

Supplementary Information

A Study of Procyanidin Binding to Histatin 5 using Electrospray Ionization Tandem Mass Spectrometry (ESI-MS/MS) and Molecular Simulations

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PDB coordinates for procyanidins:

Procyanidin B1 compact rotamer:

HETATM	1	O1	UNK	1	27.536	19.487	89.064	0.00	0.00	O
HETATM	2	C2	UNK	1	26.822	18.510	88.315	0.00	0.00	C
HETATM	3	C3	UNK	1	26.178	17.484	89.257	0.00	0.00	C
HETATM	4	C4	UNK	1	27.279	16.765	90.064	0.00	0.00	C
HETATM	5	C5	UNK	1	29.135	17.413	91.657	0.00	0.00	C
HETATM	6	C6	UNK	1	30.061	18.337	92.148	0.00	0.00	C
HETATM	7	C7	UNK	1	30.131	19.621	91.612	0.00	0.00	C
HETATM	8	C8	UNK	1	29.263	19.981	90.582	0.00	0.00	C
HETATM	9	C9	UNK	1	28.340	19.063	90.079	0.00	0.00	C
HETATM	10	C10	UNK	1	28.269	17.769	90.612	0.00	0.00	C
HETATM	11	O11	UNK	1	29.687	16.964	88.513	0.00	0.00	O
HETATM	12	C12	UNK	1	31.053	17.028	88.129	0.00	0.00	C
HETATM	13	C13	UNK	1	31.199	16.332	86.771	0.00	0.00	C
HETATM	14	C14	UNK	1	30.843	14.857	86.959	0.00	0.00	C
HETATM	15	C15	UNK	1	28.900	13.462	87.759	0.00	0.00	C
HETATM	16	C16	UNK	1	27.724	13.316	88.494	0.00	0.00	C
HETATM	17	C17	UNK	1	27.209	14.384	89.232	0.00	0.00	C
HETATM	18	C18	UNK	1	27.870	15.623	89.246	0.00	0.00	C
HETATM	19	C19	UNK	1	29.055	15.758	88.503	0.00	0.00	C
HETATM	20	C20	UNK	1	29.574	14.688	87.760	0.00	0.00	C
HETATM	21	C21	UNK	1	25.800	19.223	87.453	0.00	0.00	C
HETATM	22	C22	UNK	1	25.385	18.643	86.246	0.00	0.00	C
HETATM	23	C23	UNK	1	24.442	19.274	85.433	0.00	0.00	C
HETATM	24	C24	UNK	1	23.897	20.503	85.816	0.00	0.00	C
HETATM	25	C25	UNK	1	24.303	21.090	87.016	0.00	0.00	C
HETATM	26	C26	UNK	1	25.245	20.455	87.827	0.00	0.00	C
HETATM	27	C27	UNK	1	31.411	18.499	88.090	0.00	0.00	C
HETATM	28	C28	UNK	1	30.618	19.418	87.388	0.00	0.00	C
HETATM	29	C29	UNK	1	30.936	20.779	87.374	0.00	0.00	C
HETATM	30	C30	UNK	1	32.065	21.235	88.059	0.00	0.00	C
HETATM	31	C31	UNK	1	32.864	20.328	88.754	0.00	0.00	C
HETATM	32	C32	UNK	1	32.540	18.972	88.771	0.00	0.00	C
HETATM	33	O33	UNK	1	25.254	18.114	90.156	0.00	0.00	O
HETATM	34	O34	UNK	1	29.068	16.155	92.171	0.00	0.00	O
HETATM	35	O35	UNK	1	31.054	20.489	92.107	0.00	0.00	O
HETATM	36	O36	UNK	1	32.546	16.408	86.299	0.00	0.00	O
HETATM	37	O37	UNK	1	29.409	12.425	87.040	0.00	0.00	O

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Procyanidin B1 extended rotamer:

HETATM	1	O1	UNK	1	24.636	17.768	89.372	0.00	0.00	O
HETATM	2	C2	UNK	1	24.807	16.418	89.785	0.00	0.00	C
HETATM	3	C3	UNK	1	25.983	16.306	90.764	0.00	0.00	C
HETATM	4	C4	UNK	1	27.279	16.765	90.064	0.00	0.00	C
HETATM	5	C5	UNK	1	28.128	18.854	88.916	0.00	0.00	C
HETATM	6	C6	UNK	1	27.907	20.041	88.212	0.00	0.00	C
HETATM	7	C7	UNK	1	26.611	20.452	87.908	0.00	0.00	C
HETATM	8	C8	UNK	1	25.531	19.672	88.320	0.00	0.00	C
HETATM	9	C9	UNK	1	25.741	18.481	89.016	0.00	0.00	C
HETATM	10	C10	UNK	1	27.043	18.061	89.319	0.00	0.00	C
HETATM	11	O11	UNK	1	28.873	14.647	91.164	0.00	0.00	O
HETATM	12	C12	UNK	1	29.282	13.462	91.833	0.00	0.00	C
HETATM	13	C13	UNK	1	30.482	12.879	91.080	0.00	0.00	C
HETATM	14	C14	UNK	1	30.009	12.477	89.682	0.00	0.00	C
HETATM	15	C15	UNK	1	28.927	13.542	87.668	0.00	0.00	C
HETATM	16	C16	UNK	1	28.161	14.551	87.085	0.00	0.00	C
HETATM	17	C17	UNK	1	27.636	15.584	87.862	0.00	0.00	C
HETATM	18	C18	UNK	1	27.870	15.623	89.246	0.00	0.00	C
HETATM	19	C19	UNK	1	28.642	14.599	89.823	0.00	0.00	C
HETATM	20	C20	UNK	1	29.172	13.561	89.045	0.00	0.00	C
HETATM	21	C21	UNK	1	23.504	15.935	90.391	0.00	0.00	C
HETATM	22	C22	UNK	1	23.180	14.572	90.344	0.00	0.00	C
HETATM	23	C23	UNK	1	21.990	14.098	90.897	0.00	0.00	C
HETATM	24	C24	UNK	1	21.099	14.984	91.508	0.00	0.00	C
HETATM	25	C25	UNK	1	21.412	16.345	91.561	0.00	0.00	C
HETATM	26	C26	UNK	1	22.603	16.815	91.007	0.00	0.00	C
HETATM	27	C27	UNK	1	29.608	13.872	93.254	0.00	0.00	C
HETATM	28	C28	UNK	1	30.463	14.953	93.517	0.00	0.00	C
HETATM	29	C29	UNK	1	30.744	15.346	94.828	0.00	0.00	C
HETATM	30	C30	UNK	1	30.175	14.649	95.898	0.00	0.00	C
HETATM	31	C31	UNK	1	29.330	13.570	95.648	0.00	0.00	C
HETATM	32	C32	UNK	1	29.047	13.185	94.338	0.00	0.00	C
HETATM	33	O33	UNK	1	25.760	17.101	91.936	0.00	0.00	O
HETATM	34	O34	UNK	1	29.392	18.443	89.207	0.00	0.00	O
HETATM	35	O35	UNK	1	26.436	21.607	87.210	0.00	0.00	O
HETATM	36	O36	UNK	1	30.979	11.709	91.734	0.00	0.00	O
HETATM	37	O37	UNK	1	29.440	12.530	86.916	0.00	0.00	O
HETATM	38	O38	UNK	1	26.895	16.569	87.282	0.00	0.00	O
HETATM	39	O39	UNK	1	21.719	12.767	90.828	0.00	0.00	O
HETATM	40	O40	UNK	1	19.945	14.495	92.039	0.00	0.00	O
HETATM	41	O41	UNK	1	31.556	16.406	95.093	0.00	0.00	O
HETATM	42	O42	UNK	1	30.425	15.009	97.185	0.00	0.00	O

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Procyanidin B2 compact rotamer:

HETATM	1	C1	UNK	1	-31.207	27.871	22.310	0.00	0.00	C
HETATM	2	C2	UNK	1	-30.468	26.944	21.560	0.00	0.00	C
HETATM	3	C3	UNK	1	-29.941	25.814	22.200	0.00	0.00	C
HETATM	4	C4	UNK	1	-30.155	25.616	23.565	0.00	0.00	C
HETATM	5	C5	UNK	1	-30.904	26.530	24.305	0.00	0.00	C
HETATM	6	C6	UNK	1	-31.424	27.658	23.674	0.00	0.00	C
HETATM	7	C9	UNK	1	-29.105	26.266	19.561	0.00	0.00	C
HETATM	8	C10	UNK	1	-29.266	24.846	20.121	0.00	0.00	C
HETATM	9	C11	UNK	1	-30.250	27.160	20.079	0.00	0.00	C
HETATM	10	O14	UNK	1	-29.213	24.869	21.542	0.00	0.00	O
HETATM	11	O15	UNK	1	-31.721	28.966	21.687	0.00	0.00	O
HETATM	12	O16	UNK	1	-31.147	26.350	25.631	0.00	0.00	O
HETATM	13	C17	UNK	1	-28.188	23.907	19.618	0.00	0.00	C
HETATM	14	C18	UNK	1	-26.996	23.702	20.329	0.00	0.00	C
HETATM	15	C19	UNK	1	-26.010	22.837	19.845	0.00	0.00	C
HETATM	16	C20	UNK	1	-26.209	22.165	18.636	0.00	0.00	C
HETATM	17	C21	UNK	1	-27.390	22.361	17.922	0.00	0.00	C
HETATM	18	C22	UNK	1	-28.371	23.224	18.408	0.00	0.00	C
HETATM	19	O26	UNK	1	-27.843	26.832	19.941	0.00	0.00	O
HETATM	20	O27	UNK	1	-24.849	22.631	20.525	0.00	0.00	O
HETATM	21	O28	UNK	1	-25.269	21.317	18.138	0.00	0.00	O
HETATM	22	C34	UNK	1	-33.736	26.783	17.523	0.00	0.00	C
HETATM	23	C35	UNK	1	-33.656	26.010	18.686	0.00	0.00	C
HETATM	24	C36	UNK	1	-32.529	26.125	19.511	0.00	0.00	C
HETATM	25	C37	UNK	1	-31.481	27.005	19.194	0.00	0.00	C
HETATM	26	C38	UNK	1	-31.580	27.771	18.022	0.00	0.00	C
HETATM	27	C39	UNK	1	-32.700	27.657	17.197	0.00	0.00	C
HETATM	28	C41	UNK	1	-34.413	24.090	20.165	0.00	0.00	C
HETATM	29	C42	UNK	1	-33.607	24.852	21.226	0.00	0.00	C
HETATM	30	C43	UNK	1	-34.776	25.062	19.038	0.00	0.00	C
HETATM	31	O46	UNK	1	-32.423	25.374	20.642	0.00	0.00	O
HETATM	32	O47	UNK	1	-34.835	26.672	16.727	0.00	0.00	O
HETATM	33	O48	UNK	1	-30.571	28.624	17.693	0.00	0.00	O
HETATM	34	C49	UNK	1	-33.195	24.005	22.413	0.00	0.00	C
HETATM	35	C50	UNK	1	-33.851	24.150	23.645	0.00	0.00	C
HETATM	36	C51	UNK	1	-33.468	23.395	24.757	0.00	0.00	C
HETATM	37	C52	UNK	1	-32.418	22.478	24.648	0.00	0.00	C
HETATM	38	C53	UNK	1	-31.759	22.326	23.429	0.00	0.00	C
HETATM	39	C54	UNK	1	-32.142	23.084	22.323	0.00	0.00	C
HETATM	40	O58	UNK	1	-33.675	22.997	19.608	0.00	0.00	O
HETATM	41	O59	UNK	1	-34.090	23.533	25.961	0.00	0.00	O
HETATM	42	O60	UNK	1	-32.019	21.732	25.712	0.00	0.00	O
HETATM	43	H7	UNK	1	-29.738	24.718	24.048	0.00	0.00	H
HETATM	44	H8	UNK	1	-32.013	28.379	24.264	0.00	0.00	H
HETATM	45	H12	UNK	1	-29.152	26.229	18.448	0.00	0.00	H
HETATM	46	H13	UNK	1	-30.249	24.433	19.803	0.00	0.00	H
HETATM	47	H23	UNK	1	-26.833	24.232	21.282	0.00	0.00	H

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Procyanidin B2 extended rotamer:

