	62.488	1.00190.29		1SG4137
ATOM	4137	CA	PRO	513	93.796	23.599	63.847	1.00190.29		1SG4138
ATOM	4138	CD	PRO	513	92.129	22.788	62.322	1.00190.29		1SG4139
ATOM	4139	CB	PRO	513	92.493	23.431	64.629	1.00190.29		1SG4140
ATOM	4140	CG	PRO	513	91.400	23.362	63.547	1.00190.29		1SG4141
ATOM	4141	C	PRO	513	94.925	22.867	64.483	1.00190.29		1SG4142
ATOM	4142	O	PRO	513	94.793	21.686	64.800	1.00190.29		1SG4143
ATOM	4143	N	GLU	514	96.048	23.585	64.676	1.00126.61		1SG4144
ATOM	4144	CA	GLU	514	97.200	23.014	65.294	1.00126.61		1SG4145
ATOM	4145	CB	GLU	514	98.063	22.130	64.384	1.00126.61		1SG4146
ATOM	4146	CG	GLU	514	99.092	21.305	65.166	1.00126.61		1SG4147
ATOM	4147	CD	GLU	514	98.356	20.139	65.816	1.00126.61		1SG4148
ATOM	4148	OE1	GLU	514	97.597	19.446	65.087	1.00126.61		1SG4149
ATOM	4149	OE2	GLU	514	98.534	19.930	67.046	1.00126.61		1SG4150
ATOM	4150	C	GLU	514	98.053	24.145	65.752	1.00126.61		1SG4151
ATOM	4151	O	GLU	514	97.779	25.307	65.453	1.00126.61		1SG4152
ATOM	4152	N	SER	515	99.114	23.816	66.511	1.00	75.12	1SG4153
ATOM	4153	CA	SER	515	99.991	24.813	67.039	1.00	75.12	1SG4154
ATOM	4154	CB	SER	515	100.960	24.274	68.104	1.00	75.12	1SG4155
ATOM	4155	OG	SER	515	100.231	23.780	69.216	1.00	75.12	1SG4156
ATOM	4156	C	SER	515	100.820	25.348	65.924	1.00	75.12	1SG4157
ATOM	4157	O	SER	515	100.884	24.775	64.837	1.00	75.12	1SG4158
ATOM	4158	N	THR	516	101.459	26.504	66.174	1.00	37.75	1SG4159
ATOM	4159	CA	THR	516	102.286	27.097	65.175	1.00	37.75	1SG4160
ATOM	4160	CB	THR	516	102.893	28.394	65.627	1.00	37.75	1SG4161
ATOM	4161	OG1	THR	516	101.875	29.315	65.989	1.00	37.75	1SG4162
ATOM	4162	CG2	THR	516	103.739	28.969	64.480	1.00	37.75	1SG4163
ATOM	4163	C	THR	516	103.406	26.148	64.926	1.00	37.75	1SG4164
ATOM	4164	O	THR	516	103.760	25.862	63.784	1.00	37.75	1SG4165
ATOM	4165	N	VAL	517	103.979	25.607	66.013	1.00	50.35	1SG4166
ATOM	4166	CA	VAL	517	105.135	24.781	65.871	1.00	50.35	1SG4167
ATOM	4167	CB	VAL	517	105.650	24.310	67.198	1.00	50.35	1SG4168
ATOM	4168	CG1	VAL	517	106.835	23.360	66.961	1.00	50.35	1SG4169
ATOM	4169	CG2	VAL	517	105.985	25.543	68.054	1.00	50.35	1SG4170
ATOM	4170	C	VAL	517	104.862	23.555	65.059	1.00	50.35	1SG4171
ATOM	4171	O	VAL	517	105.442	23.379	63.989	1.00	50.35	1SG4172
ATOM	4172	N	GLU	518	103.956	22.674	65.528	1.00	96.78	1SG4173
ATOM	4173	CA	GLU	518	103.867	21.422	64.832	1.00	96.78	1SG4174
ATOM	4174	CB	GLU	518	102.981	20.387	65.549	1.00	96.78	1SG4175
ATOM	4175	CG	GLU	518	103.510	19.887	66.894	1.00	96.78	1SG4176
ATOM	4176	CD	GLU	518	102.495	18.881	67.424	1.00	96.78	1SG4177
ATOM	4177	OE1	GLU	518	102.268	17.853	66.731	1.00	96.78	1SG4178
ATOM	4178	OE2	GLU	518	101.928	19.127	68.523	1.00	96.78	1SG4179
ATOM	4179	C	GLU	518	103.288	21.535	63.469	1.00	96.78	1SG4180
ATOM	4180	O	GLU	518	103.978	21.398	62.462	1.00	96.78	1SG4181
ATOM	4181	N	ASP	519	101.986	21.840	63.395	1.00	48.57	1SG4182
ATOM	4182	CA	ASP	519	101.412	21.808	62.093	1.00	48.57	1SG4183
ATOM	4183	CB	ASP	519	99.875	21.832	62.076	1.00	48.57	1SG4184
ATOM	4184	CG	ASP	519	99.389	20.418	62.374	1.00	48.57	1SG4185
ATOM	4185	OD1	ASP	519	100.259	19.522	62.545	1.00	48.57	1SG4186
ATOM	4186	OD2	ASP	519	98.147	20.211	62.424	1.00	48.57	1SG4187
ATOM	4187	C	ASP	519	101.904	22.949	61.295	1.00	48.57	1SG4188

