

# Documentation of MULTICOM

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MULTICOM is a Protein Tertiary Structure Predictor Using Multi-Template Combination.

MULTICOM was ranked among the best protein tertiary structure predictors during the 8th and 9th Critical Assessments of Techniques for Protein Structure Prediction (CASP8,9) in 2008 and 2010, respectively.

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There is an example for Protein Tertiary Structure Prediction using MULTICOM.

## **Input sequence:**

MNLRWTSEAKTKLKNIPFFARSQAKARIEQLARQAEQDIVTPELVEQARLEFGQ

## **Prediction results:**

Protein template structures (PDB code + chain id) used to generate the model and the e-values of their alignments with the target (smaller, more significant):

2KRUA 2.1e-28

2L09A 1.2e-23

PFRMAT TS

TARGET query

AUTHOR MULTICOM

METHOD Z. Wang, J. Eickholt and J. Cheng. MULTICOM: a multi-level combination METHOD approach to protein structure prediction and its assessment in CASP8.

METHOD Bioinformatics. 26(7):882-888, 2010.

MODEL 1

PDB TEMPLATE PARENT 2KRUA 2L09A

ATOM	1	N	MET	1	8.270	-12.198	0.663	1.00	81.71	1SG	2
ATOM	2	CA	MET	1	8.403	-10.771	1.037	1.00	81.71	1SG	3
ATOM	3	CB	MET	1	9.815	-10.263	0.720	1.00	81.71	1SG	4
ATOM	4	CG	MET	1	10.901	-10.971	1.530	1.00	81.71	1SG	5
ATOM	5	SD	MET	1	10.775	-10.723	3.327	1.00	81.71	1SG	6
ATOM	6	CE	MET	1	9.415	-11.901	3.573	1.00	81.71	1SG	7
ATOM	7	C	MET	1	7.411	-9.953	0.280	1.00	81.71	1SG	8
ATOM	8	O	MET	1	6.475	-9.411	0.864	1.00	81.71	1SG	9
ATOM	9	N	ASN	2	7.590	-9.841	-1.051	1.00	57.13	1SG	10
ATOM	10	CA	ASN	2	6.662	-9.067	-1.819	1.00	57.13	1SG	11
ATOM	11	CB	ASN	2	7.267	-8.427	-3.080	1.00	57.13	1SG	12

ATOM	12	CG	ASN	2	7.727	-9.548	-3.998	1.00	57.13	1SG	13
ATOM	13	OD1	ASN	2	6.948	-10.114	-4.764	1.00	57.13	1SG	14
ATOM	14	ND2	ASN	2	9.043	-9.877	-3.922	1.00	57.13	1SG	15
ATOM	15	C	ASN	2	5.548	-9.966	-2.250	1.00	57.13	1SG	16
ATOM	16	O	ASN	2	5.727	-11.170	-2.421	1.00	57.13	1SG	17
ATOM	17	N	LEU	3	4.342	-9.389	-2.394	1.00103.48		1SG	18
ATOM	18	CA	LEU	3	3.196	-10.139	-2.816	1.00103.48		1SG	19
ATOM	19	CB	LEU	3	1.847	-9.555	-2.344	1.00103.48		1SG	20
ATOM	20	CG	LEU	3	1.619	-9.638	-0.818	1.00103.48		1SG	21
ATOM	21	CD1	LEU	3	2.594	-8.748	-0.032	1.00103.48		1SG	22
ATOM	22	CD2	LEU	3	0.149	-9.369	-0.462	1.00103.48		1SG	23
ATOM	23	C	LEU	3	3.183	-10.166	-4.308	1.00103.48		1SG	24
ATOM	24	O	LEU	3	3.974	-9.489	-4.962	1.00103.48		1SG	25
ATOM	25	N	ARG	4	2.293	-11.000	-4.883	1.00115.69		1SG	26
ATOM	26	CA	ARG	4	2.209	-11.089	-6.309	1.00115.69		1SG	27
ATOM	27	CB	ARG	4	1.456	-12.330	-6.808	1.00115.69		1SG	28
ATOM	28	CG	ARG	4	2.150	-13.653	-6.503	1.00115.69		1SG	29
ATOM	29	CD	ARG	4	1.521	-14.816	-7.267	1.00115.69		1SG	30
ATOM	30	NE	ARG	4	1.709	-14.526	-8.716	1.00115.69		1SG	31
ATOM	31	CZ	ARG	4	1.302	-15.427	-9.658	1.00115.69		1SG	32
ATOM	32	NH1	ARG	4	0.704	-16.591	-9.272	1.00115.69		1SG	33
ATOM	33	NH2	ARG	4	1.493	-15.163	-10.983	1.00115.69		1SG	34
ATOM	34	C	ARG	4	1.449	-9.904	-6.807	1.00115.69		1SG	35
ATOM	35	O	ARG	4	0.365	-9.587	-6.320	1.00115.69		1SG	36
ATOM	36	N	TRP	5	2.004	-9.222	-7.822	1.00	74.37	1SG	37
ATOM	37	CA	TRP	5	1.347	-8.076	-8.371	1.00	74.37	1SG	38
ATOM	38	CB	TRP	5	2.281	-6.866	-8.542	1.00	74.37	1SG	39
ATOM	39	CG	TRP	5	2.658	-6.190	-7.250	1.00	74.37	1SG	40
ATOM	40	CD2	TRP	5	2.194	-4.883	-6.870	1.00	74.37	1SG	41
ATOM	41	CD1	TRP	5	3.480	-6.616	-6.248	1.00	74.37	1SG	42
ATOM	42	NE1	TRP	5	3.546	-5.662	-5.262	1.00	74.37	1SG	43
ATOM	43	CE2	TRP	5	2.764	-4.589	-5.634	1.00	74.37	1SG	44
ATOM	44	CE3	TRP	5	1.365	-4.004	-7.503	1.00	74.37	1SG	45
ATOM	45	CZ2	TRP	5	2.513	-3.401	-5.008	1.00	74.37	1SG	46
ATOM	46	CZ3	TRP	5	1.114	-2.808	-6.869	1.00	74.37	1SG	47
ATOM	47	CH2	TRP	5	1.676	-2.513	-5.645	1.00	74.37	1SG	48
ATOM	48	C	TRP	5	0.846	-8.448	-9.726	1.00	74.37	1SG	49
ATOM	49	O	TRP	5	1.568	-9.032	-10.533	1.00	74.37	1SG	50