HETATM	1	C1	-0.1	1	-30.660	7.057	-3.907	0.00	0.00	C
HETATM	2	C3	-0.1	1	-29.558	5.279	-2.680	0.00	0.00	C
HETATM	3	C5	-0.1	1	-28.360	7.309	-3.172	0.00	0.00	C
HETATM	4	C13	-0.1	1	-35.065	2.497	-2.683	0.00	0.00	C
HETATM	5	C16	-0.1	1	-34.869	4.195	-4.879	0.00	0.00	C
HETATM	6	C17	-0.1	1	-34.042	4.425	-3.770	0.00	0.00	C
HETATM	7	C18	-0.1	1	-34.161	3.560	-2.671	0.00	0.00	C
HETATM	8	O23	-0.1	1	-31.790	4.982	-3.366	0.00	0.00	O
HETATM	9	C24	-0.1	1	-33.946	10.812	-4.012	0.00	0.00	C
HETATM	10	C26	-0.1	1	-32.596	8.766	-3.941	0.00	0.00	C
HETATM	11	C28	-0.1	1	-33.211	9.908	-1.891	0.00	0.00	C
HETATM	12	C38	-0.1	1	-32.512	10.118	-10.127	0.00	0.00	C
HETATM	13	C39	-0.1	1	-32.766	10.360	-8.777	0.00	0.00	C
HETATM	14	C40	-0.1	1	-34.029	10.110	-8.225	0.00	0.00	C
HETATM	15	C41	-0.1	1	-35.034	9.614	-9.066	0.00	0.00	C
HETATM	16	O46	-0.1	1	-33.310	9.649	-6.020	0.00	0.00	O
HETATM	17	O49	-0.1	1	-36.768	1.250	-3.840	0.00	0.00	O
HETATM	18	O51	-0.1	1	-36.552	2.954	-6.000	0.00	0.00	O
HETATM	19	O53	-0.1	1	-34.515	11.855	-1.882	0.00	0.00	O
HETATM	20	O55	-0.1	1	-31.886	7.922	-1.821	0.00	0.00	O
HETATM	21	O59	-0.1	1	-27.282	5.582	-1.955	0.00	0.00	O
HETATM	22	O61	-0.1	1	-29.456	9.055	-4.394	0.00	0.00	O
HETATM	23	O63	-0.1	1	-33.301	9.369	-12.274	0.00	0.00	O
HETATM	24	O65	-0.1	1	-35.793	8.880	-11.192	0.00	0.00	O
HETATM	25	C2	0.00	1	-30.687	5.782	-3.326	0.00	0.00	C
HETATM	26	C4	0.00	1	-28.393	6.041	-2.593	0.00	0.00	C
HETATM	27	C6	0.00	1	-29.483	7.817	-3.830	0.00	0.00	C
HETATM	28	C14	0.00	1	-35.876	2.278	-3.797	0.00	0.00	C
HETATM	29	C15	0.00	1	-35.776	3.134	-4.897	0.00	0.00	C
HETATM	30	C25	0.00	1	-33.293	9.752	-4.661	0.00	0.00	C
HETATM	31	C27	0.00	1	-32.561	8.860	-2.541	0.00	0.00	C
HETATM	32	C29	0.00	1	-33.903	10.879	-2.611	0.00	0.00	C
HETATM	33	C36	0.00	1	-34.787	9.368	-10.418	0.00	0.00	C
HETATM	34	C37	0.00	1	-33.520	9.621	-10.954	0.00	0.00	C
HETATM	35	H22	0.00	1	-33.382	6.209	-2.841	0.00	0.00	H
HETATM	36	H45	0.00	1	-35.301	9.892	-6.513	0.00	0.00	H
HETATM	37	H7	0.11	1	-27.437	7.908	-3.103	0.00	0.00	H
HETATM	38	H19	0.11	1	-35.133	1.833	-1.805	0.00	0.00	H
HETATM	39	H20	0.11	1	-34.818	4.852	-5.762	0.00	0.00	H
HETATM	40	H21	0.11	1	-33.531	3.716	-1.777	0.00	0.00	H
HETATM	41	H30	0.11	1	-33.184	9.975	-0.790	0.00	0.00	H
HETATM	42	H42	0.11	1	-31.506	10.320	-10.533	0.00	0.00	H
HETATM	43	H43	0.11	1	-31.953	10.746	-8.138	0.00	0.00	H
HETATM	44	H44	0.11	1	-36.039	9.400	-8.662	0.00	0.00	H
HETATM	45	H48	0.11	1	-29.599	4.275	-2.226	0.00	0.00	H
HETATM	46	H50	0.14	1	-36.773	0.706	-3.033	0.00	0.00	H
HETATM	47	H52	0.14	1	-37.142	2.186	-5.896	0.00	0.00	H
HETATM	48	H54	0.14	1	-35.074	12.477	-2.376	0.00	0.00	H

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Procyanidin B3 compact rotamer:

HETATM	1	C1	UNK	1	38.055	-20.522	33.292	0.00	0.00	C
HETATM	2	C2	UNK	1	37.527	-21.712	33.807	0.00	0.00	C
HETATM	3	C3	UNK	1	36.987	-22.695	32.962	0.00	0.00	C
HETATM	4	C4	UNK	1	36.995	-22.475	31.577	0.00	0.00	C
HETATM	5	C5	UNK	1	37.527	-21.292	31.059	0.00	0.00	C
HETATM	6	C6	UNK	1	38.052	-20.316	31.908	0.00	0.00	C
HETATM	7	C8	UNK	1	38.325	-21.171	36.004	0.00	0.00	C
HETATM	8	C9	UNK	1	38.119	-19.689	35.662	0.00	0.00	C
HETATM	9	O11	UNK	1	38.898	-18.849	36.520	0.00	0.00	O
HETATM	10	O13	UNK	1	36.482	-23.420	30.743	0.00	0.00	O
HETATM	11	O15	UNK	1	38.568	-19.161	31.407	0.00	0.00	O
HETATM	12	C17	UNK	1	38.497	-22.366	39.626	0.00	0.00	C
HETATM	13	C18	UNK	1	37.166	-22.267	40.028	0.00	0.00	C
HETATM	14	C19	UNK	1	36.202	-21.806	39.126	0.00	0.00	C
HETATM	15	C20	UNK	1	36.580	-21.450	37.828	0.00	0.00	C
HETATM	16	C21	UNK	1	37.917	-21.546	37.413	0.00	0.00	C
HETATM	17	C22	UNK	1	38.870	-22.008	38.330	0.00	0.00	C
HETATM	18	O27	UNK	1	37.500	-21.953	35.149	0.00	0.00	O
HETATM	19	O28	UNK	1	36.831	-22.623	41.297	0.00	0.00	O
HETATM	20	O30	UNK	1	34.908	-21.715	39.539	0.00	0.00	O
HETATM	21	C32	UNK	1	35.338	-23.760	34.606	0.00	0.00	C
HETATM	22	C33	UNK	1	35.393	-24.446	35.826	0.00	0.00	C

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Procyanidin B3 extended rotamer:

HETATM	1	C1	UNK	1	38.055	-20.522	33.292	0.00	0.00	C
HETATM	2	C2	UNK	1	37.527	-21.712	33.807	0.00	0.00	C
HETATM	3	C3	UNK	1	36.987	-22.695	32.962	0.00	0.00	C
HETATM	4	C4	UNK	1	36.995	-22.475	31.577	0.00	0.00	C
HETATM	5	C5	UNK	1	37.527	-21.292	31.059	0.00	0.00	C
HETATM	6	C6	UNK	1	38.052	-20.316	31.908	0.00	0.00	C
HETATM	7	C8	UNK	1	38.325	-21.171	36.004	0.00	0.00	C
HETATM	8	C9	UNK	1	38.119	-19.689	35.662	0.00	0.00	C
HETATM	9	O11	UNK	1	38.898	-18.849	36.520	0.00	0.00	O
HETATM	10	O13	UNK	1	36.482	-23.420	30.743	0.00	0.00	O
HETATM	11	O15	UNK	1	38.568	-19.161	31.407	0.00	0.00	O
HETATM	12	C17	UNK	1	38.497	-22.366	39.626	0.00	0.00	C
HETATM	13	C18	UNK	1	37.166	-22.267	40.028	0.00	0.00	C
HETATM	14	C19	UNK	1	36.202	-21.806	39.126	0.00	0.00	C
HETATM	15	C20	UNK	1	36.580	-21.450	37.828	0.00	0.00	C
HETATM	16	C21	UNK	1	37.917	-21.546	37.413	0.00	0.00	C
HETATM	17	C22	UNK	1	38.870	-22.008	38.330	0.00	0.00	C
HETATM	18	O27	UNK	1	37.500	-21.953	35.149	0.00	0.00	O
HETATM	19	O28	UNK	1	36.831	-22.623	41.297	0.00	0.00	O
HETATM	20	O30	UNK	1	34.908	-21.715	39.539	0.00	0.00	O
HETATM	21	C32	UNK	1	37.341	-25.170	33.511	0.00	0.00	C
HETATM	22	C33	UNK	1	36.881	-26.409	33.043	0.00	0.00	C
HETATM	23	C34	UNK	1	37.745	-27.501	32.960	0.00	0.00	C
HETATM	24	C35	UNK	1	39.074	-27.385	33.365	0.00	0.00	C
HETATM	25	C36	UNK	1	39.532	-26.165	33.857	0.00	0.00	C
HETATM	26	C37	UNK	1	38.675	-25.063	33.935	0.00	0.00	C
HETATM	27	C40	UNK	1	34.624	-25.709	33.192	0.00	0.00	C
HETATM	28	C41	UNK	1	36.411	-23.973	33.556	0.00	0.00	C

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Procyanidin B4 compact rotamer

HETATM	1	C1	UNK	1	-8.250	4.304	16.216	0.00	0.00	C
HETATM	2	C2	UNK	1	-7.179	5.118	15.823	0.00	0.00	C
HETATM	3	C3	UNK	1	-5.877	4.886	16.295	0.00	0.00	C
HETATM	4	C4	UNK	1	-5.656	3.811	17.168	0.00	0.00	C
HETATM	5	C5	UNK	1	-6.720	2.995	17.559	0.00	0.00	C
HETATM	6	C6	UNK	1	-8.011	3.237	17.090	0.00	0.00	C
HETATM	7	C8	UNK	1	-8.536	6.187	14.167	0.00	0.00	C
HETATM	8	C9	UNK	1	-9.777	5.953	15.041	0.00	0.00	C
HETATM	9	O11	UNK	1	-9.916	6.952	16.059	0.00	0.00	O
HETATM	10	O13	UNK	1	-4.399	3.566	17.630	0.00	0.00	O
HETATM	11	O15	UNK	1	-9.051	2.444	17.468	0.00	0.00	O
HETATM	12	C17	UNK	1	-8.850	8.717	11.329	0.00	0.00	C
HETATM	13	C18	UNK	1	-8.508	9.912	11.960	0.00	0.00	C
HETATM	14	C19	UNK	1	-8.177	9.908	13.318	0.00	0.00	C
HETATM	15	C20	UNK	1	-8.190	8.706	14.032	0.00	0.00	C
HETATM	16	C21	UNK	1	-8.535	7.498	13.408	0.00	0.00	C
HETATM	17	C22	UNK	1	-8.864	7.520	12.046	0.00	0.00	C
HETATM	18	O27	UNK	1	-7.369	6.170	14.979	0.00	0.00	O
HETATM	19	O28	UNK	1	-8.503	11.063	11.235	0.00	0.00	O
HETATM	20	O30	UNK	1	-7.848	11.086	13.915	0.00	0.00	O
HETATM	21	C32	UNK	1	-4.931	7.262	16.147	0.00	0.00	C
HETATM	22	C33	UNK	1	-4.686	8.222	15.157	0.00	0.00	C
HETATM	23	C34	UNK	1	-4.904	9.575	15.413	0.00	0.00	C
HETATM	24	C35	UNK	1	-5.348	9.999	16.663	0.00	0.00	C
HETATM	25	C36	UNK	1	-5.567	9.054	17.665	0.00	0.00	C
HETATM	26	C37	UNK	1	-5.357	7.694	17.414	0.00	0.00	C
HETATM	27	C40	UNK	1	-3.555	6.646	13.793	0.00	0.00	C
HETATM	28	C41	UNK	1	-4.733	5.788	15.851	0.00	0.00	C
HETATM	29	C42	UNK	1	-4.444	5.529	14.353	0.00	0.00	C
HETATM	30	O44	UNK	1	-3.762	4.273	14.212	0.00	0.00	O
HETATM	31	O46	UNK	1	-5.550	11.328	16.870	0.00	0.00	O
HETATM	32	O48	UNK	1	-5.564	6.778	18.398	0.00	0.00	O
HETATM	33	C50	UNK	1	-1.756	5.942	10.497	0.00	0.00	C
HETATM	34	C51	UNK	1	-2.768	6.158	9.563	0.00	0.00	C