Supplementary material 1.txt

ATOM	4188	O	ASP	519	102.267	22.784	60.133	1.00	48.57	1SG4189
ATOM	4189	N	ALA	520	101.947	24.146	61.899	1.00	77.58	1SG4190
ATOM	4190	CA	ALA	520	102.227	25.234	61.027	1.00	77.58	1SG4191
ATOM	4191	CB	ALA	520	102.105	26.600	61.725	1.00	77.58	1SG4192
ATOM	4192	C	ALA	520	103.603	25.152	60.441	1.00	77.58	1SG4193
ATOM	4193	O	ALA	520	103.741	24.979	59.233	1.00	77.58	1SG4194
ATOM	4194	N	LEU	521	104.656	25.192	61.281	1.00	95.08	1SG4195
ATOM	4195	CA	LEU	521	105.991	25.215	60.744	1.00	95.08	1SG4196
ATOM	4196	CB	LEU	521	107.060	25.652	61.764	1.00	95.08	1SG4197
ATOM	4197	CG	LEU	521	107.006	27.152	62.114	1.00	95.08	1SG4198
ATOM	4198	CD2	LEU	521	105.688	27.535	62.800	1.00	95.08	1SG4199
ATOM	4199	CD1	LEU	521	107.321	28.017	60.883	1.00	95.08	1SG4200
ATOM	4200	C	LEU	521	106.400	23.890	60.190	1.00	95.08	1SG4201
ATOM	4201	O	LEU	521	106.942	23.814	59.088	1.00	95.08	1SG4202
ATOM	4202	N	ASN	522	106.134	22.802	60.937	1.00	33.02	1SG4203
ATOM	4203	CA	ASN	522	106.622	21.515	60.535	1.00	33.02	1SG4204
ATOM	4204	CB	ASN	522	106.364	20.403	61.566	1.00	33.02	1SG4205
ATOM	4205	CG	ASN	522	107.239	20.690	62.778	1.00	33.02	1SG4206
ATOM	4206	OD1	ASN	522	108.103	21.565	62.735	1.00	33.02	1SG4207
ATOM	4207	ND2	ASN	522	107.024	19.929	63.884	1.00	33.02	1SG4208
ATOM	4208	C	ASN	522	105.985	21.113	59.251	1.00	33.02	1SG4209
ATOM	4209	O	ASN	522	106.647	20.555	58.377	1.00	33.02	1SG4210
ATOM	4210	N	HIS	523	104.678	21.383	59.096	1.00	61.89	1SG4211
ATOM	4211	CA	HIS	523	104.026	20.977	57.888	1.00	61.89	1SG4212
ATOM	4212	ND1	HIS	523	101.322	19.200	56.974	1.00	61.89	1SG4213
ATOM	4213	CG	HIS	523	101.783	20.487	56.813	1.00	61.89	1SG4214
ATOM	4214	CB	HIS	523	102.512	21.246	57.881	1.00	61.89	1SG4215
ATOM	4215	NE2	HIS	523	100.761	19.820	54.915	1.00	61.89	1SG4216
ATOM	4216	CD2	HIS	523	101.433	20.851	55.549	1.00	61.89	1SG4217
ATOM	4217	CE1	HIS	523	100.719	18.850	55.811	1.00	61.89	1SG4218
ATOM	4218	C	HIS	523	104.643	21.742	56.763	1.00	61.89	1SG4219
ATOM	4219	O	HIS	523	104.906	21.191	55.698	1.00	61.89	1SG4220
ATOM	4220	N	VAL	524	104.925	23.038	56.994	1.00	38.04	1SG4221
ATOM	4221	CA	VAL	524	105.483	23.904	55.995	1.00	38.04	1SG4222
ATOM	4222	CB	VAL	524	105.725	25.285	56.527	1.00	38.04	1SG4223
ATOM	4223	CG1	VAL	524	106.600	26.049	55.529	1.00	38.04	1SG4224
ATOM	4224	CG2	VAL	524	104.363	25.960	56.756	1.00	38.04	1SG4225
ATOM	4225	C	VAL	524	106.796	23.353	55.538	1.00	38.04	1SG4226
ATOM	4226	O	VAL	524	107.104	23.374	54.346	1.00	38.04	1SG4227
ATOM	4227	N	ASN	525	107.605	22.839	56.479	1.00	37.24	1SG4228
ATOM	4228	CA	ASN	525	108.887	22.310	56.119	1.00	37.24	1SG4229
ATOM	4229	CB	ASN	525	109.683	21.784	57.326	1.00	37.24	1SG4230
ATOM	4230	CG	ASN	525	110.119	22.980	58.159	1.00	37.24	1SG4231
ATOM	4231	OD1	ASN	525	110.736	22.823	59.211	1.00	37.24	1SG4232
ATOM	4232	ND2	ASN	525	109.789	24.210	57.680	1.00	37.24	1SG4233
ATOM	4233	C	ASN	525	108.674	21.160	55.189	1.00	37.24	1SG4234
ATOM	4234	O	ASN	525	109.413	20.986	54.221	1.00	37.24	1SG4235
ATOM	4235	N	GLY	526	107.636	20.349	55.457	1.00	19.06	1SG4236
ATOM	4236	CA	GLY	526	107.378	19.186	54.662	1.00	19.06	1SG4237
ATOM	4237	C	GLY	526	107.110	19.608	53.255	1.00	19.06	1SG4238
ATOM	4238	O	GLY	526	107.533	18.938	52.315	1.00	19.06	1SG4239
ATOM	4239	N	LEU	527	106.381	20.725	53.066	1.00	89.15	1SG4240
ATOM	4240	CA	LEU	527	106.071	21.163	51.735	1.00	89.15	1SG4241
ATOM	4241	CB	LEU	527	105.079	22.334	51.653	1.00	89.15	1SG4242
ATOM	4242	CG	LEU	527	103.615	21.965	51.963	1.00	89.15	1SG4243
ATOM	4243	CD2	LEU	527	102.673	23.138	51.644	1.00	89.15	1SG4244
ATOM	4244	CD1	LEU	527	103.446	21.446	53.396	1.00	89.15	1SG4245
ATOM	4245	C	LEU	527	107.330	21.545	51.021	1.00	89.15	1SG4246
ATOM	4246	O	LEU	527	107.442	21.348	49.814	1.00	89.15	1SG4247
ATOM	4247	N	LEU	528	108.309	22.126	51.738	1.00	37.01	1SG4248
ATOM	4248	CA	LEU	528	109.548	22.514	51.125	1.00	37.01	1SG4249
ATOM	4249	CB	LEU	528	110.509	23.182	52.122	1.00	37.01	1SG4250
ATOM	4250	CG	LEU	528	109.975	24.498	52.714	1.00	37.01	1SG4251
ATOM	4251	CD2	LEU	528	109.559	25.475	51.605	1.00	37.01	1SG4252
ATOM	4252	CD1	LEU	528	110.982	25.113	53.699	1.00	37.01	1SG4253
ATOM	4253	C	LEU	528	110.245	21.285	50.629	1.00	37.01	1SG4254
ATOM	4254	O	LEU	528	110.800	21.276	49.531	1.00	37.01	1SG4255
ATOM	4255	N	GLY	529	110.238	20.209	51.440	1.00	18.48	1SG4256
ATOM	4256	CA	GLY	529	110.920	18.998	51.082	1.00	18.48	1SG4257
ATOM	4257	C	GLY	529	110.298	18.428	49.848	1.00	18.48	1SG4258
ATOM	4258	O	GLY	529	110.997	17.962	48.950	1.00	18.48	1SG4259

Supplementary material 1.txt

ATOM	4259	N	ASN	530	108.956	18.452	49.776	1.00	26.26	1SG4260
ATOM	4260	CA	ASN	530	108.247	17.905	48.657	1.00	26.26	1SG4261
ATOM	4261	CB	ASN	530	106.722	18.054	48.802	1.00	26.26	1SG4262
ATOM	4262	CG	ASN	530	106.280	17.228	50.000	1.00	26.26	1SG4263
ATOM	4263	OD1	ASN	530	106.700	16.084	50.168	1.00	26.26	1SG4264
ATOM	4264	ND2	ASN	530	105.416	17.822	50.866	1.00	26.26	1SG4265
ATOM	4265	C	ASN	530	108.642	18.679	47.443	1.00	26.26	1SG4266
ATOM	4266	O	ASN	530	108.861	18.114	46.373	1.00	26.26	1SG4267
ATOM	4267	N	CYS	531	108.759	20.009	47.598	1.00	32.10	1SG4268
ATOM	4268	CA	CYS	531	109.079	20.884	46.509	1.00	32.10	1SG4269
ATOM	4269	CB	CYS	531	109.147	22.359	46.925	1.00	32.10	1SG4270
ATOM	4270	SG	CYS	531	107.533	22.982	47.462	1.00	32.10	1SG4271
ATOM	4271	C	CYS	531	110.426	20.531	45.977	1.00	32.10	1SG4272
ATOM	4272	O	CYS	531	110.650	20.563	44.768	1.00	32.10	1SG4273
ATOM	4273	N	LEU	532	111.366	20.200	46.876	1.00	39.46	1SG4274
ATOM	4274	CA	LEU	532	112.701	19.877	46.463	1.00	39.46	1SG4275
ATOM	4275	CB	LEU	532	113.643	19.595	47.646	1.00	39.46	1SG4276
ATOM	4276	CG	LEU	532	113.877	20.815	48.555	1.00	39.46	1SG4277
ATOM	4277	CD2	LEU	532	114.272	22.058	47.740	1.00	39.46	1SG4278
ATOM	4278	CD1	LEU	532	114.883	20.493	49.672	1.00	39.46	1SG4279
ATOM	4279	C	LEU	532	112.678	18.640	45.617	1.00	39.46	1SG4280
ATOM	4280	O	LEU	532	113.374	18.560	44.606	1.00	39.46	1SG4281
ATOM	4281	N	LEU	533	111.882	17.627	46.011	1.00	86.47	1SG4282
ATOM	4282	CA	LEU	533	111.833	16.418	45.242	1.00	86.47	1SG4283
ATOM	4283	CB	LEU	533	110.987	15.300	45.880	1.00	86.47	1SG4284
ATOM	4284	CG	LEU	533	111.680	14.577	47.051	1.00	86.47	1SG4285
ATOM	4285	CD2	LEU	533	110.850	13.375	47.528	1.00	86.47	1SG4286
ATOM	4286	CD1	LEU	533	112.032	15.540	48.192	1.00	86.47	1SG4287
ATOM	4287	C	LEU	533	111.256	16.719	43.897	1.00	86.47	1SG4288
ATOM	4288	O	LEU	533	111.678	16.137	42.899	1.00	86.47	1SG4289
ATOM	4289	N	GLU	534	110.255	17.619	43.842	1.00	80.47	1SG4290
ATOM	4290	CA	GLU	534	109.618	17.946	42.600	1.00	80.47	1SG4291
ATOM	4291	CB	GLU	534	108.367	18.815	42.761	1.00	80.47	1SG4292
ATOM	4292	CG	GLU	534	107.235	18.109	43.510	1.00	80.47	1SG4293
ATOM	4293	CD	GLU	534	106.875	16.842	42.745	1.00	80.47	1SG4294
ATOM	4294	OE1	GLU	534	106.533	16.952	41.538	1.00	80.47	1SG4295
ATOM	4295	OE2	GLU	534	106.936	15.745	43.362	1.00	80.47	1SG4296
ATOM	4296	C	GLU	534	110.576	18.656	41.693	1.00	80.47	1SG4297
ATOM	4297	O	GLU	534	110.540	18.463	40.479	1.00	80.47	1SG4298
ATOM	4298	N	MET	535	111.441	19.525	42.248	1.00	77.13	1SG4299
ATOM	4299	CA	MET	535	112.392	20.221	41.429	1.00	77.13	1SG4300
ATOM	4300	CB	MET	535	113.205	21.271	42.205	1.00	77.13	1SG4301
ATOM	4301	CG	MET	535	112.366	22.483	42.617	1.00	77.13	1SG4302
ATOM	4302	SD	MET	535	113.269	23.760	43.542	1.00	77.13	1SG4303
ATOM	4303	CE	MET	535	113.182	22.870	45.122	1.00	77.13	1SG4304
ATOM	4304	C	MET	535	113.337	19.219	40.844	1.00	77.13	1SG4305
ATOM	4305	O	MET	535	113.709	19.303	39.674	1.00	77.13	1SG4306
ATOM	4306	N	ASN	536	113.734	18.219	41.648	1.00	45.07	1SG4307
ATOM	4307	CA	ASN	536	114.665	17.222	41.204	1.00	45.07	1SG4308
ATOM	4308	CB	ASN	536	115.038	16.213	42.303	1.00	45.07	1SG4309
ATOM	4309	CG	ASN	536	115.989	16.905	43.273	1.00	45.07	1SG4310
ATOM	4310	OD1	ASN	536	116.823	17.712	42.869	1.00	45.07	1SG4311
ATOM	4311	ND2	ASN	536	115.869	16.576	44.588	1.00	45.07	1SG4312
ATOM	4312	C	ASN	536	114.068	16.460	40.055	1.00	45.07	1SG4313
ATOM	4313	O	ASN	536	114.775	16.098	39.118	1.00	45.07	1SG4314
ATOM	4314	N	TRP	537	112.751	16.180	40.110	1.00	106.73	1SG4315
ATOM	4315	CA	TRP	537	112.067	15.441	39.084	1.00	106.73	1SG4316
ATOM	4316	CB	TRP	537	110.602	15.127	39.429	1.00	106.73	1SG4317
ATOM	4317	CG	TRP	537	109.899	14.374	38.326	1.00	106.73	1SG4318
ATOM	4318	CD2	TRP	537	109.272	15.012	37.204	1.00	106.73	1SG4319
ATOM	4319	CD1	TRP	537	109.741	13.031	38.146	1.00	106.73	1SG4320
ATOM	4320	NE1	TRP	537	109.060	12.792	36.976	1.00	106.73	1SG4321
ATOM	4321	CE2	TRP	537	108.765	14.003	36.385	1.00	106.73	1SG4322
ATOM	4322	CE3	TRP	537	109.136	16.331	36.878	1.00	106.73	1SG4323
ATOM	4323	CZ2	TRP	537	108.110	14.299	35.224	1.00	106.73	1SG4324
ATOM	4324	CZ3	TRP	537	108.471	16.628	35.709	1.00	106.73	1SG4325
ATOM	4325	CH2	TRP	537	107.969	15.631	34.899	1.00	106.73	1SG4326
ATOM	4326	C	TRP	537	112.036	16.211	37.801	1.00	106.73	1SG4327
ATOM	4327	O	TRP	537	112.169	15.639	36.720	1.00	106.73	1SG4328
ATOM	4328	N	LYS	538	111.838	17.537	37.882	1.00	120.34	1SG4329
ATOM	4329	CA	LYS	538	111.680	18.320	36.692	1.00	120.34	1SG4330