ATOM	50	N	THR	6	-0.428	-8.111	-10.001	1.00	41.19	1SG	51
ATOM	51	CA	THR	6	-1.024	-8.405	-11.269	1.00	41.19	1SG	52
ATOM	52	CB	THR	6	-2.522	-8.439	-11.216	1.00	41.19	1SG	53
ATOM	53	OG1	THR	6	-3.021	-7.200	-10.736	1.00	41.19	1SG	54
ATOM	54	CG2	THR	6	-2.955	-9.585	-10.286	1.00	41.19	1SG	55
ATOM	55	C	THR	6	-0.595	-7.352	-12.241	1.00	41.19	1SG	56
ATOM	56	O	THR	6	-0.089	-6.298	-11.860	1.00	41.19	1SG	57
ATOM	57	N	SER	7	-0.784	-7.630	-13.544	1.00	27.55	1SG	58
ATOM	58	CA	SER	7	-0.347	-6.728	-14.569	1.00	27.55	1SG	59
ATOM	59	CB	SER	7	-0.626	-7.264	-15.982	1.00	27.55	1SG	60
ATOM	60	OG	SER	7	0.114	-8.456	-16.199	1.00	27.55	1SG	61
ATOM	61	C	SER	7	-1.078	-5.435	-14.419	1.00	27.55	1SG	62
ATOM	62	O	SER	7	-0.504	-4.362	-14.595	1.00	27.55	1SG	63
ATOM	63	N	GLU	8	-2.380	-5.507	-14.094	1.00	115.66	1SG	64
ATOM	64	CA	GLU	8	-3.151	-4.313	-13.932	1.00	115.66	1SG	65
ATOM	65	CB	GLU	8	-4.669	-4.570	-13.820	1.00	115.66	1SG	66
ATOM	66	CG	GLU	8	-5.082	-5.675	-12.845	1.00	115.66	1SG	67
ATOM	67	CD	GLU	8	-5.233	-6.969	-13.638	1.00	115.66	1SG	68
ATOM	68	OE1	GLU	8	-4.789	-6.991	-14.816	1.00	115.66	1SG	69
ATOM	69	OE2	GLU	8	-5.799	-7.946	-13.077	1.00	115.66	1SG	70
ATOM	70	C	GLU	8	-2.659	-3.555	-12.737	1.00	115.66	1SG	71
ATOM	71	O	GLU	8	-2.592	-2.327	-12.768	1.00	115.66	1SG	72
ATOM	72	N	ALA	9	-2.290	-4.268	-11.655	1.00	32.12	1SG	73
ATOM	73	CA	ALA	9	-1.821	-3.631	-10.456	1.00	32.12	1SG	74
ATOM	74	CB	ALA	9	-1.507	-4.634	-9.332	1.00	32.12	1SG	75
ATOM	75	C	ALA	9	-0.557	-2.890	-10.759	1.00	32.12	1SG	76
ATOM	76	O	ALA	9	-0.349	-1.775	-10.282	1.00	32.12	1SG	77
ATOM	77	N	LYS	10	0.321	-3.492	-11.579	1.00	109.02	1SG	78
ATOM	78	CA	LYS	10	1.573	-2.870	-11.899	1.00	109.02	1SG	79
ATOM	79	CB	LYS	10	2.401	-3.681	-12.908	1.00	109.02	1SG	80
ATOM	80	CG	LYS	10	2.945	-4.989	-12.337	1.00	109.02	1SG	81
ATOM	81	CD	LYS	10	3.936	-4.782	-11.190	1.00	109.02	1SG	82
ATOM	82	CE	LYS	10	4.442	-6.091	-10.578	1.00	109.02	1SG	83
ATOM	83	NZ	LYS	10	5.151	-6.892	-11.601	1.00	109.02	1SG	84
ATOM	84	C	LYS	10	1.292	-1.559	-12.559	1.00	109.02	1SG	85
ATOM	85	O	LYS	10	1.935	-0.553	-12.260	1.00	109.02	1SG	86
ATOM	86	N	THR	11	0.309	-1.537	-13.477	1.00	23.72	1SG	87
ATOM	87	CA	THR	11	0.000	-0.335	-14.197	1.00	23.72	1SG	88