HETATM	35	C52 UNK	1	-4.043	6.535	9.997	0.00	0.00	C
HETATM	36	C53 UNK	1	-4.293	6.691	11.363	0.00	0.00	C
HETATM	37	C54 UNK	1	-3.280	6.477	12.311	0.00	0.00	C
HETATM	38	C55 UNK	1	-2.009	6.099	11.860	0.00	0.00	C
HETATM	39	O60 UNK	1	-4.232	7.890	13.919	0.00	0.00	O
HETATM	40	O61 UNK	1	-2.491	5.997	8.241	0.00	0.00	O
HETATM	41	O63 UNK	1	-5.018	6.742	9.070	0.00	0.00	O
HETATM	42	C66 UNK	1	-9.645	4.581	15.710	0.00	0.00	C
HETATM	43	H7 UNK	1	-6.538	2.152	18.246	0.00	0.00	H
HETATM	44	H10 UNK	1	-10.690	5.953	14.400	0.00	0.00	H
HETATM	45	H12 UNK	1	-10.425	7.677	15.702	0.00	0.00	H
HETATM	46	H14 UNK	1	-4.338	2.804	18.232	0.00	0.00	H
HETATM	47	H16 UNK	1	-8.800	1.727	18.076	0.00	0.00	H
HETATM	48	H23 UNK	1	-9.110	8.718	10.257	0.00	0.00	H
HETATM	49	H24 UNK	1	-7.922	8.707	15.102	0.00	0.00	H
HETATM	50	H25 UNK	1	-9.137	6.586	11.526	0.00	0.00	H
HETATM	51	H26 UNK	1	-8.462	5.358	13.427	0.00	0.00	H
HETATM	52	H29 UNK	1	-8.247	11.824	11.785	0.00	0.00	H
HETATM	53	H31 UNK	1	-7.643	10.999	14.863	0.00	0.00	H
HETATM	54	H38 UNK	1	-4.718	10.318	14.619	0.00	0.00	H
HETATM	55	H39 UNK	1	-5.909	9.382	18.660	0.00	0.00	H
HETATM	56	H43 UNK	1	-5.390	5.509	13.767	0.00	0.00	H
HETATM	57	H45 UNK	1	-4.415	3.578	14.166	0.00	0.00	H
HETATM	58	H47 UNK	1	-5.857	11.538	17.769	0.00	0.00	H
HETATM	59	H49 UNK	1	-5.873	7.159	19.239	0.00	0.00	H
HETATM	60	H56 UNK	1	-0.750	5.643	10.156	0.00	0.00	H
HETATM	61	H57 UNK	1	-5.301	6.989	11.699	0.00	0.00	H
HETATM	62	H58 UNK	1	-1.195	5.920	12.584	0.00	0.00	H
HETATM	63	H59 UNK	1	-2.594	6.686	14.354	0.00	0.00	H
HETATM	64	H62 UNK	1	-3.275	6.176	7.691	0.00	0.00	H
HETATM	65	H64 UNK	1	-5.873	7.005	9.455	0.00	0.00	H
HETATM	66	H65 UNK	1	-3.812	5.506	16.415	0.00	0.00	H
HETATM	67	H67 UNK	1	-9.906	3.789	14.970	0.00	0.00	H
HETATM	68	H68 UNK	1	-10.384	4.498	16.538	0.00	0.00	H
CONNECT	1	2							
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CONNECT 68 42
END

Procyanidin B4 extended rotamer:

HETATM	1	C1	UNK	1	13.943	51.505	-30.872	0.00	0.00	C
HETATM	2	C2	UNK	1	14.017	50.153	-30.514	0.00	0.00	C
HETATM	3	C3	UNK	1	13.016	49.246	-30.903	0.00	0.00	C
HETATM	4	C4	UNK	1	11.938	49.714	-31.668	0.00	0.00	C
HETATM	5	C5	UNK	1	11.868	51.059	-32.034	0.00	0.00	C
HETATM	6	C6	UNK	1	12.861	51.955	-31.638	0.00	0.00	C
HETATM	7	C8	UNK	1	16.218	50.464	-29.586	0.00	0.00	C
HETATM	8	C9	UNK	1	15.833	51.914	-29.252	0.00	0.00	C
HETATM	9	O11	UNK	1	15.062	51.999	-28.048	0.00	0.00	O
HETATM	10	O13	UNK	1	10.961	48.848	-32.054	0.00	0.00	O
HETATM	11	O15	UNK	1	12.795	53.269	-31.988	0.00	0.00	O
HETATM	12	C17	UNK	1	19.266	49.287	-27.619	0.00	0.00	C
HETATM	13	C18	UNK	1	18.685	48.606	-26.550	0.00	0.00	C
HETATM	14	C19	UNK	1	17.293	48.524	-26.456	0.00	0.00	C
HETATM	15	C20	UNK	1	16.494	49.124	-27.434	0.00	0.00	C
HETATM	16	C21	UNK	1	17.068	49.811	-28.514	0.00	0.00	C
HETATM	17	C22	UNK	1	18.465	49.883	-28.593	0.00	0.00	C
HETATM	18	O27	UNK	1	15.046	49.674	-29.757	0.00	0.00	O
HETATM	19	O28	UNK	1	19.492	48.034	-25.615	0.00	0.00	O
HETATM	20	O30	UNK	1	16.745	47.854	-25.405	0.00	0.00	O
HETATM	21	C32	UNK	1	12.962	46.781	-31.626	0.00	0.00	C
HETATM	22	C33	UNK	1	12.115	45.673	-31.495	0.00	0.00	C
HETATM	23	C34	UNK	1	11.960	44.770	-32.548	0.00	0.00	C
HETATM	24	C35	UNK	1	12.667	44.942	-33.737	0.00	0.00	C
HETATM	25	C36	UNK	1	13.537	46.023	-33.863	0.00	0.00	C
HETATM	26	C37	UNK	1	13.690	46.938	-32.817	0.00	0.00	C
HETATM	27	C40	UNK	1	11.937	46.004	-29.160	0.00	0.00	C
HETATM	28	C41	UNK	1	13.095	47.781	-30.495	0.00	0.00	C
HETATM	29	C42	UNK	1	12.066	47.517	-29.373	0.00	0.00	C
HETATM	30	O44	UNK	1	12.516	48.125	-28.153	0.00	0.00	O
HETATM	31	O46	UNK	1	12.543	44.076	-34.778	0.00	0.00	O
HETATM	32	O48	UNK	1	14.549	47.986	-32.944	0.00	0.00	O
HETATM	33	C50	UNK	1	10.555	44.766	-25.822	0.00	0.00	C
HETATM	34	C51	UNK	1	9.184	44.964	-25.982	0.00	0.00	C
HETATM	35	C52	UNK	1	8.697	45.502	-27.176	0.00	0.00	C
HETATM	36	C53	UNK	1	9.586	45.837	-28.202	0.00	0.00	C
HETATM	37	C54	UNK	1	10.967	45.641	-28.052	0.00	0.00	C
HETATM	38	C55	UNK	1	11.439	45.102	-26.848	0.00	0.00	C
HETATM	39	O60	UNK	1	11.422	45.421	-30.351	0.00	0.00	O
HETATM	40	O61	UNK	1	8.346	44.627	-24.965	0.00	0.00	O

HETATM	41	O63 UNK	1	7.355	45.688	-27.311	0.00	0.00	O
HETATM	42	C66 UNK	1	15.006	52.472	-30.412	0.00	0.00	C
HETATM	43	H7 UNK	1	11.018	51.418	-32.638	0.00	0.00	H
HETATM	44	H10 UNK	1	16.756	52.530	-29.142	0.00	0.00	H
HETATM	45	H12 UNK	1	15.663	52.020	-27.306	0.00	0.00	H
HETATM	46	H14 UNK	1	10.260	49.253	-32.594	0.00	0.00	H
HETATM	47	H16 UNK	1	12.012	53.496	-32.520	0.00	0.00	H
HETATM	48	H23 UNK	1	20.365	49.354	-27.694	0.00	0.00	H
HETATM	49	H24 UNK	1	15.396	49.056	-27.352	0.00	0.00	H
HETATM	50	H25 UNK	1	18.946	50.418	-29.431	0.00	0.00	H
HETATM	51	H26 UNK	1	16.792	50.456	-30.541	0.00	0.00	H
HETATM	52	H29 UNK	1	18.970	47.590	-24.923	0.00	0.00	H
HETATM	53	H31 UNK	1	15.772	47.839	-25.417	0.00	0.00	H
HETATM	54	H38 UNK	1	11.281	43.910	-32.426	0.00	0.00	H
HETATM	55	H39 UNK	1	14.104	46.151	-34.800	0.00	0.00	H
HETATM	56	H43 UNK	1	11.069	47.926	-29.652	0.00	0.00	H
HETATM	57	H45 UNK	1	12.270	49.048	-28.166	0.00	0.00	H
HETATM	58	H47 UNK	1	11.918	43.350	-34.606	0.00	0.00	H
HETATM	59	H49 UNK	1	15.003	48.026	-33.803	0.00	0.00	H
HETATM	60	H56 UNK	1	10.942	44.342	-24.879	0.00	0.00	H
HETATM	61	H57 UNK	1	9.196	46.262	-29.142	0.00	0.00	H
HETATM	62	H58 UNK	1	12.521	44.940	-26.700	0.00	0.00	H
HETATM	63	H59 UNK	1	12.936	45.568	-28.934	0.00	0.00	H
HETATM	64	H62 UNK	1	7.418	44.812	-25.196	0.00	0.00	H
HETATM	65	H64 UNK	1	7.097	46.065	-28.171	0.00	0.00	H
HETATM	66	H65 UNK	1	14.105	47.583	-30.064	0.00	0.00	H
HETATM	67	H67 UNK	1	15.678	52.689	-31.274	0.00	0.00	H
HETATM	68	H68 UNK	1	14.551	53.442	-30.108	0.00	0.00	H
CONECT	1	2							
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CONECT	2	1							
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CONECT 68 42
END

PDB coordinates for 6 Histatin conformers:

Histatin conformer 1:

ATOM	1	N	ASP	1	-0.753	-1.254	-0.000	1.00	1.00	TAG N1+
ATOM	2	CA	ASP	1	0.000	0.000	0.000	1.00	1.00	TAG C
ATOM	3	C	ASP	1	-0.977	1.136	0.278	1.00	1.00	TAG C
ATOM	4	O	ASP	1	-0.823	1.876	1.260	1.00	1.00	TAG O
ATOM	5	CB	ASP	1	0.960	0.376	-1.135	1.00	1.00	TAG C
ATOM	6	CG	ASP	1	1.770	1.663	-0.847	1.00	1.00	TAG C
ATOM	7	OD1	ASP	1	1.890	2.102	0.330	1.00	1.00	TAG O
ATOM	8	OD2	ASP	1	2.303	2.244	-1.824	1.00	1.00	TAG O
ATOM	9	1H	ASP	1	-0.117	-2.025	-0.000	1.00	1.00	TAG H
ATOM	10	2H	ASP	1	-1.329	-1.298	0.816	1.00	1.00	TAG H
ATOM	11	3H	ASP	1	-1.329	-1.298	-0.816	1.00	1.00	TAG H
ATOM	12	HA	ASP	1	0.619	-0.185	0.890	1.00	1.00	TAG H
ATOM	13	1HB	ASP	1	1.657	-0.458	-1.309	1.00	1.00	TAG H
ATOM	14	2HB	ASP	1	0.385	0.512	-2.063	1.00	1.00	TAG H
ATOM	15	H01	ASP	1	2.345	3.187	-1.652	1.00	1.00	TAG H
ATOM	16	N	SER	2	-1.967	1.311	-0.528	1.00	1.00	TAG N
ATOM	17	CA	SER	2	-2.992	2.337	-0.341	1.00	1.00	TAG C
ATOM	18	C	SER	2	-4.416	1.801	-0.329	1.00	1.00	TAG C
ATOM	19	O	SER	2	-5.328	2.145	0.408	1.00	1.00	TAG O
ATOM	20	CB	SER	2	-2.874	3.386	-1.449	1.00	1.00	TAG C
ATOM	21	OG	SER	2	-3.946	4.308	-1.377	1.00	1.00	TAG O
ATOM	22	H	SER	2	-2.106	0.753	-1.346	1.00	1.00	TAG H
ATOM	23	HA	SER	2	-2.807	2.770	0.653	1.00	1.00	TAG H
ATOM	24	1HB	SER	2	-1.917	3.920	-1.357	1.00	1.00	TAG H
ATOM	25	2HB	SER	2	-2.873	2.892	-2.432	1.00	1.00	TAG H
ATOM	26	HG	SER	2	-3.853	4.986	-2.106	1.00	1.00	TAG H
ATOM	27	N	HIS	3	-4.661	0.820	-1.300	1.00	0.00	TAG N
ATOM	28	CA	HIS	3	-5.959	0.168	-1.448	1.00	0.00	TAG C
ATOM	29	C	HIS	3	-6.059	-1.049	-0.561	1.00	0.00	TAG C
ATOM	30	O	HIS	3	-6.895	-1.115	0.383	1.00	0.00	TAG O
ATOM	31	CB	HIS	3	-6.074	-0.235	-2.927	1.00	0.00	TAG C
ATOM	32	CG	HIS	3	-6.002	0.948	-3.848	1.00	0.00	TAG C
ATOM	33	CD2	HIS	3	-4.928	1.173	-4.698	1.00	0.00	TAG C
ATOM	34	ND1	HIS	3	-6.968	1.944	-3.973	1.00	0.00	TAG N
ATOM	35	CE1	HIS	3	-6.384	2.716	-4.908	1.00	0.00	TAG C
ATOM	36	NE2	HIS	3	-5.173	2.328	-5.394	1.00	0.00	TAG N
ATOM	37	H	HIS	3	-3.919	0.556	-1.913	1.00	0.00	TAG H
ATOM	38	HA	HIS	3	-6.730	0.877	-1.100	1.00	0.00	TAG H
ATOM	39	2HB	HIS	3	-7.028	-0.764	-3.125	1.00	0.00	TAG H
ATOM	40	3HB	HIS	3	-5.276	-0.945	-3.230	1.00	0.00	TAG H
ATOM	41	2HD	HIS	3	-4.058	0.527	-4.774	1.00	0.00	TAG H
ATOM	42	1HE	HIS	3	-6.913	3.604	-5.227	1.00	0.00	TAG H
ATOM	43	2HE	HIS	3	-4.582	2.783	-6.104	1.00	0.00	TAG H
ATOM	44	N	ALA	4	-5.202	-2.035	-0.778	1.00	1.00	TAG N