Supplementary material 1.txt

ATOM	4330	CB	LYS	538	111.277	19.776	36.956	1.00120.34	1SG4331
ATOM	4331	CG	LYS	538	110.724	20.425	35.690	1.00120.34	1SG4332
ATOM	4332	CD	LYS	538	109.455	19.743	35.173	1.00120.34	1SG4333
ATOM	4333	CE	LYS	538	108.996	20.247	33.804	1.00120.34	1SG4334
ATOM	4334	NZ	LYS	538	107.961	19.341	33.261	1.00120.34	1SG4335
ATOM	4335	C	LYS	538	112.935	18.298	35.876	1.00120.34	1SG4336
ATOM	4336	O	LYS	538	112.888	18.392	34.652	1.00120.34	1SG4337
ATOM	4337	N	PHE	539	114.100	18.208	36.534	1.00109.41	1SG4338
ATOM	4338	CA	PHE	539	115.361	18.169	35.849	1.00109.41	1SG4339
ATOM	4339	CB	PHE	539	116.577	18.205	36.789	1.00109.41	1SG4340
ATOM	4340	CG	PHE	539	116.753	19.590	37.308	1.00109.41	1SG4341
ATOM	4341	CD1	PHE	539	117.421	20.528	36.555	1.00109.41	1SG4342
ATOM	4342	CD2	PHE	539	116.269	19.952	38.544	1.00109.41	1SG4343
ATOM	4343	CE1	PHE	539	117.597	21.808	37.020	1.00109.41	1SG4344
ATOM	4344	CE2	PHE	539	116.443	21.232	39.015	1.00109.41	1SG4345
ATOM	4345	CZ	PHE	539	117.108	22.163	38.253	1.00109.41	1SG4346
ATOM	4346	C	PHE	539	115.473	16.905	35.050	1.00109.41	1SG4347
ATOM	4347	O	PHE	539	116.078	16.888	33.981	1.00109.41	1SG4348
ATOM	4348	N	LEU	540	114.909	15.796	35.552	1.0076.41	1SG4349
ATOM	4349	CA	LEU	540	115.131	14.535	34.915	1.0076.41	1SG4350
ATOM	4350	CB	LEU	540	114.492	13.355	35.669	1.0076.41	1SG4351
ATOM	4351	CG	LEU	540	115.105	13.106	37.060	1.0076.41	1SG4352
ATOM	4352	CD2	LEU	540	116.630	12.948	36.972	1.0076.41	1SG4353
ATOM	4353	CD1	LEU	540	114.431	11.919	37.767	1.0076.41	1SG4354
ATOM	4354	C	LEU	540	114.622	14.510	33.517	1.0076.41	1SG4355
ATOM	4355	O	LEU	540	113.456	14.798	33.245	1.0076.41	1SG4356
ATOM	4356	N	LYS	541	115.542	14.202	32.581	1.00131.13	1SG4357
ATOM	4357	CA	LYS	541	115.174	13.972	31.225	1.00131.13	1SG4358
ATOM	4358	CB	LYS	541	116.384	13.679	30.320	1.00131.13	1SG4359
ATOM	4359	CG	LYS	541	117.450	14.775	30.265	1.00131.13	1SG4360
ATOM	4360	CD	LYS	541	118.750	14.295	29.615	1.00131.13	1SG4361
ATOM	4361	CE	LYS	541	119.819	15.380	29.479	1.00131.13	1SG4362
ATOM	4362	NZ	LYS	541	121.015	14.822	28.808	1.00131.13	1SG4363
ATOM	4363	C	LYS	541	114.419	12.693	31.268	1.00131.13	1SG4364
ATOM	4364	O	LYS	541	113.276	12.621	30.830	1.00131.13	1SG4365
ATOM	4365	N	LYS	542	115.038	11.654	31.875	1.00257.18	1SG4366
ATOM	4366	CA	LYS	542	114.454	10.342	31.896	1.00257.18	1SG4367
ATOM	4367	CB	LYS	542	113.241	10.227	32.843	1.00257.18	1SG4368
ATOM	4368	CG	LYS	542	112.707	8.803	33.038	1.00257.18	1SG4369
ATOM	4369	CD	LYS	542	113.718	7.837	33.660	1.00257.18	1SG4370
ATOM	4370	CE	LYS	542	114.538	7.062	32.623	1.00257.18	1SG4371
ATOM	4371	NZ	LYS	542	115.497	6.165	33.305	1.00257.18	1SG4372
ATOM	4372	C	LYS	542	114.065	10.026	30.486	1.00257.18	1SG4373
ATOM	4373	O	LYS	542	114.609	10.595	29.539	1.00257.18	1SG4374
ATOM	4374	N	GLN	543	113.157	9.065	30.272	1.00264.08	1SG4375
ATOM	4375	CA	GLN	543	112.751	8.917	28.914	1.00264.08	1SG4376
ATOM	4376	CB	GLN	543	111.777	7.749	28.676	1.00264.08	1SG4377
ATOM	4377	CG	GLN	543	111.349	7.585	27.216	1.00264.08	1SG4378
ATOM	4378	CD	GLN	543	110.422	6.379	27.134	1.00264.08	1SG4379
ATOM	4379	OE1	GLN	543	110.169	5.710	28.134	1.00264.08	1SG4380
ATOM	4380	NE2	GLN	543	109.908	6.089	25.909	1.00264.08	1SG4381
ATOM	4381	C	GLN	543	112.036	10.193	28.632	1.00264.08	1SG4382
ATOM	4382	O	GLN	543	111.423	10.755	29.539	1.00264.08	1SG4383
ATOM	4383	N	ASP	544	112.089	10.676	27.374	1.00259.35	1SG4384
ATOM	4384	CA	ASP	544	111.468	11.927	27.047	1.00259.35	1SG4385
ATOM	4385	CB	ASP	544	109.930	11.854	27.042	1.00259.35	1SG4386
ATOM	4386	CG	ASP	544	109.380	13.174	26.517	1.00259.35	1SG4387
ATOM	4387	OD1	ASP	544	110.197	14.065	26.161	1.00259.35	1SG4388
ATOM	4388	OD2	ASP	544	108.128	13.308	26.468	1.00259.35	1SG4389
ATOM	4389	C	ASP	544	111.888	12.981	28.030	1.00259.35	1SG4390
ATOM	4390	O	ASP	544	111.126	13.343	28.925	1.00259.35	1SG4391
ATOM	4391	N	SER	545	113.137	13.478	27.886	1.00115.06	1SG4392
ATOM	4392	CA	SER	545	113.687	14.501	28.727	1.00115.06	1SG4393
ATOM	4393	CB	SER	545	114.969	15.132	28.158	1.00115.06	1SG4394
ATOM	4394	OG	SER	545	115.410	16.185	29.002	1.00115.06	1SG4395
ATOM	4395	C	SER	545	112.685	15.595	28.883	1.00115.06	1SG4396
ATOM	4396	O	SER	545	111.738	15.717	28.110	1.00115.06	1SG4397
ATOM	4397	N	VAL	546	112.872	16.418	29.929	1.00143.98	1SG4398
ATOM	4398	CA	VAL	546	111.917	17.428	30.262	1.00143.98	1SG4399
ATOM	4399	CB	VAL	546	112.111	18.020	31.619	1.00143.98	1SG4400
ATOM	4400	CG1	VAL	546	111.808	16.905	32.632	1.00143.98	1SG4401