ATOM	88	CB	THR	11	-1.120	-0.518	-15.179	1.00	23.72	1SG	89
ATOM	89	OG1	THR	11	-0.799	-1.535	-16.116	1.00	23.72	1SG	90
ATOM	90	CG2	THR	11	-1.356	0.814	-15.911	1.00	23.72	1SG	91
ATOM	91	C	THR	11	-0.455	0.694	-13.215	1.00	23.72	1SG	92
ATOM	92	O	THR	11	-0.068	1.859	-13.297	1.00	23.72	1SG	93
ATOM	93	N	LYS	12	-1.293	0.275	-12.250	1.00	90.89	1SG	94
ATOM	94	CA	LYS	12	-1.833	1.180	-11.278	1.00	90.89	1SG	95
ATOM	95	CB	LYS	12	-2.806	0.505	-10.295	1.00	90.89	1SG	96
ATOM	96	CG	LYS	12	-4.090	-0.010	-10.946	1.00	90.89	1SG	97
ATOM	97	CD	LYS	12	-4.922	1.083	-11.619	1.00	90.89	1SG	98
ATOM	98	CE	LYS	12	-6.219	0.561	-12.239	1.00	90.89	1SG	99
ATOM	99	NZ	LYS	12	-6.980	1.677	-12.843	1.00	90.89	1SG	100
ATOM	100	C	LYS	12	-0.721	1.748	-10.450	1.00	90.89	1SG	101
ATOM	101	O	LYS	12	-0.722	2.935	-10.133	1.00	90.89	1SG	102
ATOM	102	N	LEU	13	0.263	0.910	-10.074	1.00	53.34	1SG	103
ATOM	103	CA	LEU	13	1.346	1.342	-9.234	1.00	53.34	1SG	104
ATOM	104	CB	LEU	13	2.319	0.204	-8.882	1.00	53.34	1SG	105
ATOM	105	CG	LEU	13	3.496	0.638	-7.984	1.00	53.34	1SG	106
ATOM	106	CD1	LEU	13	3.018	1.144	-6.615	1.00	53.34	1SG	107
ATOM	107	CD2	LEU	13	4.543	-0.484	-7.868	1.00	53.34	1SG	108
ATOM	108	C	LEU	13	2.132	2.400	-9.940	1.00	53.34	1SG	109
ATOM	109	O	LEU	13	2.569	3.370	-9.327	1.00	53.34	1SG	110
ATOM	110	N	LYS	14	2.341	2.247	-11.261	1.00	95.57	1SG	111
ATOM	111	CA	LYS	14	3.123	3.219	-11.965	1.00	95.57	1SG	112
ATOM	112	CB	LYS	14	3.476	2.837	-13.418	1.00	95.57	1SG	113
ATOM	113	CG	LYS	14	2.325	2.825	-14.423	1.00	95.57	1SG	114
ATOM	114	CD	LYS	14	2.852	2.788	-15.862	1.00	95.57	1SG	115
ATOM	115	CE	LYS	14	1.769	2.763	-16.940	1.00	95.57	1SG	116
ATOM	116	NZ	LYS	14	2.391	2.860	-18.282	1.00	95.57	1SG	117
ATOM	117	C	LYS	14	2.412	4.537	-11.950	1.00	95.57	1SG	118
ATOM	118	O	LYS	14	3.046	5.590	-12.000	1.00	95.57	1SG	119
ATOM	119	N	ASN	15	1.069	4.508	-11.896	1.00	53.90	1SG	120
ATOM	120	CA	ASN	15	0.260	5.693	-11.909	1.00	53.90	1SG	121
ATOM	121	CB	ASN	15	-1.244	5.377	-11.956	1.00	53.90	1SG	122
ATOM	122	CG	ASN	15	-1.539	4.822	-13.343	1.00	53.90	1SG	123
ATOM	123	OD1	ASN	15	-0.874	5.183	-14.313	1.00	53.90	1SG	124
ATOM	124	ND2	ASN	15	-2.559	3.928	-13.447	1.00	53.90	1SG	125
ATOM	125	C	ASN	15	0.530	6.525	-10.685	1.00	53.90	1SG	126

ATOM	126	O	ASN	15	0.455	7.750	-10.752	1.00	53.90	1SG	127
ATOM	127	N	ILE	16	0.826	5.902	-9.525	1.00	150.81	1SG	128
ATOM	128	CA	ILE	16	1.074	6.662	-8.325	1.00	150.81	1SG	129
ATOM	129	CB	ILE	16	1.064	5.883	-7.037	1.00	150.81	1SG	130
ATOM	130	CG2	ILE	16	-0.359	5.385	-6.784	1.00	150.81	1SG	131
ATOM	131	CG1	ILE	16	2.128	4.783	-7.026	1.00	150.81	1SG	132
ATOM	132	CD1	ILE	16	2.227	4.064	-5.683	1.00	150.81	1SG	133
ATOM	133	C	ILE	16	2.388	7.371	-8.410	1.00	150.81	1SG	134
ATOM	134	O	ILE	16	3.313	6.951	-9.104	1.00	150.81	1SG	135
ATOM	135	N	PRO	17	2.456	8.480	-7.717	1.00	77.41	1SG	136
ATOM	136	CA	PRO	17	3.644	9.287	-7.712	1.00	77.41	1SG	137
ATOM	137	CD	PRO	17	1.267	9.246	-7.378	1.00	77.41	1SG	138
ATOM	138	CB	PRO	17	3.274	10.561	-6.961	1.00	77.41	1SG	139
ATOM	139	CG	PRO	17	1.758	10.693	-7.202	1.00	77.41	1SG	140
ATOM	140	C	PRO	17	4.777	8.521	-7.112	1.00	77.41	1SG	141
ATOM	141	O	PRO	17	4.550	7.723	-6.205	1.00	77.41	1SG	142
ATOM	142	N	PHE	18	6.004	8.773	-7.600	1.00	51.53	1SG	143
ATOM	143	CA	PHE	18	7.166	8.025	-7.222	1.00	51.53	1SG	144
ATOM	144	CB	PHE	18	8.422	8.439	-7.999	1.00	51.53	1SG	145
ATOM	145	CG	PHE	18	9.521	7.568	-7.502	1.00	51.53	1SG	146
ATOM	146	CD1	PHE	18	9.695	6.307	-8.023	1.00	51.53	1SG	147
ATOM	147	CD2	PHE	18	10.370	8.005	-6.511	1.00	51.53	1SG	148
ATOM	148	CE1	PHE	18	10.705	5.494	-7.570	1.00	51.53	1SG	149
ATOM	149	CE2	PHE	18	11.382	7.194	-6.053	1.00	51.53	1SG	150
ATOM	150	CZ	PHE	18	11.551	5.939	-6.582	1.00	51.53	1SG	151
ATOM	151	C	PHE	18	7.469	8.181	-5.770	1.00	51.53	1SG	152
ATOM	152	O	PHE	18	7.850	7.218	-5.107	1.00	51.53	1SG	153
ATOM	153	N	PHE	19	7.326	9.401	-5.228	1.00	60.48	1SG	154
ATOM	154	CA	PHE	19	7.693	9.603	-3.857	1.00	60.48	1SG	155
ATOM	155	CB	PHE	19	7.377	11.024	-3.363	1.00	60.48	1SG	156
ATOM	156	CG	PHE	19	8.135	11.982	-4.212	1.00	60.48	1SG	157
ATOM	157	CD1	PHE	19	9.476	12.200	-4.000	1.00	60.48	1SG	158
ATOM	158	CD2	PHE	19	7.495	12.666	-5.220	1.00	60.48	1SG	159
ATOM	159	CE1	PHE	19	10.173	13.087	-4.785	1.00	60.48	1SG	160
ATOM	160	CE2	PHE	19	8.184	13.554	-6.009	1.00	60.48	1SG	161
ATOM	161	CZ	PHE	19	9.524	13.763	-5.791	1.00	60.48	1SG	162
ATOM	162	C	PHE	19	6.867	8.687	-3.008	1.00	60.48	1SG	163
ATOM	163	O	PHE	19	7.393	7.994	-2.140	1.00	60.48	1SG	164