ATOM	45	CA	ALA	4	-5.192	-3.266	-0.011	1.00	1.00	TAG	C
ATOM	46	C	ALA	4	-4.714	-2.982	1.424	1.00	1.00	TAG	C
ATOM	47	O	ALA	4	-5.377	-3.380	2.377	1.00	1.00	TAG	O
ATOM	48	CB	ALA	4	-4.266	-4.278	-0.684	1.00	1.00	TAG	C
ATOM	49	H	ALA	4	-4.512	-2.005	-1.501	1.00	1.00	TAG	H
ATOM	50	HA	ALA	4	-6.209	-3.681	0.030	1.00	1.00	TAG	H
ATOM	51	1HB	ALA	4	-4.258	-5.212	-0.102	1.00	1.00	TAG	H
ATOM	52	2HB	ALA	4	-4.625	-4.484	-1.702	1.00	1.00	TAG	H
ATOM	53	3HB	ALA	4	-3.247	-3.867	-0.732	1.00	1.00	TAG	H
ATOM	54	N	LYS	5	-3.619	-2.328	1.601	1.00	1.00	TAG	N
ATOM	55	CA	LYS	5	-3.104	-1.996	2.924	1.00	1.00	TAG	C
ATOM	56	C	LYS	5	-4.103	-1.123	3.673	1.00	1.00	TAG	C
ATOM	57	O	LYS	5	-4.500	-1.455	4.775	1.00	1.00	TAG	O
ATOM	58	CB	LYS	5	-1.757	-1.275	2.809	1.00	1.00	TAG	C
ATOM	59	CG	LYS	5	-0.625	-2.187	2.408	1.00	1.00	TAG	C
ATOM	60	CD	LYS	5	0.677	-1.429	2.265	1.00	1.00	TAG	C
ATOM	61	CE	LYS	5	1.780	-2.386	1.825	1.00	1.00	TAG	C
ATOM	62	NZ	LYS	5	3.031	-1.688	1.433	1.00	1.00	TAG	N
ATOM	63	H	LYS	5	-3.045	-2.002	0.850	1.00	1.00	TAG	H
ATOM	64	HA	LYS	5	-2.956	-2.931	3.485	1.00	1.00	TAG	H
ATOM	65	1HB	LYS	5	-1.845	-0.464	2.070	1.00	1.00	TAG	H
ATOM	66	2HB	LYS	5	-1.516	-0.805	3.775	1.00	1.00	TAG	H
ATOM	67	1HG	LYS	5	-0.508	-2.980	3.161	1.00	1.00	TAG	H
ATOM	68	2HG	LYS	5	-0.870	-2.680	1.456	1.00	1.00	TAG	H
ATOM	69	1HD	LYS	5	0.564	-0.620	1.530	1.00	1.00	TAG	H
ATOM	70	2HD	LYS	5	0.947	-0.958	3.223	1.00	1.00	TAG	H
ATOM	71	1HE	LYS	5	1.998	-3.088	2.643	1.00	1.00	TAG	H
ATOM	72	2HE	LYS	5	1.420	-2.986	0.976	1.00	1.00	TAG	H
ATOM	73	H01	LYS	5	3.285	-1.023	2.150	1.00	1.00	TAG	H
ATOM	74	H02	LYS	5	2.887	-1.203	0.559	1.00	1.00	TAG	H
ATOM	75	N	ARG	6	-4.521	-0.029	3.077	1.00	1.00	TAG	N
ATOM	76	CA	ARG	6	-5.451	0.928	3.704	1.00	1.00	TAG	C
ATOM	77	C	ARG	6	-6.815	0.288	3.908	1.00	1.00	TAG	C
ATOM	78	O	ARG	6	-7.336	0.249	5.033	1.00	1.00	TAG	O
ATOM	79	CB	ARG	6	-5.604	2.222	2.893	1.00	1.00	TAG	C
ATOM	80	CG	ARG	6	-4.366	3.070	2.832	1.00	1.00	TAG	C
ATOM	81	CD	ARG	6	-3.997	3.621	4.188	1.00	1.00	TAG	C
ATOM	82	NE	ARG	6	-2.577	3.954	4.232	1.00	1.00	TAG	N
ATOM	83	CZ	ARG	6	-2.057	4.953	4.936	1.00	1.00	TAG	C
ATOM	84	NH1	ARG	6	-2.848	5.783	5.619	1.00	1.00	TAG	N
ATOM	85	NH2	ARG	6	-0.742	5.161	4.903	1.00	1.00	TAG	N1+
ATOM	86	H	ARG	6	-4.238	0.233	2.155	1.00	1.00	TAG	H
ATOM	87	HA	ARG	6	-5.016	1.199	4.678	1.00	1.00	TAG	H
ATOM	88	1HB	ARG	6	-5.905	1.962	1.867	1.00	1.00	TAG	H
ATOM	89	2HB	ARG	6	-6.421	2.818	3.327	1.00	1.00	TAG	H
ATOM	90	1HG	ARG	6	-3.530	2.471	2.440	1.00	1.00	TAG	H
ATOM	91	2HG	ARG	6	-4.524	3.901	2.129	1.00	1.00	TAG	H
ATOM	92	1HD	ARG	6	-4.597	4.517	4.402	1.00	1.00	TAG	H
ATOM	93	2HD	ARG	6	-4.231	2.882	4.968	1.00	1.00	TAG	H
ATOM	94	HE	ARG	6	-1.950	3.390	3.693	1.00	1.00	TAG	H
ATOM	95	H01	ARG	6	-3.848	5.639	5.623	1.00	1.00	TAG	H

ATOM	96	H02	ARG	6	-2.447	6.555	6.132	1.00	1.00	TAG	H
ATOM	97	H03	ARG	6	-0.420	5.430	5.822	1.00	1.00	TAG	H
ATOM	98	H04	ARG	6	-0.533	5.897	4.244	1.00	1.00	TAG	H
ATOM	99	H05	ARG	6	-0.274	4.312	4.618	1.00	1.00	TAG	H
ATOM	100	N	HIS	7	-7.432	-0.226	2.855	1.00	1.00	TAG	N
ATOM	101	CA	HIS	7	-8.772	-0.793	2.911	1.00	1.00	TAG	C
ATOM	102	C	HIS	7	-8.825	-2.297	3.184	1.00	1.00	TAG	C
ATOM	103	O	HIS	7	-9.644	-2.786	3.977	1.00	1.00	TAG	O
ATOM	104	CB	HIS	7	-9.569	-0.423	1.666	1.00	1.00	TAG	C
ATOM	105	CG	HIS	7	-10.133	0.960	1.717	1.00	1.00	TAG	C
ATOM	106	CD2	HIS	7	-9.488	2.050	1.174	1.00	1.00	TAG	C
ATOM	107	ND1	HIS	7	-11.273	1.442	2.276	1.00	1.00	TAG	N
ATOM	108	CE1	HIS	7	-11.292	2.796	2.065	1.00	1.00	TAG	C
ATOM	109	NE2	HIS	7	-10.204	3.144	1.396	1.00	1.00	TAG	N
ATOM	110	H	HIS	7	-7.020	-0.262	1.945	1.00	1.00	TAG	H
ATOM	111	HA	HIS	7	-9.243	-0.336	3.793	1.00	1.00	TAG	H
ATOM	112	1HB	HIS	7	-8.920	-0.515	0.784	1.00	1.00	TAG	H
ATOM	113	2HB	HIS	7	-10.390	-1.143	1.537	1.00	1.00	TAG	H
ATOM	114	HD1	HIS	7	-11.971	0.907	2.754	1.00	1.00	TAG	H
ATOM	115	HD2	HIS	7	-8.528	2.017	0.638	1.00	1.00	TAG	H
ATOM	116	HE1	HIS	7	-12.084	3.483	2.398	1.00	1.00	TAG	H
ATOM	117	N	HIS	8	-7.942	-3.062	2.524	1.00	1.00	TAG	N
ATOM	118	CA	HIS	8	-8.024	-4.516	2.535	1.00	1.00	TAG	C
ATOM	119	C	HIS	8	-7.639	-5.173	3.861	1.00	1.00	TAG	C
ATOM	120	O	HIS	8	-7.288	-6.359	3.894	1.00	1.00	TAG	O
ATOM	121	CB	HIS	8	-7.244	-5.111	1.370	1.00	1.00	TAG	C
ATOM	122	CG	HIS	8	-7.989	-5.063	0.075	1.00	1.00	TAG	C
ATOM	123	CD2	HIS	8	-8.919	-5.897	-0.454	1.00	1.00	TAG	C
ATOM	124	ND1	HIS	8	-7.839	-4.038	-0.834	1.00	1.00	TAG	N
ATOM	125	CE1	HIS	8	-8.645	-4.241	-1.868	1.00	1.00	TAG	C
ATOM	126	NE2	HIS	8	-9.309	-5.367	-1.657	1.00	1.00	TAG	N
ATOM	127	H	HIS	8	-7.181	-2.696	1.988	1.00	1.00	TAG	H
ATOM	128	HA	HIS	8	-9.092	-4.747	2.413	1.00	1.00	TAG	H
ATOM	129	1HB	HIS	8	-6.293	-4.569	1.259	1.00	1.00	TAG	H
ATOM	130	2HB	HIS	8	-6.993	-6.156	1.603	1.00	1.00	TAG	H
ATOM	131	HD2	HIS	8	-9.292	-6.828	-0.002	1.00	1.00	TAG	H
ATOM	132	HE1	HIS	8	-8.744	-3.587	-2.747	1.00	1.00	TAG	H
ATOM	133	HE2	HIS	8	-9.986	-5.767	-2.275	1.00	1.00	TAG	H
ATOM	134	N	GLY	9	-7.888	-4.361	4.956	1.00	1.00	TAG	N
ATOM	135	CA	GLY	9	-7.682	-4.810	6.344	1.00	1.00	TAG	C
ATOM	136	C	GLY	9	-6.309	-5.442	6.609	1.00	1.00	TAG	C
ATOM	137	O	GLY	9	-6.198	-6.481	7.266	1.00	1.00	TAG	O
ATOM	138	H	GLY	9	-8.221	-3.421	4.879	1.00	1.00	TAG	H
ATOM	139	1HA	GLY	9	-7.812	-3.950	7.017	1.00	1.00	TAG	H
ATOM	140	2HA	GLY	9	-8.463	-5.540	6.600	1.00	1.00	TAG	H
ATOM	141	N	TYR	10	-5.292	-4.815	6.069	1.00	0.00	TAG	N
ATOM	142	CA	TYR	10	-3.921	-5.266	6.293	1.00	0.00	TAG	C
ATOM	143	C	TYR	10	-3.261	-4.467	7.390	1.00	0.00	TAG	C
ATOM	144	O	TYR	10	-2.087	-4.617	7.648	1.00	0.00	TAG	O
ATOM	145	CB	TYR	10	-3.066	-5.108	5.002	1.00	0.00	TAG	C
ATOM	146	CG	TYR	10	-3.519	-5.906	3.774	1.00	0.00	TAG	C