Supplementary material 1.txt

ATOM	4401	CG2	VAL	546	113.532	18.599	31.720	1.00143.98	1SG4402
ATOM	4402	C	VAL	546	111.896	18.516	29.248	1.00143.98	1SG4403
ATOM	4403	O	VAL	546	112.875	18.825	28.570	1.00143.98	1SG4404
ATOM	4404	N	PRO	547	110.715	19.059	29.133	1.00171.70	1SG4405
ATOM	4405	CA	PRO	547	110.407	20.122	28.227	1.00171.70	1SG4406
ATOM	4406	CD	PRO	547	109.550	18.576	29.851	1.00171.70	1SG4407
ATOM	4407	CB	PRO	547	108.889	20.307	28.293	1.00171.70	1SG4408
ATOM	4408	CG	PRO	547	108.495	19.674	29.641	1.00171.70	1SG4409
ATOM	4409	C	PRO	547	111.170	21.336	28.611	1.00171.70	1SG4410
ATOM	4410	O	PRO	547	111.243	21.639	29.800	1.00171.70	1SG4411
ATOM	4411	N	LEU	548	111.720	22.047	27.611	1.00160.40	1SG4412
ATOM	4412	CA	LEU	548	112.490	23.232	27.827	1.00160.40	1SG4413
ATOM	4413	CB	LEU	548	111.986	24.138	28.967	1.00160.40	1SG4414
ATOM	4414	CG	LEU	548	110.635	24.812	28.654	1.00160.40	1SG4415
ATOM	4415	CD2	LEU	548	110.287	25.879	29.703	1.00160.40	1SG4416
ATOM	4416	CD1	LEU	548	109.517	23.776	28.459	1.00160.40	1SG4417
ATOM	4417	C	LEU	548	113.901	22.834	28.090	1.00160.40	1SG4418
ATOM	4418	O	LEU	548	114.171	21.814	28.723	1.00160.40	1SG4419
ATOM	4419	N	SER	549	114.844	23.649	27.581	1.00 38.99	1SG4420
ATOM	4420	CA	SER	549	116.232	23.343	27.735	1.00 38.99	1SG4421
ATOM	4421	CB	SER	549	117.165	24.278	26.946	1.00 38.99	1SG4422
ATOM	4422	OG	SER	549	116.955	24.111	25.551	1.00 38.99	1SG4423
ATOM	4423	C	SER	549	116.563	23.474	29.181	1.00 38.99	1SG4424
ATOM	4424	O	SER	549	115.869	24.151	29.938	1.00 38.99	1SG4425
ATOM	4425	N	CYS	550	117.652	22.803	29.590	1.00 42.14	1SG4426
ATOM	4426	CA	CYS	550	118.077	22.784	30.955	1.00 42.14	1SG4427
ATOM	4427	CB	CYS	550	119.287	21.868	31.193	1.00 42.14	1SG4428
ATOM	4428	SG	CYS	550	119.786	21.824	32.938	1.00 42.14	1SG4429
ATOM	4429	C	CYS	550	118.467	24.174	31.329	1.00 42.14	1SG4430
ATOM	4430	O	CYS	550	118.318	24.583	32.478	1.00 42.14	1SG4431
ATOM	4431	N	LYS	551	118.956	24.945	30.344	1.00 86.04	1SG4432
ATOM	4432	CA	LYS	551	119.442	26.270	30.584	1.00 86.04	1SG4433
ATOM	4433	CB	LYS	551	119.846	26.954	29.270	1.00 86.04	1SG4434
ATOM	4434	CG	LYS	551	120.724	28.193	29.430	1.00 86.04	1SG4435
ATOM	4435	CD	LYS	551	121.406	28.582	28.117	1.00 86.04	1SG4436
ATOM	4436	CE	LYS	551	122.295	27.468	27.557	1.00 86.04	1SG4437
ATOM	4437	NZ	LYS	551	122.701	27.784	26.170	1.00 86.04	1SG4438
ATOM	4438	C	LYS	551	118.338	27.064	31.215	1.00 86.04	1SG4439
ATOM	4439	O	LYS	551	118.576	27.866	32.117	1.00 86.04	1SG4440
ATOM	4440	N	LYS	552	117.100	26.873	30.730	1.00128.18	1SG4441
ATOM	4441	CA	LYS	552	115.928	27.534	31.237	1.00128.18	1SG4442
ATOM	4442	CB	LYS	552	114.714	27.395	30.306	1.00128.18	1SG4443
ATOM	4443	CG	LYS	552	114.818	28.305	29.083	1.00128.18	1SG4444
ATOM	4444	CD	LYS	552	115.977	27.953	28.149	1.00128.18	1SG4445
ATOM	4445	CE	LYS	552	116.139	28.944	26.996	1.00128.18	1SG4446
ATOM	4446	NZ	LYS	552	116.497	30.277	27.531	1.00128.18	1SG4447
ATOM	4447	C	LYS	552	115.558	27.016	32.601	1.00128.18	1SG4448
ATOM	4448	O	LYS	552	114.924	27.713	33.389	1.00128.18	1SG4449
ATOM	4449	N	TYR	553	115.924	25.757	32.894	1.00104.75	1SG4450
ATOM	4450	CA	TYR	553	115.626	25.040	34.108	1.00104.75	1SG4451
ATOM	4451	CB	TYR	553	115.957	23.538	34.054	1.00104.75	1SG4452
ATOM	4452	CG	TYR	553	114.745	22.848	33.530	1.00104.75	1SG4453
ATOM	4453	CD1	TYR	553	113.721	22.587	34.407	1.00104.75	1SG4454
ATOM	4454	CD2	TYR	553	114.609	22.461	32.215	1.00104.75	1SG4455
ATOM	4455	CE1	TYR	553	112.579	21.954	33.991	1.00104.75	1SG4456
ATOM	4456	CE2	TYR	553	113.462	21.823	31.792	1.00104.75	1SG4457
ATOM	4457	CZ	TYR	553	112.444	21.569	32.683	1.00104.75	1SG4458
ATOM	4458	OH	TYR	553	111.262	20.917	32.274	1.00104.75	1SG4459
ATOM	4459	C	TYR	553	116.260	25.608	35.333	1.00104.75	1SG4460
ATOM	4460	O	TYR	553	115.803	25.328	36.437	1.00104.75	1SG4461
ATOM	4461	N	SER	554	117.350	26.372	35.185	1.00114.08	1SG4462
ATOM	4462	CA	SER	554	118.150	26.852	36.279	1.00114.08	1SG4463
ATOM	4463	CB	SER	554	119.351	27.685	35.798	1.00114.08	1SG4464
ATOM	4464	OG	SER	554	120.233	26.869	35.043	1.00114.08	1SG4465
ATOM	4465	C	SER	554	117.380	27.707	37.297	1.00114.08	1SG4466
ATOM	4466	O	SER	554	118.022	28.303	38.159	1.00114.08	1SG4467
ATOM	4467	N	PHE	555	116.012	27.766	37.279	1.00192.56	1SG4468
ATOM	4468	CA	PHE	555	115.147	28.405	38.251	1.00192.56	1SG4469
ATOM	4469	CB	PHE	555	113.659	28.371	37.923	1.00192.56	1SG4470
ATOM	4470	CG	PHE	555	113.216	29.534	38.723	1.00192.56	1SG4471
ATOM	4471	CD1	PHE	555	113.439	30.811	38.270	1.00192.56	1SG4472