ATOM	164	N	ALA	20	5.543	8.716	-3.249	1.00	74.45	1SG 165
ATOM	165	CA	ALA	20	4.480	8.004	-2.589	1.00	74.45	1SG 166
ATOM	166	CB	ALA	20	3.081	8.541	-2.943	1.00	74.45	1SG 167
ATOM	167	C	ALA	20	4.464	6.528	-2.867	1.00	74.45	1SG 168
ATOM	168	O	ALA	20	3.897	5.769	-2.086	1.00	74.45	1SG 169
ATOM	169	N	ARG	21	5.004	6.078	-4.014	1.00	192.17	1SG 170
ATOM	170	CA	ARG	21	4.811	4.709	-4.410	1.00	192.17	1SG 171
ATOM	171	CB	ARG	21	5.326	4.391	-5.824	1.00	192.17	1SG 172
ATOM	172	CG	ARG	21	6.804	4.670	-6.056	1.00	192.17	1SG 173
ATOM	173	CD	ARG	21	7.155	4.735	-7.543	1.00	192.17	1SG 174
ATOM	174	NE	ARG	21	6.942	3.383	-8.132	1.00	192.17	1SG 175
ATOM	175	CZ	ARG	21	6.437	3.269	-9.395	1.00	192.17	1SG 176
ATOM	176	NH1	ARG	21	6.063	4.388	-10.079	1.00	192.17	1SG 177
ATOM	177	NH2	ARG	21	6.298	2.041	-9.974	1.00	192.17	1SG 178
ATOM	178	C	ARG	21	5.323	3.711	-3.413	1.00	192.17	1SG 179
ATOM	179	O	ARG	21	4.667	2.694	-3.191	1.00	192.17	1SG 180
ATOM	180	N	SER	22	6.485	3.936	-2.776	1.00	28.08	1SG 181
ATOM	181	CA	SER	22	6.929	2.968	-1.812	1.00	28.08	1SG 182
ATOM	182	CB	SER	22	8.280	3.336	-1.176	1.00	28.08	1SG 183
ATOM	183	OG	SER	22	8.661	2.342	-0.236	1.00	28.08	1SG 184
ATOM	184	C	SER	22	5.911	2.923	-0.716	1.00	28.08	1SG 185
ATOM	185	O	SER	22	5.585	1.855	-0.196	1.00	28.08	1SG 186
ATOM	186	N	GLN	23	5.373	4.102	-0.349	1.00	39.96	1SG 187
ATOM	187	CA	GLN	23	4.398	4.202	0.699	1.00	39.96	1SG 188
ATOM	188	CB	GLN	23	3.951	5.653	0.946	1.00	39.96	1SG 189
ATOM	189	CG	GLN	23	2.888	5.782	2.038	1.00	39.96	1SG 190
ATOM	190	CD	GLN	23	3.537	5.460	3.373	1.00	39.96	1SG 191
ATOM	191	OE1	GLN	23	4.344	6.234	3.886	1.00	39.96	1SG 192
ATOM	192	NE2	GLN	23	3.181	4.284	3.954	1.00	39.96	1SG 193
ATOM	193	C	GLN	23	3.174	3.438	0.301	1.00	39.96	1SG 194
ATOM	194	O	GLN	23	2.633	2.668	1.091	1.00	39.96	1SG 195
ATOM	195	N	ALA	24	2.711	3.627	-0.948	1.00	35.95	1SG 196
ATOM	196	CA	ALA	24	1.513	2.994	-1.421	1.00	35.95	1SG 197
ATOM	197	CB	ALA	24	1.113	3.462	-2.831	1.00	35.95	1SG 198
ATOM	198	C	ALA	24	1.700	1.509	-1.474	1.00	35.95	1SG 199
ATOM	199	O	ALA	24	0.820	0.748	-1.077	1.00	35.95	1SG 200
ATOM	200	N	LYS	25	2.875	1.055	-1.940	1.00	127.72	1SG 201
ATOM	201	CA	LYS	25	3.119	-0.346	-2.111	1.00	127.72	1SG 202