ATOM	147	CD1	TYR	10	-4.425	-6.963	3.905	1.00	0.00	TAG	C
ATOM	148	CD2	TYR	10	-3.030	-5.569	2.508	1.00	0.00	TAG	C
ATOM	149	CE1	TYR	10	-4.840	-7.670	2.780	1.00	0.00	TAG	C
ATOM	150	CE2	TYR	10	-3.446	-6.277	1.385	1.00	0.00	TAG	C
ATOM	151	CZ	TYR	10	-4.351	-7.328	1.522	1.00	0.00	TAG	C
ATOM	152	OH	TYR	10	-4.763	-8.023	0.420	1.00	0.00	TAG	O
ATOM	153	H	TYR	10	-5.457	-4.016	5.494	1.00	0.00	TAG	H
ATOM	154	HA	TYR	10	-3.940	-6.326	6.609	1.00	0.00	TAG	H
ATOM	155	2HB	TYR	10	-2.016	-5.391	5.214	1.00	0.00	TAG	H
ATOM	156	3HB	TYR	10	-2.994	-4.032	4.739	1.00	0.00	TAG	H
ATOM	157	1HD	TYR	10	-4.814	-7.232	4.877	1.00	0.00	TAG	H
ATOM	158	2HD	TYR	10	-2.336	-4.748	2.393	1.00	0.00	TAG	H
ATOM	159	1HE	TYR	10	-5.545	-8.482	2.878	1.00	0.00	TAG	H
ATOM	160	2HE	TYR	10	-3.066	-6.003	0.412	1.00	0.00	TAG	H
ATOM	161	HH	TYR	10	-4.331	-7.652	-0.352	1.00	0.00	TAG	H
ATOM	162	N	LYS	11	-3.892	-3.668	8.085	1.00	1.00	TAG	N
ATOM	163	CA	LYS	11	-3.294	-2.737	9.036	1.00	1.00	TAG	C
ATOM	164	C	LYS	11	-2.940	-3.472	10.314	1.00	1.00	TAG	C
ATOM	165	O	LYS	11	-1.829	-3.281	10.829	1.00	1.00	TAG	O
ATOM	166	CB	LYS	11	-4.267	-1.595	9.331	1.00	1.00	TAG	C
ATOM	167	CG	LYS	11	-3.735	-0.527	10.264	1.00	1.00	TAG	C
ATOM	168	CD	LYS	11	-4.484	0.771	10.024	1.00	1.00	TAG	C
ATOM	169	CE	LYS	11	-4.027	1.883	10.948	1.00	1.00	TAG	C
ATOM	170	NZ	LYS	11	-4.621	1.712	12.291	1.00	1.00	TAG	N
ATOM	171	H	LYS	11	-4.888	-3.589	8.046	1.00	1.00	TAG	H
ATOM	172	HA	LYS	11	-2.377	-2.314	8.602	1.00	1.00	TAG	H
ATOM	173	1HB	LYS	11	-4.552	-1.121	8.380	1.00	1.00	TAG	H
ATOM	174	2HB	LYS	11	-5.184	-2.018	9.768	1.00	1.00	TAG	H
ATOM	175	1HG	LYS	11	-3.854	-0.845	11.310	1.00	1.00	TAG	H
ATOM	176	2HG	LYS	11	-2.658	-0.379	10.094	1.00	1.00	TAG	H
ATOM	177	1HD	LYS	11	-4.343	1.085	8.979	1.00	1.00	TAG	H
ATOM	178	2HD	LYS	11	-5.562	0.600	10.166	1.00	1.00	TAG	H
ATOM	179	1HE	LYS	11	-2.930	1.880	11.021	1.00	1.00	TAG	H
ATOM	180	2HE	LYS	11	-4.319	2.858	10.531	1.00	1.00	TAG	H
ATOM	181	H01	LYS	11	-4.641	2.603	12.767	1.00	1.00	TAG	H
ATOM	182	H02	LYS	11	-4.067	1.057	12.824	1.00	1.00	TAG	H
ATOM	183	N	ARG	12	-3.728	-4.258	10.860	1.00	1.00	TAG	N
ATOM	184	CA	ARG	12	-3.534	-4.912	12.144	1.00	1.00	TAG	C
ATOM	185	C	ARG	12	-2.344	-5.830	11.877	1.00	1.00	TAG	C
ATOM	186	O	ARG	12	-1.641	-6.104	12.999	1.00	1.00	TAG	O
ATOM	187	CB	ARG	12	-4.797	-5.705	12.494	1.00	1.00	TAG	C
ATOM	188	CG	ARG	12	-4.753	-6.411	13.848	1.00	1.00	TAG	C
ATOM	189	CD	ARG	12	-6.139	-6.871	14.282	1.00	1.00	TAG	C
ATOM	190	NE	ARG	12	-6.897	-7.440	13.171	1.00	1.00	TAG	N
ATOM	191	CZ	ARG	12	-8.153	-7.110	12.872	1.00	1.00	TAG	C
ATOM	192	NH1	ARG	12	-8.806	-6.212	13.606	1.00	1.00	TAG	N
ATOM	193	NH2	ARG	12	-8.751	-7.666	11.821	1.00	1.00	TAG	N1+
ATOM	194	H	ARG	12	-4.597	-4.509	10.435	1.00	1.00	TAG	H
ATOM	195	HA	ARG	12	-3.353	-4.231	12.987	1.00	1.00	TAG	H
ATOM	196	1HB	ARG	12	-5.658	-5.021	12.481	1.00	1.00	TAG	H
ATOM	197	2HB	ARG	12	-4.970	-6.457	11.710	1.00	1.00	TAG	H

ATOM	198	1HG	ARG	12	-4.079	-7.278	13.790	1.00	1.00	TAG	H
ATOM	199	2HG	ARG	12	-4.337	-5.730	14.605	1.00	1.00	TAG	H
ATOM	200	1HD	ARG	12	-6.042	-7.620	15.081	1.00	1.00	TAG	H
ATOM	201	2HD	ARG	12	-6.692	-6.019	14.705	1.00	1.00	TAG	H
ATOM	202	HE	ARG	12	-6.444	-8.122	12.596	1.00	1.00	TAG	H
ATOM	203	1HH1	ARG	12	-8.354	-5.781	14.387	1.00	1.00	TAG	H
ATOM	204	2HH1	ARG	12	-9.749	-5.968	13.377	1.00	1.00	TAG	H
ATOM	205	H01	ARG	12	-8.993	-8.622	12.038	1.00	1.00	TAG	H
ATOM	206	H02	ARG	12	-8.125	-7.648	11.028	1.00	1.00	TAG	H
ATOM	207	H03	ARG	12	-9.590	-7.149	11.599	1.00	1.00	TAG	H
ATOM	208	N	LYS	13	-2.090	-6.451	10.909	1.00	1.00	TAG	N
ATOM	209	CA	LYS	13	-0.848	-7.156	10.616	1.00	1.00	TAG	C
ATOM	210	C	LYS	13	0.189	-6.186	10.065	1.00	1.00	TAG	C
ATOM	211	O	LYS	13	1.265	-6.032	10.662	1.00	1.00	TAG	O
ATOM	212	CB	LYS	13	-1.098	-8.286	9.611	1.00	1.00	TAG	C
ATOM	213	CG	LYS	13	-1.827	-9.464	10.209	1.00	1.00	TAG	C
ATOM	214	CD	LYS	13	-2.089	-10.538	9.175	1.00	1.00	TAG	C
ATOM	215	CE	LYS	13	-2.859	-11.688	9.819	1.00	1.00	TAG	C
ATOM	216	NZ	LYS	13	-3.363	-12.673	8.830	1.00	1.00	TAG	N
ATOM	217	H	LYS	13	-2.755	-6.546	10.167	1.00	1.00	TAG	H
ATOM	218	HA	LYS	13	-0.466	-7.594	11.549	1.00	1.00	TAG	H
ATOM	219	1HB	LYS	13	-1.682	-7.894	8.766	1.00	1.00	TAG	H
ATOM	220	2HB	LYS	13	-0.134	-8.627	9.206	1.00	1.00	TAG	H
ATOM	221	1HG	LYS	13	-1.232	-9.885	11.034	1.00	1.00	TAG	H
ATOM	222	2HG	LYS	13	-2.781	-9.127	10.641	1.00	1.00	TAG	H
ATOM	223	1HD	LYS	13	-2.665	-10.121	8.336	1.00	1.00	TAG	H
ATOM	224	2HD	LYS	13	-1.138	-10.906	8.762	1.00	1.00	TAG	H
ATOM	225	1HE	LYS	13	-2.206	-12.201	10.540	1.00	1.00	TAG	H
ATOM	226	2HE	LYS	13	-3.708	-11.280	10.388	1.00	1.00	TAG	H
ATOM	227	H01	LYS	13	-3.573	-13.543	9.298	1.00	1.00	TAG	H
ATOM	228	H02	LYS	13	-2.659	-12.831	8.123	1.00	1.00	TAG	H
ATOM	229	N	PHE	14	-0.041	-5.505	8.993	1.00	0.00	TAG	N
ATOM	230	CA	PHE	14	1.006	-4.765	8.296	1.00	0.00	TAG	C
ATOM	231	C	PHE	14	1.222	-3.409	8.924	1.00	0.00	TAG	C
ATOM	232	O	PHE	14	2.115	-2.644	8.478	1.00	0.00	TAG	O
ATOM	233	CB	PHE	14	0.618	-4.569	6.799	1.00	0.00	TAG	C
ATOM	234	CG	PHE	14	0.563	-5.838	5.934	1.00	0.00	TAG	C
ATOM	235	CD1	PHE	14	1.154	-7.018	6.400	1.00	0.00	TAG	C
ATOM	236	CD2	PHE	14	-0.015	-5.814	4.662	1.00	0.00	TAG	C
ATOM	237	CE1	PHE	14	1.183	-8.153	5.597	1.00	0.00	TAG	C
ATOM	238	CE2	PHE	14	0.006	-6.953	3.862	1.00	0.00	TAG	C
ATOM	239	CZ	PHE	14	0.608	-8.121	4.329	1.00	0.00	TAG	C
ATOM	240	H	PHE	14	-0.972	-5.483	8.626	1.00	0.00	TAG	H
ATOM	241	HA	PHE	14	1.955	-5.331	8.368	1.00	0.00	TAG	H
ATOM	242	2HB	PHE	14	1.321	-3.855	6.326	1.00	0.00	TAG	H
ATOM	243	3HB	PHE	14	-0.360	-4.049	6.733	1.00	0.00	TAG	H
ATOM	244	1HD	PHE	14	1.631	-7.041	7.371	1.00	0.00	TAG	H
ATOM	245	2HD	PHE	14	-0.464	-4.905	4.286	1.00	0.00	TAG	H
ATOM	246	1HE	PHE	14	1.669	-9.049	5.954	1.00	0.00	TAG	H
ATOM	247	2HE	PHE	14	-0.435	-6.927	2.877	1.00	0.00	TAG	H
ATOM	248	HZ	PHE	14	0.637	-9.001	3.705	1.00	0.00	TAG	H

ATOM	249	N	HIS	15	0.515	-3.093	10.006	1.00	1.00	TAG N
ATOM	250	CA	HIS	15	0.674	-1.815	10.739	1.00	1.00	TAG C
ATOM	251	C	HIS	15	1.749	-1.967	11.792	1.00	1.00	TAG C
ATOM	252	O	HIS	15	2.691	-1.137	11.858	1.00	1.00	TAG O
ATOM	253	CB	HIS	15	-0.773	-1.537	11.442	1.00	1.00	TAG C
ATOM	254	CG	HIS	15	-0.566	-0.300	12.285	1.00	1.00	TAG C
ATOM	255	CD2	HIS	15	-0.391	0.983	11.917	1.00	1.00	TAG C
ATOM	256	ND1	HIS	15	-0.631	-0.257	13.671	1.00	1.00	TAG N
ATOM	257	CE1	HIS	15	-0.377	1.035	14.017	1.00	1.00	TAG C
ATOM	258	NE2	HIS	15	-0.299	1.804	12.932	1.00	1.00	TAG N
ATOM	259	H	HIS	15	-0.183	-3.699	10.387	1.00	1.00	TAG H
ATOM	260	HA	HIS	15	0.970	-0.986	10.079	1.00	1.00	TAG H
ATOM	261	1HB	HIS	15	-1.559	-1.378	10.687	1.00	1.00	TAG H
ATOM	262	2HB	HIS	15	-1.087	-2.391	12.058	1.00	1.00	TAG H
ATOM	263	HD1	HIS	15	-0.825	-1.019	14.289	1.00	1.00	TAG H
ATOM	264	HD2	HIS	15	-0.330	1.309	10.868	1.00	1.00	TAG H
ATOM	265	HE1	HIS	15	-0.254	1.394	15.049	1.00	1.00	TAG H
ATOM	266	N	GLU	16	1.692	-2.972	12.641	1.00	1.00	TAG N
ATOM	267	CA	GLU	16	2.590	-3.130	13.782	1.00	1.00	TAG C
ATOM	268	C	GLU	16	3.910	-3.713	13.294	1.00	1.00	TAG C
ATOM	269	O	GLU	16	4.977	-3.172	13.631	1.00	1.00	TAG O
ATOM	270	CB	GLU	16	1.976	-4.067	14.816	1.00	1.00	TAG C
ATOM	271	CG	GLU	16	2.805	-4.218	16.081	1.00	1.00	TAG C
ATOM	272	CD	GLU	16	2.301	-5.325	16.988	1.00	1.00	TAG C
ATOM	273	OE1	GLU	16	1.544	-6.196	16.509	1.00	1.00	TAG O
ATOM	274	OE2	GLU	16	2.685	-5.354	18.180	1.00	1.00	TAG O
ATOM	275	H	GLU	16	1.020	-3.709	12.563	1.00	1.00	TAG H
ATOM	276	HA	GLU	16	2.756	-2.149	14.249	1.00	1.00	TAG H
ATOM	277	1HB	GLU	16	0.977	-3.694	15.086	1.00	1.00	TAG H
ATOM	278	2HB	GLU	16	1.836	-5.059	14.361	1.00	1.00	TAG H
ATOM	279	1HG	GLU	16	3.850	-4.424	15.806	1.00	1.00	TAG H
ATOM	280	2HG	GLU	16	2.798	-3.267	16.634	1.00	1.00	TAG H
ATOM	281	H01	GLU	16	2.929	-6.252	18.417	1.00	1.00	TAG H
ATOM	282	N	LYS	17	3.889	-4.776	12.521	1.00	1.00	TAG N
ATOM	283	CA	LYS	17	5.076	-5.545	12.164	1.00	1.00	TAG C
ATOM	284	C	LYS	17	5.746	-4.920	10.957	1.00	1.00	TAG C
ATOM	285	O	LYS	17	6.970	-4.755	10.934	1.00	1.00	TAG O
ATOM	286	CB	LYS	17	4.691	-6.996	11.866	1.00	1.00	TAG C
ATOM	287	CG	LYS	17	5.852	-7.911	11.541	1.00	1.00	TAG C
ATOM	288	CD	LYS	17	5.460	-9.346	11.843	1.00	1.00	TAG C
ATOM	289	CE	LYS	17	6.565	-10.330	11.510	1.00	1.00	TAG C
ATOM	290	NZ	LYS	17	6.611	-10.581	10.055	1.00	1.00	TAG N1+
ATOM	291	H	LYS	17	3.048	-5.136	12.118	1.00	1.00	TAG H
ATOM	292	HA	LYS	17	5.782	-5.536	13.008	1.00	1.00	TAG H
ATOM	293	1HB	LYS	17	4.155	-7.403	12.736	1.00	1.00	TAG H
ATOM	294	2HB	LYS	17	3.986	-7.006	11.021	1.00	1.00	TAG H
ATOM	295	1HG	LYS	17	6.128	-7.809	10.481	1.00	1.00	TAG H
ATOM	296	2HG	LYS	17	6.735	-7.626	12.131	1.00	1.00	TAG H
ATOM	297	1HD	LYS	17	5.202	-9.436	12.908	1.00	1.00	TAG H
ATOM	298	2HD	LYS	17	4.557	-9.605	11.270	1.00	1.00	TAG H
ATOM	299	1HE	LYS	17	7.533	-9.935	11.851	1.00	1.00	TAG H