Supplementary material 1.txt

ATOM	4472	CD2	PHE	555	112.631	29.361	39.942	1.00192.56	1SG4473
ATOM	4473	CE1	PHE	555	113.037	31.897	39.007	1.00192.56	1SG4474
ATOM	4474	CE2	PHE	555	112.224	30.438	40.686	1.00192.56	1SG4475
ATOM	4475	CZ	PHE	555	112.429	31.711	40.220	1.00192.56	1SG4476
ATOM	4476	C	PHE	555	115.423	27.725	39.565	1.00192.56	1SG4477
ATOM	4477	O	PHE	555	115.009	28.174	40.634	1.00192.56	1SG4478
ATOM	4478	N	HIS	556	116.085	26.556	39.488	1.00 62.87	1SG4479
ATOM	4479	CA	HIS	556	116.555	25.836	40.629	1.00 62.87	1SG4480
ATOM	4480	ND1	HIS	556	116.719	22.649	41.703	1.00 62.87	1SG4481
ATOM	4481	CG	HIS	556	117.598	23.658	41.382	1.00 62.87	1SG4482
ATOM	4482	CB	HIS	556	117.389	24.606	40.241	1.00 62.87	1SG4483
ATOM	4483	NE2	HIS	556	118.384	22.530	43.171	1.00 62.87	1SG4484
ATOM	4484	CD2	HIS	556	118.608	23.573	42.288	1.00 62.87	1SG4485
ATOM	4485	CE1	HIS	556	117.237	22.006	42.779	1.00 62.87	1SG4486
ATOM	4486	C	HIS	556	117.443	26.769	41.400	1.00 62.87	1SG4487
ATOM	4487	O	HIS	556	117.467	26.740	42.629	1.00 62.87	1SG4488
ATOM	4488	N	VAL	557	118.195	27.633	40.691	1.00 63.77	1SG4489
ATOM	4489	CA	VAL	557	119.066	28.591	41.308	1.00 63.77	1SG4490
ATOM	4490	CB	VAL	557	119.619	29.556	40.330	1.00 63.77	1SG4491
ATOM	4491	CG1	VAL	557	120.130	30.722	41.173	1.00 63.77	1SG4492
ATOM	4492	CG2	VAL	557	120.681	28.868	39.456	1.00 63.77	1SG4493
ATOM	4493	C	VAL	557	118.296	29.458	42.249	1.00 63.77	1SG4494
ATOM	4494	O	VAL	557	118.756	29.738	43.354	1.00 63.77	1SG4495
ATOM	4495	N	LEU	558	117.106	29.926	41.833	1.00100.28	1SG4496
ATOM	4496	CA	LEU	558	116.376	30.811	42.692	1.00100.28	1SG4497
ATOM	4497	CB	LEU	558	115.146	31.488	42.059	1.00100.28	1SG4498
ATOM	4498	CG	LEU	558	115.554	32.507	40.972	1.00100.28	1SG4499
ATOM	4499	CD2	LEU	558	114.546	33.656	40.833	1.00100.28	1SG4500
ATOM	4500	CD1	LEU	558	115.916	31.813	39.650	1.00100.28	1SG4501
ATOM	4501	C	LEU	558	116.005	30.087	43.947	1.00100.28	1SG4502
ATOM	4502	O	LEU	558	115.953	30.689	45.017	1.00100.28	1SG4503
ATOM	4503	N	ALA	559	115.716	28.777	43.849	1.00 33.48	1SG4504
ATOM	4504	CA	ALA	559	115.397	27.999	45.013	1.00 33.48	1SG4505
ATOM	4505	CB	ALA	559	115.021	26.546	44.678	1.00 33.48	1SG4506
ATOM	4506	C	ALA	559	116.600	27.956	45.910	1.00 33.48	1SG4507
ATOM	4507	O	ALA	559	116.478	28.009	47.132	1.00 33.48	1SG4508
ATOM	4508	N	ARG	560	117.805	27.838	45.321	1.00 53.84	1SG4509
ATOM	4509	CA	ARG	560	119.023	27.733	46.078	1.00 53.84	1SG4510
ATOM	4510	CB	ARG	560	120.253	27.498	45.185	1.00 53.84	1SG4511
ATOM	4511	CG	ARG	560	120.195	26.170	44.429	1.00 53.84	1SG4512
ATOM	4512	CD	ARG	560	121.466	25.851	43.641	1.00 53.84	1SG4513
ATOM	4513	NE	ARG	560	121.261	24.529	42.986	1.00 53.84	1SG4514
ATOM	4514	CZ	ARG	560	122.330	23.798	42.558	1.00 53.84	1SG4515
ATOM	4515	NH1	ARG	560	123.597	24.266	42.749	1.00 53.84	1SG4516
ATOM	4516	NH2	ARG	560	122.131	22.598	41.938	1.00 53.84	1SG4517
ATOM	4517	C	ARG	560	119.272	28.992	46.853	1.00 53.84	1SG4518
ATOM	4518	O	ARG	560	119.708	28.945	48.002	1.00 53.84	1SG4519
ATOM	4519	N	SER	561	119.002	30.155	46.235	1.00 75.82	1SG4520
ATOM	4520	CA	SER	561	119.279	31.430	46.837	1.00 75.82	1SG4521
ATOM	4521	CB	SER	561	118.935	32.596	45.896	1.00 75.82	1SG4522
ATOM	4522	OG	SER	561	119.226	33.837	46.522	1.00 75.82	1SG4523
ATOM	4523	C	SER	561	118.487	31.611	48.100	1.00 75.82	1SG4524
ATOM	4524	O	SER	561	119.001	32.139	49.085	1.00 75.82	1SG4525
ATOM	4525	N	ILE	562	117.209	31.189	48.108	1.00120.19	1SG4526
ATOM	4526	CA	ILE	562	116.374	31.369	49.265	1.00120.19	1SG4527
ATOM	4527	CB	ILE	562	114.933	30.980	49.026	1.00120.19	1SG4528
ATOM	4528	CG2	ILE	562	114.847	29.467	48.782	1.00120.19	1SG4529
ATOM	4529	CG1	ILE	562	114.040	31.468	50.176	1.00120.19	1SG4530
ATOM	4530	CD1	ILE	562	113.826	32.978	50.183	1.00120.19	1SG4531
ATOM	4531	C	ILE	562	116.908	30.557	50.406	1.00120.19	1SG4532
ATOM	4532	O	ILE	562	116.989	31.040	51.535	1.00120.19	1SG4533
ATOM	4533	N	GLN	563	117.317	29.303	50.133	1.00 72.51	1SG4534
ATOM	4534	CA	GLN	563	117.774	28.418	51.165	1.00 72.51	1SG4535
ATOM	4535	CB	GLN	563	118.210	27.053	50.604	1.00 72.51	1SG4536
ATOM	4536	CG	GLN	563	117.067	26.227	50.011	1.00 72.51	1SG4537
ATOM	4537	CD	GLN	563	116.368	25.509	51.156	1.00 72.51	1SG4538
ATOM	4538	OE1	GLN	563	116.948	24.638	51.802	1.00 72.51	1SG4539
ATOM	4539	NE2	GLN	563	115.086	25.880	51.417	1.00 72.51	1SG4540
ATOM	4540	C	GLN	563	118.980	29.010	51.824	1.00 72.51	1SG4541
ATOM	4541	O	GLN	563	119.087	29.012	53.050	1.00 72.51	1SG4542
ATOM	4542	N	PHE	564	119.922	29.535	51.021	1.00 53.81	1SG4543