ATOM	202	CB	LYS	25	4.531	-0.611	-2.658	1.00127.72	1SG 203
ATOM	203	CG	LYS	25	4.767	-2.040	-3.131	1.00127.72	1SG 204
ATOM	204	CD	LYS	25	4.671	-3.093	-2.037	1.00127.72	1SG 205
ATOM	205	CE	LYS	25	4.982	-4.491	-2.566	1.00127.72	1SG 206
ATOM	206	NZ	LYS	25	6.424	-4.771	-2.445	1.00127.72	1SG 207
ATOM	207	C	LYS	25	2.973	-1.022	-0.783	1.00127.72	1SG 208
ATOM	208	O	LYS	25	2.396	-2.105	-0.690	1.00127.72	1SG 209
ATOM	209	N	ALA	26	3.480	-0.389	0.289	1.00 27.28	1SG 210
ATOM	210	CA	ALA	26	3.390	-0.980	1.591	1.00 27.28	1SG 211
ATOM	211	CB	ALA	26	4.066	-0.130	2.679	1.00 27.28	1SG 212
ATOM	212	C	ALA	26	1.944	-1.111	1.955	1.00 27.28	1SG 213
ATOM	213	O	ALA	26	1.526	-2.123	2.514	1.00 27.28	1SG 214
ATOM	214	N	ARG	27	1.143	-0.076	1.645	1.00 87.55	1SG 215
ATOM	215	CA	ARG	27	-0.250	-0.055	1.992	1.00 87.55	1SG 216
ATOM	216	CB	ARG	27	-0.906	1.291	1.636	1.00 87.55	1SG 217
ATOM	217	CG	ARG	27	-0.195	2.498	2.257	1.00 87.55	1SG 218
ATOM	218	CD	ARG	27	-0.260	2.545	3.783	1.00 87.55	1SG 219
ATOM	219	NE	ARG	27	-1.692	2.710	4.151	1.00 87.55	1SG 220
ATOM	220	CZ	ARG	27	-2.054	3.654	5.067	1.00 87.55	1SG 221
ATOM	221	NH1	ARG	27	-1.100	4.440	5.646	1.00 87.55	1SG 222
ATOM	222	NH2	ARG	27	-3.370	3.821	5.387	1.00 87.55	1SG 223
ATOM	223	C	ARG	27	-0.984	-1.130	1.242	1.00 87.55	1SG 224
ATOM	224	O	ARG	27	-1.786	-1.867	1.816	1.00 87.55	1SG 225
ATOM	225	N	ILE	28	-0.702	-1.258	-0.068	1.00 41.35	1SG 226
ATOM	226	CA	ILE	28	-1.406	-2.176	-0.922	1.00 41.35	1SG 227
ATOM	227	CB	ILE	28	-0.932	-2.096	-2.346	1.00 41.35	1SG 228
ATOM	228	CG2	ILE	28	-1.613	-3.220	-3.146	1.00 41.35	1SG 229
ATOM	229	CG1	ILE	28	-1.175	-0.685	-2.913	1.00 41.35	1SG 230
ATOM	230	CD1	ILE	28	-0.446	-0.420	-4.231	1.00 41.35	1SG 231
ATOM	231	C	ILE	28	-1.168	-3.577	-0.454	1.00 41.35	1SG 232
ATOM	232	O	ILE	28	-2.092	-4.385	-0.370	1.00 41.35	1SG 233
ATOM	233	N	GLU	29	0.092	-3.900	-0.128	1.00107.62	1SG 234
ATOM	234	CA	GLU	29	0.455	-5.225	0.279	1.00107.62	1SG 235
ATOM	235	CB	GLU	29	1.954	-5.359	0.563	1.00107.62	1SG 236
ATOM	236	CG	GLU	29	2.831	-4.935	-0.609	1.00107.62	1SG 237
ATOM	237	CD	GLU	29	2.354	-5.633	-1.875	1.00107.62	1SG 238
ATOM	238	OE1	GLU	29	1.233	-5.309	-2.350	1.00107.62	1SG 239
ATOM	239	OE2	GLU	29	3.114	-6.495	-2.389	1.00107.62	1SG 240

ATOM	240	C	GLU	29	-0.230	-5.534	1.570	1.00107.62	1SG 241
ATOM	241	O	GLU	29	-0.636	-6.670	1.810	1.00107.62	1SG 242
ATOM	242	N	GLN	30	-0.335	-4.522	2.454	1.00 82.61	1SG 243
ATOM	243	CA	GLN	30	-0.946	-4.683	3.743	1.00 82.61	1SG 244
ATOM	244	CB	GLN	30	-0.916	-3.394	4.576	1.00 82.61	1SG 245
ATOM	245	CG	GLN	30	0.482	-2.896	4.928	1.00 82.61	1SG 246
ATOM	246	CD	GLN	30	0.316	-1.622	5.745	1.00 82.61	1SG 247
ATOM	247	OE1	GLN	30	-0.436	-1.588	6.715	1.00 82.61	1SG 248
ATOM	248	NE2	GLN	30	1.032	-0.541	5.336	1.00 82.61	1SG 249
ATOM	249	C	GLN	30	-2.392	-4.997	3.549	1.00 82.61	1SG 250
ATOM	250	O	GLN	30	-2.957	-5.834	4.255	1.00 82.61	1SG 251
ATOM	251	N	LEU	31	-3.029	-4.314	2.578	1.00 44.56	1SG 252
ATOM	252	CA	LEU	31	-4.427	-4.486	2.305	1.00 44.56	1SG 253
ATOM	253	CB	LEU	31	-4.924	-3.560	1.179	1.00 44.56	1SG 254
ATOM	254	CG	LEU	31	-4.909	-2.065	1.555	1.00 44.56	1SG 255
ATOM	255	CD1	LEU	31	-5.415	-1.190	0.398	1.00 44.56	1SG 256
ATOM	256	CD2	LEU	31	-5.696	-1.806	2.853	1.00 44.56	1SG 257
ATOM	257	C	LEU	31	-4.648	-5.897	1.867	1.00 44.56	1SG 258
ATOM	258	O	LEU	31	-5.629	-6.528	2.250	1.00 44.56	1SG 259
ATOM	259	N	ALA	32	-3.717	-6.430	1.056	1.00 34.60	1SG 260
ATOM	260	CA	ALA	32	-3.826	-7.768	0.554	1.00 34.60	1SG 261
ATOM	261	CB	ALA	32	-2.652	-8.160	-0.362	1.00 34.60	1SG 262
ATOM	262	C	ALA	32	-3.830	-8.699	1.719	1.00 34.60	1SG 263
ATOM	263	O	ALA	32	-4.554	-9.689	1.722	1.00 34.60	1SG 264
ATOM	264	N	ARG	33	-3.008	-8.401	2.741	1.00138.62	1SG 265
ATOM	265	CA	ARG	33	-2.912	-9.221	3.914	1.00138.62	1SG 266
ATOM	266	CB	ARG	33	-1.782	-8.774	4.853	1.00138.62	1SG 267
ATOM	267	CG	ARG	33	-0.405	-9.029	4.240	1.00138.62	1SG 268
ATOM	268	CD	ARG	33	0.069	-10.473	4.424	1.00138.62	1SG 269
ATOM	269	NE	ARG	33	-0.985	-11.373	3.873	1.00138.62	1SG 270
ATOM	270	CZ	ARG	33	-0.669	-12.654	3.521	1.00138.62	1SG 271
ATOM	271	NH1	ARG	33	0.615	-13.094	3.652	1.00138.62	1SG 272
ATOM	272	NH2	ARG	33	-1.631	-13.493	3.037	1.00138.62	1SG 273
ATOM	273	C	ARG	33	-4.204	-9.189	4.662	1.00138.62	1SG 274
ATOM	274	O	ARG	33	-4.597	-10.188	5.265	1.00138.62	1SG 275
ATOM	275	N	GLN	34	-4.900	-8.035	4.662	1.00 88.64	1SG 276
ATOM	276	CA	GLN	34	-6.133	-7.991	5.391	1.00 88.64	1SG 277
ATOM	277	CB	GLN	34	-6.861	-6.637	5.303	1.00 88.64	1SG 278