ATOM	300	2HE	LYS	17	6.397	-11.276	12.046	1.00	1.00	TAG H
ATOM	301	H01	LYS	17	5.819	-10.138	9.611	1.00	1.00	TAG H
ATOM	302	H02	LYS	17	6.581	-11.576	9.883	1.00	1.00	TAG H
ATOM	303	H03	LYS	17	7.466	-10.200	9.675	1.00	1.00	TAG H
ATOM	304	N	HIS	18	4.973	-4.404	10.017	1.00	0.00	TAG N
ATOM	305	CA	HIS	18	5.427	-3.934	8.711	1.00	0.00	TAG C
ATOM	306	C	HIS	18	6.029	-2.553	8.812	1.00	0.00	TAG C
ATOM	307	O	HIS	18	7.152	-2.279	8.317	1.00	0.00	TAG O
ATOM	308	CB	HIS	18	4.186	-3.913	7.804	1.00	0.00	TAG C
ATOM	309	CG	HIS	18	4.494	-3.395	6.429	1.00	0.00	TAG C
ATOM	310	CD2	HIS	18	4.099	-2.136	5.996	1.00	0.00	TAG C
ATOM	311	ND1	HIS	18	5.192	-4.079	5.436	1.00	0.00	TAG N
ATOM	312	CE1	HIS	18	5.159	-3.159	4.455	1.00	0.00	TAG C
ATOM	313	NE2	HIS	18	4.532	-1.977	4.705	1.00	0.00	TAG N
ATOM	314	H	HIS	18	3.999	-4.330	10.216	1.00	0.00	TAG H
ATOM	315	HA	HIS	18	6.235	-4.607	8.376	1.00	0.00	TAG H
ATOM	316	2HB	HIS	18	3.385	-3.280	8.235	1.00	0.00	TAG H
ATOM	317	3HB	HIS	18	3.735	-4.921	7.689	1.00	0.00	TAG H
ATOM	318	2HD	HIS	18	3.544	-1.424	6.600	1.00	0.00	TAG H
ATOM	319	1HE	HIS	18	5.637	-3.409	3.517	1.00	0.00	TAG H
ATOM	320	2HE	HIS	18	4.408	-1.163	4.086	1.00	0.00	TAG H
ATOM	321	N	HIS	19	5.254	-1.534	9.282	1.00	0.00	TAG N
ATOM	322	CA	HIS	19	5.728	-0.156	9.191	1.00	0.00	TAG C
ATOM	323	C	HIS	19	5.987	0.420	10.563	1.00	0.00	TAG C
ATOM	324	O	HIS	19	7.071	0.994	10.905	1.00	0.00	TAG O
ATOM	325	CB	HIS	19	4.621	0.636	8.477	1.00	0.00	TAG C
ATOM	326	CG	HIS	19	5.006	2.067	8.238	1.00	0.00	TAG C
ATOM	327	CD2	HIS	19	4.434	3.124	8.932	1.00	0.00	TAG C
ATOM	328	ND1	HIS	19	5.956	2.514	7.322	1.00	0.00	TAG N
ATOM	329	CE1	HIS	19	5.877	3.840	7.537	1.00	0.00	TAG C
ATOM	330	NE2	HIS	19	5.001	4.286	8.478	1.00	0.00	TAG N
ATOM	331	H	HIS	19	4.379	-1.727	9.681	1.00	0.00	TAG H
ATOM	332	HA	HIS	19	6.699	-0.170	8.667	1.00	0.00	TAG H
ATOM	333	2HB	HIS	19	3.681	0.631	9.065	1.00	0.00	TAG H
ATOM	334	3HB	HIS	19	4.355	0.191	7.495	1.00	0.00	TAG H
ATOM	335	2HD	HIS	19	3.670	3.016	9.698	1.00	0.00	TAG H
ATOM	336	1HE	HIS	19	6.520	4.482	6.949	1.00	0.00	TAG H
ATOM	337	2HE	HIS	19	4.805	5.253	8.777	1.00	0.00	TAG H
ATOM	338	N	SER	20	4.946	0.349	11.481	1.00	1.00	TAG N
ATOM	339	CA	SER	20	4.974	1.063	12.758	1.00	1.00	TAG C
ATOM	340	C	SER	20	6.074	0.606	13.706	1.00	1.00	TAG C
ATOM	341	O	SER	20	7.028	1.267	14.086	1.00	1.00	TAG O
ATOM	342	CB	SER	20	3.625	0.900	13.464	1.00	1.00	TAG C
ATOM	343	OG	SER	20	3.674	1.456	14.765	1.00	1.00	TAG O
ATOM	344	H	SER	20	4.124	-0.199	11.327	1.00	1.00	TAG H
ATOM	345	HA	SER	20	5.182	2.115	12.511	1.00	1.00	TAG H
ATOM	346	1HB	SER	20	2.836	1.394	12.877	1.00	1.00	TAG H
ATOM	347	2HB	SER	20	3.362	-0.166	13.524	1.00	1.00	TAG H
ATOM	348	HG	SER	20	4.271	2.259	14.763	1.00	1.00	TAG H
ATOM	349	N	HIS	21	5.962	-0.688	14.167	1.00	1.00	TAG N
ATOM	350	CA	HIS	21	6.875	-1.249	15.152	1.00	1.00	TAG C

ATOM	351	C	HIS	21	8.213	-1.733	14.589	1.00	1.00	TAG C
ATOM	352	O	HIS	21	9.030	-2.488	15.128	1.00	1.00	TAG O
ATOM	353	CB	HIS	21	6.187	-2.334	15.970	1.00	1.00	TAG C
ATOM	354	CG	HIS	21	5.320	-1.792	17.060	1.00	1.00	TAG C
ATOM	355	CD2	HIS	21	3.969	-1.577	16.899	1.00	1.00	TAG C
ATOM	356	ND1	HIS	21	5.615	-1.385	18.321	1.00	1.00	TAG N
ATOM	357	CE1	HIS	21	4.451	-0.937	18.891	1.00	1.00	TAG C
ATOM	358	NE2	HIS	21	3.465	-1.062	18.014	1.00	1.00	TAG N
ATOM	359	H	HIS	21	5.254	-1.324	13.860	1.00	1.00	TAG H
ATOM	360	HA	HIS	21	7.143	-0.411	15.812	1.00	1.00	TAG H
ATOM	361	1HB	HIS	21	5.576	-2.956	15.300	1.00	1.00	TAG H
ATOM	362	2HB	HIS	21	6.952	-2.990	16.412	1.00	1.00	TAG H
ATOM	363	HD1	HIS	21	6.516	-1.408	18.756	1.00	1.00	TAG H
ATOM	364	HD2	HIS	21	3.395	-1.798	15.987	1.00	1.00	TAG H
ATOM	365	HE1	HIS	21	4.351	-0.540	19.912	1.00	1.00	TAG H
ATOM	366	N	ARG	22	8.441	-1.287	13.352	1.00	0.00	TAG N
ATOM	367	CA	ARG	22	9.602	-1.672	12.555	1.00	0.00	TAG C
ATOM	368	C	ARG	22	10.636	-0.571	12.538	1.00	0.00	TAG C
ATOM	369	O	ARG	22	11.749	-0.792	12.926	1.00	0.00	TAG O
ATOM	370	CB	ARG	22	9.128	-2.027	11.117	1.00	0.00	TAG C
ATOM	371	CG	ARG	22	10.240	-2.520	10.149	1.00	0.00	TAG C
ATOM	372	CD	ARG	22	9.685	-2.855	8.754	1.00	0.00	TAG C
ATOM	373	NE	ARG	22	10.803	-3.261	7.853	1.00	0.00	TAG N
ATOM	374	CZ	ARG	22	11.299	-4.490	7.748	1.00	0.00	TAG C
ATOM	375	NH1	ARG	22	10.853	-5.508	8.430	1.00	0.00	TAG N
ATOM	376	NH2	ARG	22	12.279	-4.691	6.925	1.00	0.00	TAG N1+
ATOM	377	H	ARG	22	7.774	-0.647	12.944	1.00	0.00	TAG H
ATOM	378	HA	ARG	22	10.065	-2.558	13.031	1.00	0.00	TAG H
ATOM	379	2HB	ARG	22	8.611	-1.145	10.685	1.00	0.00	TAG H
ATOM	380	3HB	ARG	22	8.340	-2.805	11.176	1.00	0.00	TAG H
ATOM	381	2HG	ARG	22	10.741	-3.406	10.591	1.00	0.00	TAG H
ATOM	382	3HG	ARG	22	11.031	-1.748	10.052	1.00	0.00	TAG H
ATOM	383	2HD	ARG	22	9.151	-1.968	8.348	1.00	0.00	TAG H
ATOM	384	3HD	ARG	22	8.930	-3.665	8.840	1.00	0.00	TAG H
ATOM	385	HE	ARG	22	11.266	-2.577	7.246	1.00	0.00	TAG H
ATOM	386	H01	ARG	22	10.090	-5.385	9.080	1.00	0.00	TAG H
ATOM	387	H02	ARG	22	11.270	-6.420	8.308	1.00	0.00	TAG H
ATOM	388	H03	ARG	22	12.474	-3.839	6.419	1.00	0.00	TAG H
ATOM	389	H04	ARG	22	12.028	-5.420	6.273	1.00	0.00	TAG H
ATOM	390	H05	ARG	22	13.100	-4.971	7.442	1.00	0.00	TAG H
ATOM	391	N	GLY	23	10.321	0.583	12.280	1.00	0.00	TAG N
ATOM	392	CA	GLY	23	11.224	1.724	12.164	1.00	0.00	TAG C
ATOM	393	C	GLY	23	12.412	1.388	11.296	1.00	0.00	TAG C
ATOM	394	O	GLY	23	13.469	2.035	11.393	1.00	0.00	TAG O
ATOM	395	H	GLY	23	9.343	0.763	12.133	1.00	0.00	TAG H
ATOM	396	3HA	GLY	23	11.558	1.980	13.126	0.00	0.00	TAG H
ATOM	397	HA	GLY	23	10.682	2.564	11.689	1.00	0.00	TAG H
ATOM	398	N	TYR	24	12.299	0.419	10.432	1.00	0.00	TAG N
ATOM	399	CA	TYR	24	13.306	-0.016	9.468	1.00	0.00	TAG C
ATOM	400	C	TYR	24	14.314	1.078	9.209	1.00	0.00	TAG C
ATOM	401	O	TYR	24	14.047	2.261	9.158	1.00	0.00	TAG O

ATOM	402	CB	TYR	24	12.647	-0.393	8.109	1.00	0.00	TAG	C
ATOM	403	CG	TYR	24	11.939	0.736	7.350	1.00	0.00	TAG	C
ATOM	404	CD1	TYR	24	12.635	1.519	6.424	1.00	0.00	TAG	C
ATOM	405	CD2	TYR	24	10.581	0.980	7.577	1.00	0.00	TAG	C
ATOM	406	CE1	TYR	24	11.977	2.531	5.731	1.00	0.00	TAG	C
ATOM	407	CE2	TYR	24	9.926	1.992	6.884	1.00	0.00	TAG	C
ATOM	408	CZ	TYR	24	10.624	2.767	5.960	1.00	0.00	TAG	C
ATOM	409	OH	TYR	24	9.982	3.760	5.276	1.00	0.00	TAG	O
ATOM	410	OXT	TYR	24	15.694	0.721	9.005	0.00	0.00	TAG	O
ATOM	411	H	TYR	24	11.393	-0.102	10.429	1.00	0.00	TAG	H
ATOM	412	HA	TYR	24	13.848	-0.886	9.883	1.00	0.00	TAG	H
ATOM	413	2HB	TYR	24	11.908	-1.204	8.266	1.00	0.00	TAG	H
ATOM	414	3HB	TYR	24	13.407	-0.862	7.450	1.00	0.00	TAG	H
ATOM	415	1HD	TYR	24	13.685	1.338	6.235	1.00	0.00	TAG	H
ATOM	416	2HD	TYR	24	10.030	0.375	8.284	1.00	0.00	TAG	H
ATOM	417	1HE	TYR	24	12.512	3.133	5.011	1.00	0.00	TAG	H
ATOM	418	2HE	TYR	24	8.875	2.167	7.063	1.00	0.00	TAG	H
ATOM	419	HH	TYR	24	9.065	3.778	5.556	1.00	0.00	TAG	H
ATOM	420	H01	TYR	24	15.981	1.030	8.143	0.00	0.00	TAG	H
END											

Histatin conformer 2:

ATOM	1	N	ASP	1	-0.742	-1.261	-0.005	1.00	0.00	TAG	N1+
ATOM	2	CA	ASP	1	-0.018	0.008	0.007	1.00	0.00	TAG	C
ATOM	3	C	ASP	1	-0.973	1.176	0.003	1.00	0.00	TAG	C
ATOM	4	O	ASP	1	-0.968	2.000	0.921	1.00	0.00	TAG	O
ATOM	5	CB	ASP	1	0.963	0.088	-1.197	1.00	0.00	TAG	C
ATOM	6	CG	ASP	1	2.166	-0.865	-1.133	1.00	0.00	TAG	C
ATOM	7	OD1	ASP	1	1.969	-2.097	-1.177	1.00	0.00	TAG	O
ATOM	8	OD2	ASP	1	3.307	-0.377	-0.994	1.00	0.00	TAG	O
ATOM	9	HA	ASP	1	0.566	0.064	0.945	1.00	0.00	TAG	H
ATOM	10	2HB	ASP	1	1.353	1.117	-1.298	1.00	0.00	TAG	H
ATOM	11	3HB	ASP	1	0.440	-0.126	-2.142	1.00	0.00	TAG	H
ATOM	12	H01	ASP	1	3.615	-0.533	-0.098	1.00	0.00	TAG	H
ATOM	13	H02	ASP	1	-0.910	-1.562	0.944	1.00	0.00	TAG	H
ATOM	14	H03	ASP	1	-0.193	-1.958	-0.488	1.00	0.00	TAG	H
ATOM	15	H04	ASP	1	-1.624	-1.140	-0.481	1.00	0.00	TAG	H
ATOM	16	N	SER	2	-1.812	1.277	-0.974	1.00	1.00	TAG	N
ATOM	17	CA	SER	2	-2.731	2.404	-1.133	1.00	1.00	TAG	C
ATOM	18	C	SER	2	-4.196	2.006	-1.232	1.00	1.00	TAG	C
ATOM	19	O	SER	2	-5.154	2.587	-0.745	1.00	1.00	TAG	O
ATOM	20	CB	SER	2	-2.355	3.198	-2.387	1.00	1.00	TAG	C
ATOM	21	OG	SER	2	-3.316	4.204	-2.646	1.00	1.00	TAG	O
ATOM	22	H	SER	2	-1.894	0.591	-1.698	1.00	1.00	TAG	H
ATOM	23	HA	SER	2	-2.627	3.009	-0.221	1.00	1.00	TAG	H
ATOM	24	1HB	SER	2	-1.363	3.655	-2.256	1.00	1.00	TAG	H
ATOM	25	2HB	SER	2	-2.284	2.520	-3.250	1.00	1.00	TAG	H
ATOM	26	HG	SER	2	-3.054	4.713	-3.466	1.00	1.00	TAG	H
ATOM	27	N	HIS	3	-4.416	0.839	-1.990	1.00	0.00	TAG	N

ATOM	28	CA	HIS	3	-5.736	0.224	-2.099	1.00	0.00	TAG	C
ATOM	29	C	HIS	3	-6.249	-0.203	-0.745	1.00	0.00	TAG	C
ATOM	30	O	HIS	3	-7.450	-0.055	-0.411	1.00	0.00	TAG	O
ATOM	31	CB	HIS	3	-5.571	-0.996	-3.019	1.00	0.00	TAG	C
ATOM	32	CG	HIS	3	-6.866	-1.719	-3.247	1.00	0.00	TAG	C
ATOM	33	CD2	HIS	3	-7.766	-1.352	-4.238	1.00	0.00	TAG	C
ATOM	34	ND1	HIS	3	-7.326	-2.817	-2.522	1.00	0.00	TAG	N
ATOM	35	CE1	HIS	3	-8.500	-3.029	-3.145	1.00	0.00	TAG	C
ATOM	36	NE2	HIS	3	-8.837	-2.206	-4.176	1.00	0.00	TAG	N
ATOM	37	H	HIS	3	-3.652	0.422	-2.464	1.00	0.00	TAG	H
ATOM	38	HA	HIS	3	-6.433	0.994	-2.472	1.00	0.00	TAG	H
ATOM	39	2HB	HIS	3	-4.846	-1.721	-2.597	1.00	0.00	TAG	H
ATOM	40	3HB	HIS	3	-5.162	-0.718	-4.014	1.00	0.00	TAG	H
ATOM	41	2HD	HIS	3	-7.619	-0.526	-4.927	1.00	0.00	TAG	H
ATOM	42	1HE	HIS	3	-9.114	-3.847	-2.793	1.00	0.00	TAG	H
ATOM	43	2HE	HIS	3	-9.682	-2.215	-4.765	1.00	0.00	TAG	H
ATOM	44	N	ALA	4	-5.364	-0.719	0.106	1.00	1.00	TAG	N
ATOM	45	CA	ALA	4	-5.721	-1.205	1.425	1.00	1.00	TAG	C
ATOM	46	C	ALA	4	-6.193	-0.032	2.301	1.00	1.00	TAG	C
ATOM	47	O	ALA	4	-7.248	-0.122	2.923	1.00	1.00	TAG	O
ATOM	48	CB	ALA	4	-4.511	-1.885	2.062	1.00	1.00	TAG	C
ATOM	49	H	ALA	4	-4.394	-0.823	-0.113	1.00	1.00	TAG	H
ATOM	50	HA	ALA	4	-6.539	-1.935	1.337	1.00	1.00	TAG	H
ATOM	51	1HB	ALA	4	-4.782	-2.253	3.063	1.00	1.00	TAG	H
ATOM	52	2HB	ALA	4	-4.191	-2.729	1.435	1.00	1.00	TAG	H
ATOM	53	3HB	ALA	4	-3.687	-1.161	2.149	1.00	1.00	TAG	H
ATOM	54	N	LYS	5	-5.469	1.030	2.370	1.00	1.00	TAG	N
ATOM	55	CA	LYS	5	-5.870	2.211	3.124	1.00	1.00	TAG	C
ATOM	56	C	LYS	5	-7.191	2.751	2.591	1.00	1.00	TAG	C
ATOM	57	O	LYS	5	-7.957	3.338	3.335	1.00	1.00	TAG	O
ATOM	58	CB	LYS	5	-4.788	3.292	3.042	1.00	1.00	TAG	C
ATOM	59	CG	LYS	5	-3.563	2.974	3.862	1.00	1.00	TAG	C
ATOM	60	CD	LYS	5	-2.504	4.045	3.720	1.00	1.00	TAG	C
ATOM	61	CE	LYS	5	-1.275	3.659	4.537	1.00	1.00	TAG	C
ATOM	62	NZ	LYS	5	-0.103	4.532	4.269	1.00	1.00	TAG	N
ATOM	63	H	LYS	5	-4.584	1.122	1.914	1.00	1.00	TAG	H
ATOM	64	HA	LYS	5	-6.001	1.924	4.178	1.00	1.00	TAG	H
ATOM	65	1HB	LYS	5	-4.493	3.426	1.990	1.00	1.00	TAG	H
ATOM	66	2HB	LYS	5	-5.210	4.250	3.382	1.00	1.00	TAG	H
ATOM	67	1HG	LYS	5	-3.845	2.873	4.920	1.00	1.00	TAG	H
ATOM	68	2HG	LYS	5	-3.151	2.004	3.545	1.00	1.00	TAG	H
ATOM	69	1HD	LYS	5	-2.230	4.167	2.662	1.00	1.00	TAG	H
ATOM	70	2HD	LYS	5	-2.897	5.013	4.065	1.00	1.00	TAG	H
ATOM	71	1HE	LYS	5	-1.523	3.706	5.608	1.00	1.00	TAG	H
ATOM	72	2HE	LYS	5	-1.006	2.616	4.315	1.00	1.00	TAG	H
ATOM	73	H01	LYS	5	0.144	5.033	5.111	1.00	1.00	TAG	H
ATOM	74	H02	LYS	5	-0.333	5.191	3.539	1.00	1.00	TAG	H
ATOM	75	N	ARG	6	-7.468	2.540	1.324	1.00	1.00	TAG	N
ATOM	76	CA	ARG	6	-8.708	3.009	0.679	1.00	1.00	TAG	C
ATOM	77	C	ARG	6	-9.908	2.245	1.217	1.00	1.00	TAG	C
ATOM	78	O	ARG	6	-10.874	2.847	1.709	1.00	1.00	TAG	O

ATOM	79	CB	ARG	6	-8.661	2.885	-0.850	1.00	1.00	TAG C
ATOM	80	CG	ARG	6	-7.667	3.791	-1.518	1.00	1.00	TAG C
ATOM	81	CD	ARG	6	-8.037	5.246	-1.357	1.00	1.00	TAG C
ATOM	82	NE	ARG	6	-6.856	6.090	-1.505	1.00	1.00	TAG N
ATOM	83	CZ	ARG	6	-6.862	7.313	-2.023	1.00	1.00	TAG C
ATOM	84	NH1	ARG	6	-7.988	7.832	-2.518	1.00	1.00	TAG N
ATOM	85	NH2	ARG	6	-5.721	7.994	-2.105	1.00	1.00	TAG N1+
ATOM	86	H	ARG	6	-6.856	2.047	0.706	1.00	1.00	TAG H
ATOM	87	HA	ARG	6	-8.806	4.077	0.921	1.00	1.00	TAG H
ATOM	88	1HB	ARG	6	-8.424	1.844	-1.114	1.00	1.00	TAG H
ATOM	89	2HB	ARG	6	-9.663	3.099	-1.254	1.00	1.00	TAG H
ATOM	90	1HG	ARG	6	-6.668	3.617	-1.092	1.00	1.00	TAG H
ATOM	91	2HG	ARG	6	-7.608	3.545	-2.590	1.00	1.00	TAG H
ATOM	92	1HD	ARG	6	-8.791	5.525	-2.107	1.00	1.00	TAG H
ATOM	93	2HD	ARG	6	-8.490	5.409	-0.368	1.00	1.00	TAG H
ATOM	94	HE	ARG	6	-5.979	5.722	-1.195	1.00	1.00	TAG H
ATOM	95	1HH1	ARG	6	-8.835	7.300	-2.501	1.00	1.00	TAG H
ATOM	96	2HH1	ARG	6	-7.985	8.754	-2.906	1.00	1.00	TAG H
ATOM	97	H01	ARG	6	-5.439	8.292	-1.182	1.00	1.00	TAG H
ATOM	98	H02	ARG	6	-5.853	8.803	-2.695	1.00	1.00	TAG H
ATOM	99	H03	ARG	6	-5.004	7.402	-2.500	1.00	1.00	TAG H
ATOM	100	N	HIS	7	-9.901	0.877	1.143	1.00	0.00	TAG N
ATOM	101	CA	HIS	7	-11.086	0.117	1.530	1.00	0.00	TAG C
ATOM	102	C	HIS	7	-10.739	-0.951	2.539	1.00	0.00	TAG C
ATOM	103	O	HIS	7	-11.681	-1.463	3.238	1.00	0.00	TAG O
ATOM	104	CB	HIS	7	-11.632	-0.519	0.241	1.00	0.00	TAG C
ATOM	105	CG	HIS	7	-12.019	0.508	-0.782	1.00	0.00	TAG C
ATOM	106	CD2	HIS	7	-11.263	0.757	-1.919	1.00	0.00	TAG C
ATOM	107	ND1	HIS	7	-13.149	1.322	-0.734	1.00	0.00	TAG N
ATOM	108	CE1	HIS	7	-12.979	2.020	-1.872	1.00	0.00	TAG C
ATOM	109	NE2	HIS	7	-11.887	1.745	-2.636	1.00	0.00	TAG N
ATOM	110	H	HIS	7	-9.099	0.408	0.829	1.00	0.00	TAG H
ATOM	111	HA	HIS	7	-11.780	0.813	2.033	1.00	0.00	TAG H
ATOM	112	2HB	HIS	7	-12.523	-1.145	0.449	1.00	0.00	TAG H
ATOM	113	3HB	HIS	7	-10.897	-1.203	-0.231	1.00	0.00	TAG H
ATOM	114	2HD	HIS	7	-10.340	0.241	-2.169	1.00	0.00	TAG H
ATOM	115	1HE	HIS	7	-13.725	2.763	-2.121	1.00	0.00	TAG H
ATOM	116	2HE	HIS	7	-11.594	2.169	-3.528	1.00	0.00	TAG H
ATOM	117	N	HIS	8	-9.444	-1.344	2.755	1.00	0.00	TAG N
ATOM	118	CA	HIS	8	-9.153	-2.419	3.700	1.00	0.00	TAG C
ATOM	119	C	HIS	8	-8.439	-1.889	4.920	1.00	0.00	TAG C
ATOM	120	O	HIS	8	-8.326	-2.668	5.925	1.00	0.00	TAG O
ATOM	121	CB	HIS	8	-8.263	-3.424	2.951	1.00	0.00	TAG C
ATOM	122	CG	HIS	8	-8.999	-4.127	1.849	1.00	0.00	TAG C
ATOM	123	CD2	HIS	8	-10.372	-4.014	1.672	1.00	0.00	TAG C
ATOM	124	ND1	HIS	8	-8.429	-4.957	0.886	1.00	0.00	TAG N
ATOM	125	CE1	HIS	8	-9.530	-5.293	0.190	1.00	0.00	TAG C
ATOM	126	NE2	HIS	8	-10.723	-4.775	0.587	1.00	0.00	TAG N
ATOM	127	H	HIS	8	-8.720	-0.898	2.265	1.00	0.00	TAG H
ATOM	128	HA	HIS	8	-10.117	-2.825	4.051	1.00	0.00	TAG H
ATOM	129	2HB	HIS	8	-7.863	-4.195	3.639	1.00	0.00	TAG H