Supplementary material 1.txt

ATOM	4543	CA	PHE	564	121.143	30.067	51.555	1.00	53.81	1SG4544
ATOM	4544	CB	PHE	564	122.165	30.452	50.472	1.00	53.81	1SG4545
ATOM	4545	CG	PHE	564	123.455	30.671	51.185	1.00	53.81	1SG4546
ATOM	4546	CD1	PHE	564	124.323	29.619	51.368	1.00	53.81	1SG4547
ATOM	4547	CD2	PHE	564	123.788	31.909	51.685	1.00	53.81	1SG4548
ATOM	4548	CE1	PHE	564	125.515	29.798	52.027	1.00	53.81	1SG4549
ATOM	4549	CE2	PHE	564	124.980	32.092	52.347	1.00	53.81	1SG4550
ATOM	4550	CZ	PHE	564	125.847	31.039	52.516	1.00	53.81	1SG4551
ATOM	4551	C	PHE	564	120.853	31.305	52.348	1.00	53.81	1SG4552
ATOM	4552	O	PHE	564	121.457	31.553	53.390	1.00	53.81	1SG4553
ATOM	4553	N	MET	565	119.920	32.125	51.837	1.00163.64		1SG4554
ATOM	4554	CA	MET	565	119.585	33.408	52.381	1.00163.64		1SG4555
ATOM	4555	CB	MET	565	118.544	34.139	51.510	1.00163.64		1SG4556
ATOM	4556	CG	MET	565	118.567	35.663	51.645	1.00163.64		1SG4557
ATOM	4557	SD	MET	565	119.823	36.498	50.620	1.00163.64		1SG4558
ATOM	4558	CE	MET	565	121.238	35.449	51.063	1.00163.64		1SG4559
ATOM	4559	C	MET	565	118.986	33.294	53.756	1.00163.64		1SG4560
ATOM	4560	O	MET	565	119.285	34.112	54.625	1.00163.64		1SG4561
ATOM	4561	N	TYR	566	118.127	32.285	54.021	1.00209.40		1SG4562
ATOM	4562	CA	TYR	566	117.446	32.351	55.287	1.00209.40		1SG4563
ATOM	4563	CB	TYR	566	115.931	32.113	55.173	1.00209.40		1SG4564
ATOM	4564	CG	TYR	566	115.311	33.277	54.480	1.00209.40		1SG4565
ATOM	4565	CD1	TYR	566	115.420	33.433	53.117	1.00209.40		1SG4566
ATOM	4566	CD2	TYR	566	114.601	34.210	55.201	1.00209.40		1SG4567
ATOM	4567	CE1	TYR	566	114.837	34.509	52.488	1.00209.40		1SG4568
ATOM	4568	CE2	TYR	566	114.016	35.286	54.577	1.00209.40		1SG4569
ATOM	4569	CZ	TYR	566	114.134	35.438	53.217	1.00209.40		1SG4570
ATOM	4570	OH	TYR	566	113.533	36.542	52.575	1.00209.40		1SG4571
ATOM	4571	C	TYR	566	117.945	31.362	56.296	1.00209.40		1SG4572
ATOM	4572	O	TYR	566	117.487	30.219	56.328	1.00209.40		1SG4573
ATOM	4573	N	ASN	567	118.870	31.802	57.183	1.00237.75		1SG4574
ATOM	4574	CA	ASN	567	119.239	30.985	58.303	1.00237.75		1SG4575
ATOM	4575	CB	ASN	567	120.669	31.248	58.831	1.00237.75		1SG4576
ATOM	4576	CG	ASN	567	120.857	32.688	59.310	1.00237.75		1SG4577
ATOM	4577	OD1	ASN	567	121.828	32.971	60.010	1.00237.75		1SG4578
ATOM	4578	ND2	ASN	567	119.929	33.613	58.946	1.00237.75		1SG4579
ATOM	4579	C	ASN	567	118.220	31.348	59.337	1.00237.75		1SG4580
ATOM	4580	O	ASN	567	118.516	31.825	60.432	1.00237.75		1SG4581
ATOM	4581	N	GLN	568	116.954	31.086	58.973	1.00131.74		1SG4582
ATOM	4582	CA	GLN	568	115.794	31.398	59.749	1.00131.74		1SG4583
ATOM	4583	CB	GLN	568	115.759	30.724	61.131	1.00131.74		1SG4584
ATOM	4584	CG	GLN	568	115.581	29.206	61.063	1.00131.74		1SG4585
ATOM	4585	CD	GLN	568	115.341	28.696	62.477	1.00131.74		1SG4586
ATOM	4586	OE1	GLN	568	116.120	28.953	63.393	1.00131.74		1SG4587
ATOM	4587	NE2	GLN	568	114.215	27.956	62.665	1.00131.74		1SG4588
ATOM	4588	C	GLN	568	115.696	32.877	59.947	1.00131.74		1SG4589
ATOM	4589	O	GLN	568	115.002	33.333	60.855	1.00131.74		1SG4590
ATOM	4590	N	GLY	569	116.336	33.675	59.068	1.00	32.43	1SG4591
ATOM	4591	CA	GLY	569	116.250	35.100	59.222	1.00	32.43	1SG4592
ATOM	4592	C	GLY	569	116.254	35.714	57.859	1.00	32.43	1SG4593
ATOM	4593	O	GLY	569	116.890	35.204	56.938	1.00	32.43	1SG4594
ATOM	4594	N	ASP	570	115.543	36.850	57.704	1.00	58.07	1SG4595
ATOM	4595	CA	ASP	570	115.471	37.496	56.424	1.00	58.07	1SG4596
ATOM	4596	CB	ASP	570	114.503	38.692	56.400	1.00	58.07	1SG4597
ATOM	4597	CG	ASP	570	114.402	39.196	54.967	1.00	58.07	1SG4598
ATOM	4598	OD1	ASP	570	114.853	38.465	54.046	1.00	58.07	1SG4599
ATOM	4599	OD2	ASP	570	113.873	40.319	54.769	1.00	58.07	1SG4600
ATOM	4600	C	ASP	570	116.833	38.019	56.084	1.00	58.07	1SG4601
ATOM	4601	O	ASP	570	117.262	39.045	56.605	1.00	58.07	1SG4602
ATOM	4602	N	GLY	571	117.541	37.324	55.175	1.00	41.99	1SG4603
ATOM	4603	CA	GLY	571	118.877	37.688	54.781	1.00	41.99	1SG4604
ATOM	4604	C	GLY	571	118.900	38.979	54.017	1.00	41.99	1SG4605
ATOM	4605	O	GLY	571	119.857	39.748	54.103	1.00	41.99	1SG4606
ATOM	4606	N	PHE	572	117.873	39.202	53.181	1.00129.00		1SG4607
ATOM	4607	CA	PHE	572	117.780	40.354	52.331	1.00129.00		1SG4608
ATOM	4608	CB	PHE	572	116.562	40.197	51.407	1.00129.00		1SG4609
ATOM	4609	CG	PHE	572	116.606	41.235	50.352	1.00129.00		1SG4610
ATOM	4610	CD1	PHE	572	116.022	42.461	50.558	1.00129.00		1SG4611
ATOM	4611	CD2	PHE	572	117.233	40.967	49.158	1.00129.00		1SG4612
ATOM	4612	CE1	PHE	572	116.064	43.415	49.574	1.00129.00		1SG4613
ATOM	4613	CE2	PHE	572	117.280	41.916	48.169	1.00129.00		1SG4614