ATOM	278	CG	GLN	34	-6.136	-5.477	5.988	1.00	88.64	1SG 279
ATOM	279	CD	GLN	34	-7.017	-4.246	5.828	1.00	88.64	1SG 280
ATOM	280	OE1	GLN	34	-6.605	-3.230	5.272	1.00	88.64	1SG 281
ATOM	281	NE2	GLN	34	-8.276	-4.341	6.330	1.00	88.64	1SG 282
ATOM	282	C	GLN	34	-7.028	-9.018	4.772	1.00	88.64	1SG 283
ATOM	283	O	GLN	34	-7.707	-9.773	5.465	1.00	88.64	1SG 284
ATOM	284	N	ALA	35	-7.029	-9.050	3.428	1.00	53.08	1SG 285
ATOM	285	CA	ALA	35	-7.758	-9.969	2.603	1.00	53.08	1SG 286
ATOM	286	CB	ALA	35	-7.664	-9.627	1.106	1.00	53.08	1SG 287
ATOM	287	C	ALA	35	-7.196	-11.345	2.795	1.00	53.08	1SG 288
ATOM	288	O	ALA	35	-7.912	-12.335	2.657	1.00	53.08	1SG 289
ATOM	289	N	GLU	36	-5.892	-11.437	3.123	1.00	140.57	1SG 290
ATOM	290	CA	GLU	36	-5.188	-12.683	3.223	1.00	140.57	1SG 291
ATOM	291	CB	GLU	36	-5.888	-13.695	4.148	1.00	140.57	1SG 292
ATOM	292	CG	GLU	36	-5.079	-14.969	4.392	1.00	140.57	1SG 293
ATOM	293	CD	GLU	36	-3.931	-14.641	5.338	1.00	140.57	1SG 294
ATOM	294	OE1	GLU	36	-3.762	-13.440	5.680	1.00	140.57	1SG 295
ATOM	295	OE2	GLU	36	-3.204	-15.593	5.731	1.00	140.57	1SG 296
ATOM	296	C	GLU	36	-5.059	-13.275	1.854	1.00	140.57	1SG 297
ATOM	297	O	GLU	36	-5.173	-14.486	1.669	1.00	140.57	1SG 298
ATOM	298	N	GLN	37	-4.802	-12.407	0.850	1.00	60.67	1SG 299
ATOM	299	CA	GLN	37	-4.630	-12.843	-0.505	1.00	60.67	1SG 300
ATOM	300	CB	GLN	37	-5.546	-12.108	-1.494	1.00	60.67	1SG 301
ATOM	301	CG	GLN	37	-5.233	-10.617	-1.586	1.00	60.67	1SG 302
ATOM	302	CD	GLN	37	-6.356	-9.949	-2.358	1.00	60.67	1SG 303
ATOM	303	OE1	GLN	37	-6.882	-8.926	-1.925	1.00	60.67	1SG 304
ATOM	304	NE2	GLN	37	-6.736	-10.535	-3.524	1.00	60.67	1SG 305
ATOM	305	C	GLN	37	-3.212	-12.576	-0.910	1.00	60.67	1SG 306
ATOM	306	O	GLN	37	-2.612	-11.569	-0.540	1.00	60.67	1SG 307
ATOM	307	N	ASP	38	-2.635	-13.535	-1.655	1.00	61.46	1SG 308
ATOM	308	CA	ASP	38	-1.292	-13.495	-2.155	1.00	61.46	1SG 309
ATOM	309	CB	ASP	38	-0.834	-14.858	-2.686	1.00	61.46	1SG 310
ATOM	310	CG	ASP	38	-0.719	-15.778	-1.482	1.00	61.46	1SG 311
ATOM	311	OD1	ASP	38	0.005	-15.402	-0.522	1.00	61.46	1SG 312
ATOM	312	OD2	ASP	38	-1.351	-16.867	-1.507	1.00	61.46	1SG 313
ATOM	313	C	ASP	38	-1.159	-12.513	-3.276	1.00	61.46	1SG 314
ATOM	314	O	ASP	38	-0.095	-11.922	-3.458	1.00	61.46	1SG 315
ATOM	315	N	ILE	39	-2.221	-12.328	-4.087	1.00	176.83	1SG 316