Supplementary material 1.txt

ATOM	4614	CZ	PHE	572	116.692	43.137	48.384	1.00129.00	1SG4615
ATOM	4615	C	PHE	572	117.619	41.593	53.164	1.00129.00	1SG4616
ATOM	4616	O	PHE	572	118.315	42.588	52.962	1.00129.00	1SG4617
ATOM	4617	N	SER	573	116.676	41.559	54.123	1.00 97.24	1SG4618
ATOM	4618	CA	SER	573	116.426	42.680	54.984	1.00 97.24	1SG4619
ATOM	4619	CB	SER	573	115.188	42.465	55.865	1.00 97.24	1SG4620
ATOM	4620	OG	SER	573	114.974	43.597	56.691	1.00 97.24	1SG4621
ATOM	4621	C	SER	573	117.611	42.859	55.889	1.00 97.24	1SG4622
ATOM	4622	O	SER	573	118.064	43.984	56.097	1.00 97.24	1SG4623
ATOM	4623	N	ILE	574	118.125	41.753	56.477	1.00111.12	1SG4624
ATOM	4624	CA	ILE	574	119.297	41.865	57.303	1.00111.12	1SG4625
ATOM	4625	CB	ILE	574	119.101	41.397	58.728	1.00111.12	1SG4626
ATOM	4626	CG2	ILE	574	118.690	39.918	58.768	1.00111.12	1SG4627
ATOM	4627	CG1	ILE	574	120.346	41.723	59.564	1.00111.12	1SG4628
ATOM	4628	CD1	ILE	574	120.132	41.529	61.063	1.00111.12	1SG4629
ATOM	4629	C	ILE	574	120.408	41.103	56.637	1.00111.12	1SG4630
ATOM	4630	O	ILE	574	120.525	39.884	56.741	1.00111.12	1SG4631
ATOM	4631	N	SER	575	121.247	41.854	55.903	1.00 70.47	1SG4632
ATOM	4632	CA	SER	575	122.335	41.379	55.097	1.00 70.47	1SG4633
ATOM	4633	CB	SER	575	122.814	42.501	54.161	1.00 70.47	1SG4634
ATOM	4634	OG	SER	575	123.460	43.515	54.912	1.00 70.47	1SG4635
ATOM	4635	C	SER	575	123.535	40.957	55.893	1.00 70.47	1SG4636
ATOM	4636	O	SER	575	124.119	39.906	55.635	1.00 70.47	1SG4637
ATOM	4637	N	ASN	576	123.901	41.737	56.926	1.00107.67	1SG4638
ATOM	4638	CA	ASN	576	125.191	41.592	57.547	1.00107.67	1SG4639
ATOM	4639	CB	ASN	576	125.407	42.553	58.732	1.00107.67	1SG4640
ATOM	4640	CG	ASN	576	124.399	42.229	59.824	1.00107.67	1SG4641
ATOM	4641	OD1	ASN	576	124.762	41.730	60.888	1.00107.67	1SG4642
ATOM	4642	ND2	ASN	576	123.098	42.524	59.562	1.00107.67	1SG4643
ATOM	4643	C	ASN	576	125.452	40.198	58.029	1.00107.67	1SG4644
ATOM	4644	O	ASN	576	126.561	39.691	57.864	1.00107.67	1SG4645
ATOM	4645	N	LYS	577	124.460	39.542	58.647	1.00 77.87	1SG4646
ATOM	4646	CA	LYS	577	124.677	38.235	59.199	1.00 77.87	1SG4647
ATOM	4647	CB	LYS	577	123.477	37.726	60.016	1.00 77.87	1SG4648
ATOM	4648	CG	LYS	577	123.292	38.465	61.341	1.00 77.87	1SG4649
ATOM	4649	CD	LYS	577	121.960	38.170	62.034	1.00 77.87	1SG4650
ATOM	4650	CE	LYS	577	121.839	38.827	63.410	1.00 77.87	1SG4651
ATOM	4651	NZ	LYS	577	122.823	38.231	64.341	1.00 77.87	1SG4652
ATOM	4652	C	LYS	577	124.960	37.206	58.143	1.00 77.87	1SG4653
ATOM	4653	O	LYS	577	125.827	36.355	58.334	1.00 77.87	1SG4654
ATOM	4654	N	VAL	578	124.260	37.255	56.991	1.00100.62	1SG4655
ATOM	4655	CA	VAL	578	124.384	36.174	56.053	1.00100.62	1SG4656
ATOM	4656	CB	VAL	578	123.056	35.582	55.683	1.00100.62	1SG4657
ATOM	4657	CG1	VAL	578	123.284	34.473	54.641	1.00100.62	1SG4658
ATOM	4658	CG2	VAL	578	122.360	35.102	56.968	1.00100.62	1SG4659
ATOM	4659	C	VAL	578	125.013	36.637	54.776	1.00100.62	1SG4660
ATOM	4660	O	VAL	578	126.086	36.165	54.408	1.00100.62	1SG4661
ATOM	4661	N	ILE	579	124.347	37.561	54.056	1.00171.99	1SG4662
ATOM	4662	CA	ILE	579	124.790	37.968	52.751	1.00171.99	1SG4663
ATOM	4663	CB	ILE	579	123.809	38.794	51.962	1.00171.99	1SG4664
ATOM	4664	CG2	ILE	579	122.518	37.976	51.847	1.00171.99	1SG4665
ATOM	4665	CG1	ILE	579	123.576	40.171	52.572	1.00171.99	1SG4666
ATOM	4666	CD1	ILE	579	124.687	41.187	52.303	1.00171.99	1SG4667
ATOM	4667	C	ILE	579	126.118	38.663	52.772	1.00171.99	1SG4668
ATOM	4668	O	ILE	579	126.871	38.560	51.807	1.00171.99	1SG4669
ATOM	4669	N	LYS	580	126.443	39.406	53.846	1.00 86.75	1SG4670
ATOM	4670	CA	LYS	580	127.645	40.201	53.881	1.00 86.75	1SG4671
ATOM	4671	CB	LYS	580	127.898	40.801	55.274	1.00 86.75	1SG4672
ATOM	4672	CG	LYS	580	129.163	41.654	55.364	1.00 86.75	1SG4673
ATOM	4673	CD	LYS	580	129.301	42.385	56.700	1.00 86.75	1SG4674
ATOM	4674	CE	LYS	580	129.312	41.438	57.903	1.00 86.75	1SG4675
ATOM	4675	NZ	LYS	580	129.591	42.192	59.145	1.00 86.75	1SG4676
ATOM	4676	C	LYS	580	128.856	39.368	53.567	1.00 86.75	1SG4677
ATOM	4677	O	LYS	580	129.667	39.746	52.723	1.00 86.75	1SG4678
ATOM	4678	N	ASP	581	129.013	38.199	54.211	1.00 33.47	1SG4679
ATOM	4679	CA	ASP	581	130.197	37.414	53.994	1.00 33.47	1SG4680
ATOM	4680	CB	ASP	581	130.222	36.136	54.849	1.00 33.47	1SG4681
ATOM	4681	CG	ASP	581	130.425	36.546	56.301	1.00 33.47	1SG4682
ATOM	4682	OD1	ASP	581	131.324	37.392	56.557	1.00 33.47	1SG4683
ATOM	4683	OD2	ASP	581	129.690	36.013	57.174	1.00 33.47	1SG4684
ATOM	4684	C	ASP	581	130.265	36.988	52.560	1.00 33.47	1SG4685

Supplementary material 1.txt

ATOM	4685	O	ASP	581	131.326	37.035	51.939	1.00	33.47	1SG4686
ATOM	4686	N	GLN	582	129.124	36.568	51.986	1.00	37.94	1SG4687
ATOM	4687	CA	GLN	582	129.139	36.078	50.639	1.00	37.94	1SG4688
ATOM	4688	CB	GLN	582	127.775	35.561	50.153	1.00	37.94	1SG4689
ATOM	4689	CG	GLN	582	127.303	34.292	50.861	1.00	37.94	1SG4690
ATOM	4690	CD	GLN	582	125.978	33.892	50.231	1.00	37.94	1SG4691
ATOM	4691	OE1	GLN	582	125.024	34.667	50.200	1.00	37.94	1SG4692
ATOM	4692	NE2	GLN	582	125.921	32.643	49.695	1.00	37.94	1SG4693
ATOM	4693	C	GLN	582	129.539	37.168	49.697	1.00	37.94	1SG4694
ATOM	4694	O	GLN	582	130.323	36.939	48.778	1.00	37.94	1SG4695
ATOM	4695	N	VAL	583	129.016	38.391	49.902	1.00	100.74	1SG4696
ATOM	4696	CA	VAL	583	129.314	39.447	48.981	1.00	100.74	1SG4697
ATOM	4697	CB	VAL	583	128.585	40.734	49.248	1.00	100.74	1SG4698
ATOM	4698	CG1	VAL	583	127.071	40.461	49.199	1.00	100.74	1SG4699
ATOM	4699	CG2	VAL	583	129.085	41.331	50.566	1.00	100.74	1SG4700
ATOM	4700	C	VAL	583	130.781	39.731	49.024	1.00	100.74	1SG4701
ATOM	4701	O	VAL	583	131.395	39.967	47.987	1.00	100.74	1SG4702
ATOM	4702	N	GLN	584	131.389	39.737	50.225	1.00	126.07	1SG4703
ATOM	4703	CA	GLN	584	132.792	40.011	50.326	1.00	126.07	1SG4704
ATOM	4704	CB	GLN	584	133.230	40.259	51.784	1.00	126.07	1SG4705
ATOM	4705	CG	GLN	584	132.848	39.158	52.776	1.00	126.07	1SG4706
ATOM	4706	CD	GLN	584	134.020	38.220	52.994	1.00	126.07	1SG4707
ATOM	4707	OE1	GLN	584	134.951	38.149	52.194	1.00	126.07	1SG4708
ATOM	4708	NE2	GLN	584	133.976	37.481	54.135	1.00	126.07	1SG4709
ATOM	4709	C	GLN	584	133.586	38.921	49.668	1.00	126.07	1SG4710
ATOM	4710	O	GLN	584	134.542	39.186	48.942	1.00	126.07	1SG4711
ATOM	4711	N	LYS	585	133.197	37.654	49.872	1.00	133.18	1SG4712
ATOM	4712	CA	LYS	585	133.941	36.589	49.268	1.00	133.18	1SG4713
ATOM	4713	CB	LYS	585	133.404	35.201	49.660	1.00	133.18	1SG4714
ATOM	4714	CG	LYS	585	133.644	34.809	51.122	1.00	133.18	1SG4715
ATOM	4715	CD	LYS	585	135.127	34.716	51.494	1.00	133.18	1SG4716
ATOM	4716	CE	LYS	585	135.392	34.027	52.836	1.00	133.18	1SG4717
ATOM	4717	NZ	LYS	585	134.729	34.766	53.932	1.00	133.18	1SG4718
ATOM	4718	C	LYS	585	133.842	36.684	47.770	1.00	133.18	1SG4719
ATOM	4719	O	LYS	585	134.823	36.439	47.071	1.00	133.18	1SG4720
ATOM	4720	N	VAL	586	132.628	36.935	47.234	1.00	83.39	1SG4721
ATOM	4721	CA	VAL	586	132.427	37.003	45.809	1.00	83.39	1SG4722
ATOM	4722	CB	VAL	586	130.989	36.797	45.438	1.00	83.39	1SG4723
ATOM	4723	CG1	VAL	586	130.846	36.960	43.916	1.00	83.39	1SG4724
ATOM	4724	CG2	VAL	586	130.541	35.424	45.969	1.00	83.39	1SG4725
ATOM	4725	C	VAL	586	132.862	38.288	45.143	1.00	83.39	1SG4726
ATOM	4726	O	VAL	586	133.593	38.275	44.154	1.00	83.39	1SG4727
ATOM	4727	N	LEU	587	132.303	39.428	45.598	1.00	155.96	1SG4728
ATOM	4728	CA	LEU	587	132.535	40.734	45.036	1.00	155.96	1SG4729
ATOM	4729	CB	LEU	587	131.359	41.685	45.310	1.00	155.96	1SG4730
ATOM	4730	CG	LEU	587	130.113	41.386	44.455	1.00	155.96	1SG4731
ATOM	4731	CD2	LEU	587	129.716	39.903	44.519	1.00	155.96	1SG4732
ATOM	4732	CD1	LEU	587	130.312	41.861	43.010	1.00	155.96	1SG4733
ATOM	4733	C	LEU	587	133.789	41.454	45.454	1.00	155.96	1SG4734
ATOM	4734	O	LEU	587	134.432	42.087	44.619	1.00	155.96	1SG4735
ATOM	4735	N	ILE	588	134.095	41.513	46.770	1.00	165.01	1SG4736
ATOM	4736	CA	ILE	588	135.243	42.285	47.172	1.00	165.01	1SG4737
ATOM	4737	CB	ILE	588	135.140	42.870	48.559	1.00	165.01	1SG4738
ATOM	4738	CG2	ILE	588	135.201	41.754	49.610	1.00	165.01	1SG4739
ATOM	4739	CG1	ILE	588	136.231	43.936	48.745	1.00	165.01	1SG4740
ATOM	4740	CD1	ILE	588	136.039	45.160	47.851	1.00	165.01	1SG4741
ATOM	4741	C	ILE	588	136.574	41.602	47.042	1.00	165.01	1SG4742
ATOM	4742	O	ILE	588	137.464	42.097	46.353	1.00	165.01	1SG4743
ATOM	4743	N	VAL	589	136.734	40.411	47.656	1.00	116.04	1SG4744
ATOM	4744	CA	VAL	589	138.051	39.842	47.731	1.00	116.04	1SG4745
ATOM	4745	CB	VAL	589	138.347	39.204	49.053	1.00	116.04	1SG4746
ATOM	4746	CG1	VAL	589	137.385	38.020	49.245	1.00	116.04	1SG4747
ATOM	4747	CG2	VAL	589	139.832	38.805	49.078	1.00	116.04	1SG4748
ATOM	4748	C	VAL	589	138.234	38.792	46.691	1.00	116.04	1SG4749
ATOM	4749	O	VAL	589	137.397	37.916	46.482	1.00	116.04	1SG4750
ATOM	4750	N	PRO	590	139.348	38.924	46.023	1.00	151.86	1SG4751
ATOM	4751	CA	PRO	590	139.711	37.956	45.023	1.00	151.86	1SG4752
ATOM	4752	CD	PRO	590	139.758	40.267	45.642	1.00	151.86	1SG4753
ATOM	4753	CB	PRO	590	140.630	38.678	44.039	1.00	151.86	1SG4754
ATOM	4754	CG	PRO	590	140.242	40.157	44.190	1.00	151.86	1SG4755
ATOM	4755	C	PRO	590	140.372	36.774	45.659	1.00	151.86	1SG4756

					Supplementary material 1.txt				
ATOM	4756	O	PRO	590	140.815	36.879	46.801	1.00151.86	1SG4757
ATOM	4757	N	VAL	591	140.448	35.640	44.934	1.00123.05	1SG4758
ATOM	4758	CA	VAL	591	141.117	34.483	45.443	1.00123.05	1SG4759
ATOM	4759	CB	VAL	591	140.907	33.264	44.587	1.00123.05	1SG4760
ATOM	4760	CG1	VAL	591	139.405	32.937	44.566	1.00123.05	1SG4761
ATOM	4761	CG2	VAL	591	141.507	33.503	43.192	1.00123.05	1SG4762
ATOM	4762	C	VAL	591	142.568	34.826	45.420	1.00123.05	1SG4763
ATOM	4763	O	VAL	591	143.086	35.362	44.441	1.00123.05	1SG4764
ATOM	4764	N	PRO	592	143.220	34.499	46.499	1.00211.18	1SG4765
ATOM	4765	CA	PRO	592	144.594	34.865	46.697	1.00211.18	1SG4766
ATOM	4766	CD	PRO	592	142.518	34.305	47.758	1.00211.18	1SG4767
ATOM	4767	CB	PRO	592	144.914	34.496	48.144	1.00211.18	1SG4768
ATOM	4768	CG	PRO	592	143.551	34.616	48.854	1.00211.18	1SG4769
ATOM	4769	C	PRO	592	145.552	34.317	45.698	1.00211.18	1SG4770
ATOM	4770	O	PRO	592	146.583	34.951	45.492	1.00211.18	1SG4771
ATOM	4771	N	ILE	593	145.249	33.156	45.087	1.00110.67	1SG4772
ATOM	4772	CA	ILE	593	146.093	32.566	44.087	1.00110.67	1SG4773
ATOM	4773	CB	ILE	593	145.885	33.183	42.726	1.00110.67	1SG4774
ATOM	4774	CG2	ILE	593	146.198	34.686	42.795	1.00110.67	1SG4775
ATOM	4775	CG1	ILE	593	146.673	32.422	41.650	1.00110.67	1SG4776
ATOM	4776	CD1	ILE	593	146.319	32.853	40.227	1.00110.67	1SG4777
ATOM	4777	C	ILE	593	147.570	32.631	44.462	1.00110.67	1SG4778
ATOM	4778	O	ILE	593	147.935	32.068	45.529	1.00110.67	1SG4779
ATOM	4779	OXT	ILE	593	148.353	33.240	43.685	1.00110.67	1SG4780
END									