ATOM	316	CA	ILE	39	-2.060	-11.462	-5.220	1.00176.83	1SG 317
ATOM	317	CB	ILE	39	-2.447	-12.052	-6.549	1.00176.83	1SG 318
ATOM	318	CG2	ILE	39	-1.431	-13.140	-6.913	1.00176.83	1SG 319
ATOM	319	CG1	ILE	39	-3.909	-12.514	-6.558	1.00176.83	1SG 320
ATOM	320	CD1	ILE	39	-4.195	-13.669	-5.601	1.00176.83	1SG 321
ATOM	321	C	ILE	39	-2.838	-10.203	-5.042	1.00176.83	1SG 322
ATOM	322	O	ILE	39	-3.984	-10.204	-4.596	1.00176.83	1SG 323
ATOM	323	N	VAL	40	-2.192	-9.076	-5.395	1.00118.10	1SG 324
ATOM	324	CA	VAL	40	-2.791	-7.783	-5.258	1.00118.10	1SG 325
ATOM	325	CB	VAL	40	-1.799	-6.707	-4.919	1.00118.10	1SG 326
ATOM	326	CG1	VAL	40	-1.235	-6.985	-3.518	1.00118.10	1SG 327
ATOM	327	CG2	VAL	40	-0.715	-6.683	-6.012	1.00118.10	1SG 328
ATOM	328	C	VAL	40	-3.420	-7.408	-6.559	1.00118.10	1SG 329
ATOM	329	O	VAL	40	-2.851	-7.618	-7.631	1.00118.10	1SG 330
ATOM	330	N	THR	41	-4.650	-6.863	-6.482	1.00 59.19	1SG 331
ATOM	331	CA	THR	41	-5.354	-6.434	-7.655	1.00 59.19	1SG 332
ATOM	332	CB	THR	41	-6.811	-6.817	-7.629	1.00 59.19	1SG 333
ATOM	333	OG1	THR	41	-7.474	-6.225	-6.524	1.00 59.19	1SG 334
ATOM	334	CG2	THR	41	-6.913	-8.347	-7.548	1.00 59.19	1SG 335
ATOM	335	C	THR	41	-5.235	-4.939	-7.743	1.00 59.19	1SG 336
ATOM	336	O	THR	41	-4.828	-4.290	-6.781	1.00 59.19	1SG 337
ATOM	337	N	PRO	42	-5.552	-4.374	-8.887	1.00 75.20	1SG 338
ATOM	338	CA	PRO	42	-5.509	-2.953	-9.109	1.00 75.20	1SG 339
ATOM	339	CD	PRO	42	-6.121	-5.095	-10.014	1.00 75.20	1SG 340
ATOM	340	CB	PRO	42	-5.920	-2.744	-10.566	1.00 75.20	1SG 341
ATOM	341	CG	PRO	42	-6.746	-4.000	-10.897	1.00 75.20	1SG 342
ATOM	342	C	PRO	42	-6.457	-2.289	-8.168	1.00 75.20	1SG 343
ATOM	343	O	PRO	42	-6.309	-1.093	-7.920	1.00 75.20	1SG 344
ATOM	344	N	GLU	43	-7.456	-3.037	-7.668	1.00 42.78	1SG 345
ATOM	345	CA	GLU	43	-8.434	-2.482	-6.781	1.00 42.78	1SG 346
ATOM	346	CB	GLU	43	-9.504	-3.505	-6.368	1.00 42.78	1SG 347
ATOM	347	CG	GLU	43	-10.344	-4.046	-7.526	1.00 42.78	1SG 348
ATOM	348	CD	GLU	43	-11.195	-5.178	-6.968	1.00 42.78	1SG 349
ATOM	349	OE1	GLU	43	-12.186	-4.875	-6.254	1.00 42.78	1SG 350
ATOM	350	OE2	GLU	43	-10.854	-6.362	-7.237	1.00 42.78	1SG 351
ATOM	351	C	GLU	43	-7.742	-2.073	-5.523	1.00 42.78	1SG 352
ATOM	352	O	GLU	43	-8.021	-1.007	-4.974	1.00 42.78	1SG 353
ATOM	353	N	LEU	44	-6.827	-2.928	-5.025	1.00 99.69	1SG 354

ATOM	354	CA	LEU	44	-6.137	-2.619	-3.806	1.00	99.69	1SG 355
ATOM	355	CB	LEU	44	-5.201	-3.721	-3.271	1.00	99.69	1SG 356
ATOM	356	CG	LEU	44	-5.871	-5.049	-2.864	1.00	99.69	1SG 357
ATOM	357	CD1	LEU	44	-7.052	-4.828	-1.909	1.00	99.69	1SG 358
ATOM	358	CD2	LEU	44	-6.206	-5.923	-4.071	1.00	99.69	1SG 359
ATOM	359	C	LEU	44	-5.261	-1.435	-4.037	1.00	99.69	1SG 360
ATOM	360	O	LEU	44	-5.149	-0.557	-3.183	1.00	99.69	1SG 361
ATOM	361	N	VAL	45	-4.608	-1.388	-5.211	1.00	37.38	1SG 362
ATOM	362	CA	VAL	45	-3.689	-0.328	-5.503	1.00	37.38	1SG 363
ATOM	363	CB	VAL	45	-3.007	-0.493	-6.829	1.00	37.38	1SG 364
ATOM	364	CG1	VAL	45	-2.070	0.708	-7.048	1.00	37.38	1SG 365
ATOM	365	CG2	VAL	45	-2.295	-1.856	-6.847	1.00	37.38	1SG 366
ATOM	366	C	VAL	45	-4.440	0.959	-5.525	1.00	37.38	1SG 367
ATOM	367	O	VAL	45	-3.957	1.976	-5.029	1.00	37.38	1SG 368
ATOM	368	N	GLU	46	-5.652	0.948	-6.105	1.00	114.73	1SG 369
ATOM	369	CA	GLU	46	-6.437	2.145	-6.191	1.00	114.73	1SG 370
ATOM	370	CB	GLU	46	-7.764	1.952	-6.948	1.00	114.73	1SG 371
ATOM	371	CG	GLU	46	-7.597	1.692	-8.446	1.00	114.73	1SG 372
ATOM	372	CD	GLU	46	-7.255	3.010	-9.126	1.00	114.73	1SG 373
ATOM	373	OE1	GLU	46	-6.998	4.009	-8.402	1.00	114.73	1SG 374
ATOM	374	OE2	GLU	46	-7.250	3.032	-10.385	1.00	114.73	1SG 375
ATOM	375	C	GLU	46	-6.786	2.589	-4.809	1.00	114.73	1SG 376
ATOM	376	O	GLU	46	-6.730	3.777	-4.499	1.00	114.73	1SG 377
ATOM	377	N	GLN	47	-7.118	1.634	-3.922	1.00	117.23	1SG 378
ATOM	378	CA	GLN	47	-7.574	2.002	-2.616	1.00	117.23	1SG 379
ATOM	379	CB	GLN	47	-7.906	0.789	-1.733	1.00	117.23	1SG 380
ATOM	380	CG	GLN	47	-8.406	1.168	-0.338	1.00	117.23	1SG 381
ATOM	381	CD	GLN	47	-9.799	1.779	-0.471	1.00	117.23	1SG 382
ATOM	382	OE1	GLN	47	-10.804	1.115	-0.223	1.00	117.23	1SG 383
ATOM	383	NE2	GLN	47	-9.863	3.079	-0.868	1.00	117.23	1SG 384
ATOM	384	C	GLN	47	-6.501	2.788	-1.933	1.00	117.23	1SG 385
ATOM	385	O	GLN	47	-6.777	3.822	-1.328	1.00	117.23	1SG 386
ATOM	386	N	ALA	48	-5.238	2.337	-2.033	1.00	30.20	1SG 387
ATOM	387	CA	ALA	48	-4.169	3.030	-1.378	1.00	30.20	1SG 388
ATOM	388	CB	ALA	48	-2.812	2.322	-1.537	1.00	30.20	1SG 389
ATOM	389	C	ALA	48	-4.040	4.397	-1.969	1.00	30.20	1SG 390
ATOM	390	O	ALA	48	-3.817	5.369	-1.250	1.00	30.20	1SG 391
ATOM	391	N	ARG	49	-4.161	4.507	-3.305	1.00	125.68	1SG 392

ATOM	392	CA	ARG	49	-3.994	5.781	-3.941	1.00125.68	1SG 393
ATOM	393	CB	ARG	49	-3.991	5.676	-5.477	1.00125.68	1SG 394
ATOM	394	CG	ARG	49	-3.573	6.969	-6.176	1.00125.68	1SG 395
ATOM	395	CD	ARG	49	-3.470	6.833	-7.696	1.00125.68	1SG 396
ATOM	396	NE	ARG	49	-4.826	6.491	-8.211	1.00125.68	1SG 397
ATOM	397	CZ	ARG	49	-5.210	6.904	-9.455	1.00125.68	1SG 398
ATOM	398	NH1	ARG	49	-4.372	7.672	-10.211	1.00125.68	1SG 399
ATOM	399	NH2	ARG	49	-6.432	6.545	-9.945	1.00125.68	1SG 400
ATOM	400	C	ARG	49	-5.090	6.712	-3.515	1.00125.68	1SG 401
ATOM	401	O	ARG	49	-4.844	7.876	-3.201	1.00125.68	1SG 402
ATOM	402	N	LEU	50	-6.339	6.214	-3.482	1.00145.30	1SG 403
ATOM	403	CA	LEU	50	-7.462	7.036	-3.119	1.00145.30	1SG 404
ATOM	404	CB	LEU	50	-8.831	6.355	-3.310	1.00145.30	1SG 405
ATOM	405	CG	LEU	50	-9.324	6.336	-4.771	1.00145.30	1SG 406
ATOM	406	CD1	LEU	50	-9.642	7.761	-5.250	1.00145.30	1SG 407
ATOM	407	CD2	LEU	50	-8.352	5.615	-5.713	1.00145.30	1SG 408
ATOM	408	C	LEU	50	-7.366	7.480	-1.698	1.00145.30	1SG 409
ATOM	409	O	LEU	50	-7.643	8.638	-1.390	1.00145.30	1SG 410
ATOM	410	N	GLU	51	-6.947	6.585	-0.788	1.00 39.69	1SG 411
ATOM	411	CA	GLU	51	-6.933	6.950	0.598	1.00 39.69	1SG 412
ATOM	412	CB	GLU	51	-6.475	5.800	1.512	1.00 39.69	1SG 413
ATOM	413	CG	GLU	51	-5.062	5.307	1.203	1.00 39.69	1SG 414
ATOM	414	CD	GLU	51	-4.774	4.123	2.113	1.00 39.69	1SG 415
ATOM	415	OE1	GLU	51	-5.621	3.835	3.000	1.00 39.69	1SG 416
ATOM	416	OE2	GLU	51	-3.704	3.486	1.929	1.00 39.69	1SG 417
ATOM	417	C	GLU	51	-6.006	8.111	0.784	1.00 39.69	1SG 418
ATOM	418	O	GLU	51	-6.326	9.055	1.506	1.00 39.69	1SG 419
ATOM	419	N	PHE	52	-4.829	8.087	0.134	1.00 47.01	1SG 420
ATOM	420	CA	PHE	52	-3.914	9.179	0.299	1.00 47.01	1SG 421
ATOM	421	CB	PHE	52	-2.540	8.944	-0.356	1.00 47.01	1SG 422
ATOM	422	CG	PHE	52	-1.835	7.900	0.442	1.00 47.01	1SG 423
ATOM	423	CD1	PHE	52	-1.344	8.196	1.695	1.00 47.01	1SG 424
ATOM	424	CD2	PHE	52	-1.645	6.635	-0.066	1.00 47.01	1SG 425
ATOM	425	CE1	PHE	52	-0.688	7.240	2.436	1.00 47.01	1SG 426
ATOM	426	CE2	PHE	52	-0.990	5.677	0.670	1.00 47.01	1SG 427
ATOM	427	CZ	PHE	52	-0.511	5.977	1.922	1.00 47.01	1SG 428
ATOM	428	C	PHE	52	-4.506	10.425	-0.284	1.00 47.01	1SG 429
ATOM	429	O	PHE	52	-4.423	11.494	0.316	1.00 47.01	1SG 430

ATOM 430 N GLY 53 -5.127 10.322 -1.473 1.00 17.85 1SG 431  
ATOM 431 CA GLY 53 -5.650 11.493 -2.118 1.00 17.85 1SG 432  
ATOM 432 C GLY 53 -6.720 12.103 -1.282 1.00 17.85 1SG 433  
ATOM 433 O GLY 53 -6.766 13.320 -1.113 1.00 17.85 1SG 434  
ATOM 434 N GLN 54 -7.618 11.267 -0.737 1.00 72.74 1SG 435  
ATOM 435 CA GLN 54 -8.704 11.792 0.029 1.00 72.74 1SG 436  
ATOM 436 CB GLN 54 -10.025 11.065 -0.278 1.00 72.74 1SG 437  
ATOM 437 CG GLN 54 -9.978 9.566 0.016 1.00 72.74 1SG 438  
ATOM 438 CD GLN 54 -11.201 8.930 -0.622 1.00 72.74 1SG 439  
ATOM 439 OE1 GLN 54 -12.293 9.494 -0.611 1.00 72.74 1SG 440  
ATOM 440 NE2 GLN 54 -11.008 7.724 -1.220 1.00 72.74 1SG 441  
ATOM 441 C GLN 54 -8.383 11.652 1.512 1.00 72.74 1SG 442  
ATOM 442 O GLN 54 -8.364 10.503 2.024 1.00 72.74 1SG 443  
ATOM 443 OXT GLN 54 -8.157 12.707 2.161 1.00 72.74 1SG 444  
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