ATOM	130	3HB	HIS	8	-7.370	-2.939	2.504	1.00	0.00	TAG	H
ATOM	131	2HD	HIS	8	-11.026	-3.418	2.302	1.00	0.00	TAG	H
ATOM	132	1HE	HIS	8	-9.405	-5.958	-0.655	1.00	0.00	TAG	H
ATOM	133	2HE	HIS	8	-11.660	-4.915	0.183	1.00	0.00	TAG	H
ATOM	134	N	GLY	9	-8.157	-0.551	4.940	1.00	1.00	TAG	N
ATOM	135	CA	GLY	9	-7.411	0.121	6.019	1.00	1.00	TAG	C
ATOM	136	C01	GLY	9	-6.073	-0.582	6.408	1.00	1.00	TAG	C
ATOM	137	O01	GLY	9	-5.339	0.364	7.190	1.00	1.00	TAG	O
ATOM	138	H	GLY	9	-8.437	0.061	4.200	1.00	1.00	TAG	H
ATOM	139	1HA	GLY	9	-7.192	1.153	5.709	1.00	1.00	TAG	H
ATOM	140	2HA	GLY	9	-8.055	0.183	6.909	1.00	1.00	TAG	H
ATOM	141	N	TYR	10	-5.312	-0.890	5.371	1.00	0.00	TAG	N
ATOM	142	CA	TYR	10	-4.092	-1.652	5.624	1.00	0.00	TAG	C
ATOM	143	C	TYR	10	-4.010	-2.076	7.070	1.00	0.00	TAG	C
ATOM	144	O	TYR	10	-2.940	-2.268	7.604	1.00	0.00	TAG	O
ATOM	145	CB	TYR	10	-2.829	-0.801	5.301	1.00	0.00	TAG	C
ATOM	146	CG	TYR	10	-1.470	-1.479	5.512	1.00	0.00	TAG	C
ATOM	147	CD1	TYR	10	-0.981	-2.400	4.580	1.00	0.00	TAG	C
ATOM	148	CD2	TYR	10	-0.707	-1.168	6.641	1.00	0.00	TAG	C
ATOM	149	CE1	TYR	10	0.261	-2.998	4.776	1.00	0.00	TAG	C
ATOM	150	CE2	TYR	10	0.534	-1.767	6.834	1.00	0.00	TAG	C
ATOM	151	CZ	TYR	10	1.018	-2.682	5.901	1.00	0.00	TAG	C
ATOM	152	OH	TYR	10	2.237	-3.268	6.088	1.00	0.00	TAG	O
ATOM	153	H	TYR	10	-5.394	-0.718	4.421	1.00	0.00	TAG	H
ATOM	154	HA	TYR	10	-4.105	-2.566	5.002	1.00	0.00	TAG	H
ATOM	155	2HB	TYR	10	-2.838	0.125	5.910	1.00	0.00	TAG	H
ATOM	156	3HB	TYR	10	-2.897	-0.424	4.259	1.00	0.00	TAG	H
ATOM	157	1HD	TYR	10	-1.559	-2.647	3.701	1.00	0.00	TAG	H
ATOM	158	2HD	TYR	10	-1.071	-0.450	7.363	1.00	0.00	TAG	H
ATOM	159	1HE	TYR	10	0.644	-3.704	4.054	1.00	0.00	TAG	H
ATOM	160	2HE	TYR	10	1.117	-1.513	7.707	1.00	0.00	TAG	H
ATOM	161	HH	TYR	10	2.613	-2.934	6.905	1.00	0.00	TAG	H
ATOM	162	CA	LYS	11	-5.024	-2.727	9.133	1.00	1.00	TAG	C
ATOM	163	C	LYS	11	-4.441	-4.126	9.176	1.00	1.00	TAG	C
ATOM	164	O	LYS	11	-4.397	-4.725	10.261	1.00	1.00	TAG	O
ATOM	165	CB	LYS	11	-6.451	-2.727	9.684	1.00	1.00	TAG	C
ATOM	166	CG	LYS	11	-6.577	-3.161	11.130	1.00	1.00	TAG	C
ATOM	167	CD	LYS	11	-7.850	-2.583	11.720	1.00	1.00	TAG	C
ATOM	168	CE	LYS	11	-8.063	-3.002	13.161	1.00	1.00	TAG	C
ATOM	169	NZ	LYS	11	-8.585	-4.384	13.222	1.00	1.00	TAG	N
ATOM	170	N01	LYS	11	-5.192	-1.941	7.792	1.00	1.00	TAG	N
ATOM	171	HA	LYS	11	-4.407	-2.064	9.757	1.00	1.00	TAG	H
ATOM	172	1HB	LYS	11	-6.867	-1.714	9.583	1.00	1.00	TAG	H
ATOM	173	2HB	LYS	11	-7.068	-3.392	9.062	1.00	1.00	TAG	H
ATOM	174	1HG	LYS	11	-6.595	-4.259	11.195	1.00	1.00	TAG	H
ATOM	175	2HG	LYS	11	-5.704	-2.819	11.705	1.00	1.00	TAG	H
ATOM	176	1HD	LYS	11	-7.812	-1.485	11.663	1.00	1.00	TAG	H
ATOM	177	2HD	LYS	11	-8.711	-2.906	11.116	1.00	1.00	TAG	H
ATOM	178	1HE	LYS	11	-7.115	-2.936	13.714	1.00	1.00	TAG	H
ATOM	179	2HE	LYS	11	-8.768	-2.314	13.650	1.00	1.00	TAG	H
ATOM	180	H01	LYS	11	-6.011	-1.423	7.508	1.00	1.00	TAG	H

ATOM	181	H02	LYS	11	-8.698	-4.659	14.187	1.00	1.00	TAG	H
ATOM	182	H03	LYS	11	-7.936	-5.010	12.767	1.00	1.00	TAG	H
ATOM	183	N	ARG	12	-4.009	-4.690	8.161	1.00	1.00	TAG	N
ATOM	184	CA	ARG	12	-3.435	-6.024	8.100	1.00	1.00	TAG	C
ATOM	185	C	ARG	12	-2.534	-6.059	9.332	1.00	1.00	TAG	C
ATOM	186	O	ARG	12	-2.608	-7.238	9.991	1.00	1.00	TAG	O
ATOM	187	CB	ARG	12	-2.631	-6.161	6.803	1.00	1.00	TAG	C
ATOM	188	CG	ARG	12	-2.006	-7.536	6.581	1.00	1.00	TAG	C
ATOM	189	CD	ARG	12	-1.536	-7.710	5.143	1.00	1.00	TAG	C
ATOM	190	NE	ARG	12	-0.884	-6.506	4.633	1.00	1.00	TAG	N
ATOM	191	CZ	ARG	12	-1.163	-5.940	3.460	1.00	1.00	TAG	C
ATOM	192	NH1	ARG	12	-2.085	-6.471	2.660	1.00	1.00	TAG	N
ATOM	193	NH2	ARG	12	-0.532	-4.827	3.096	1.00	1.00	TAG	N1+
ATOM	194	H	ARG	12	-4.026	-4.244	7.266	1.00	1.00	TAG	H
ATOM	195	HA	ARG	12	-4.168	-6.843	8.096	1.00	1.00	TAG	H
ATOM	196	1HB	ARG	12	-3.290	-5.932	5.953	1.00	1.00	TAG	H
ATOM	197	2HB	ARG	12	-1.831	-5.406	6.803	1.00	1.00	TAG	H
ATOM	198	1HG	ARG	12	-1.155	-7.669	7.265	1.00	1.00	TAG	H
ATOM	199	2HG	ARG	12	-2.740	-8.318	6.826	1.00	1.00	TAG	H
ATOM	200	1HD	ARG	12	-0.836	-8.557	5.086	1.00	1.00	TAG	H
ATOM	201	2HD	ARG	12	-2.396	-7.959	4.504	1.00	1.00	TAG	H
ATOM	202	HE	ARG	12	-0.181	-6.078	5.203	1.00	1.00	TAG	H
ATOM	203	1HH1	ARG	12	-2.571	-7.299	2.938	1.00	1.00	TAG	H
ATOM	204	2HH1	ARG	12	-2.290	-6.042	1.780	1.00	1.00	TAG	H
ATOM	205	H01	ARG	12	-0.405	-4.232	3.902	1.00	1.00	TAG	H
ATOM	206	H02	ARG	12	-1.080	-4.340	2.401	1.00	1.00	TAG	H
ATOM	207	H03	ARG	12	0.370	-5.064	2.707	1.00	1.00	TAG	H
ATOM	208	N	LYS	13	-1.684	-5.305	9.649	1.00	0.00	TAG	N
ATOM	209	CA	LYS	13	-0.703	-5.502	10.713	1.00	0.00	TAG	C
ATOM	210	C	LYS	13	-1.377	-5.908	12.002	1.00	0.00	TAG	C
ATOM	211	O	LYS	13	-0.833	-6.729	12.749	1.00	0.00	TAG	O
ATOM	212	CB	LYS	13	0.121	-4.199	10.903	1.00	0.00	TAG	C
ATOM	213	CG	LYS	13	1.283	-4.348	11.917	1.00	0.00	TAG	C
ATOM	214	CD	LYS	13	2.121	-3.084	12.127	1.00	0.00	TAG	C
ATOM	215	CE	LYS	13	2.944	-2.807	10.862	1.00	0.00	TAG	C
ATOM	216	NZ	LYS	13	3.809	-1.636	11.087	1.00	0.00	TAG	N
ATOM	217	H	LYS	13	-1.629	-4.449	9.141	1.00	0.00	TAG	H
ATOM	218	HA	LYS	13	-0.028	-6.326	10.417	1.00	0.00	TAG	H
ATOM	219	2HB	LYS	13	-0.552	-3.375	11.219	1.00	0.00	TAG	H
ATOM	220	3HB	LYS	13	0.532	-3.872	9.928	1.00	0.00	TAG	H
ATOM	221	2HG	LYS	13	1.937	-5.188	11.612	1.00	0.00	TAG	H
ATOM	222	3HG	LYS	13	0.888	-4.629	12.912	1.00	0.00	TAG	H
ATOM	223	2HD	LYS	13	2.793	-3.219	12.999	1.00	0.00	TAG	H
ATOM	224	3HD	LYS	13	1.458	-2.231	12.373	1.00	0.00	TAG	H
ATOM	225	2HE	LYS	13	2.286	-2.620	9.989	1.00	0.00	TAG	H
ATOM	226	3HE	LYS	13	3.556	-3.695	10.595	1.00	0.00	TAG	H
ATOM	227	H01	LYS	13	4.024	-1.559	12.071	1.00	0.00	TAG	H
ATOM	228	H02	LYS	13	3.333	-0.800	10.779	1.00	0.00	TAG	H
ATOM	229	N	PHE	14	-2.508	-5.393	12.334	1.00	1.00	TAG	N
ATOM	230	CA	PHE	14	-3.217	-5.726	13.569	1.00	1.00	TAG	C
ATOM	231	C	PHE	14	-4.433	-6.617	13.339	1.00	1.00	TAG	C

ATOM	232	O	PHE	14	-4.730	-7.487	14.162	1.00	1.00	TAG	O
ATOM	233	CB	PHE	14	-3.591	-4.465	14.348	1.00	1.00	TAG	C
ATOM	234	CG	PHE	14	-2.401	-3.652	14.780	1.00	1.00	TAG	C
ATOM	235	CD1	PHE	14	-2.176	-2.386	14.247	1.00	1.00	TAG	C
ATOM	236	CD2	PHE	14	-1.486	-4.166	15.708	1.00	1.00	TAG	C
ATOM	237	CE1	PHE	14	-1.065	-1.633	14.638	1.00	1.00	TAG	C
ATOM	238	CE2	PHE	14	-0.374	-3.422	16.110	1.00	1.00	TAG	C
ATOM	239	CZ	PHE	14	-0.162	-2.152	15.574	1.00	1.00	TAG	C
ATOM	240	H	PHE	14	-2.991	-4.727	11.766	1.00	1.00	TAG	H
ATOM	241	HA	PHE	14	-2.517	-6.316	14.180	1.00	1.00	TAG	H
ATOM	242	1HB	PHE	14	-4.246	-3.838	13.724	1.00	1.00	TAG	H
ATOM	243	2HB	PHE	14	-4.172	-4.751	15.237	1.00	1.00	TAG	H
ATOM	244	HD1	PHE	14	-2.881	-1.974	13.510	1.00	1.00	TAG	H
ATOM	245	HD2	PHE	14	-1.646	-5.171	16.127	1.00	1.00	TAG	H
ATOM	246	HE1	PHE	14	-0.901	-0.632	14.210	1.00	1.00	TAG	H
ATOM	247	HE2	PHE	14	0.331	-3.836	16.846	1.00	1.00	TAG	H
ATOM	248	HZ	PHE	14	0.711	-1.561	15.886	1.00	1.00	TAG	H
ATOM	249	N	HIS	15	-5.117	-6.408	12.218	1.00	1.00	TAG	N
ATOM	250	CA	HIS	15	-6.235	-7.286	11.799	1.00	1.00	TAG	C
ATOM	251	C	HIS	15	-5.950	-7.844	10.423	1.00	1.00	TAG	C
ATOM	252	O	HIS	15	-6.821	-7.769	9.518	1.00	1.00	TAG	O
ATOM	253	CB	HIS	15	-7.551	-6.321	11.759	1.00	1.00	TAG	C
ATOM	254	CG	HIS	15	-8.658	-7.194	11.214	1.00	1.00	TAG	C
ATOM	255	CD2	HIS	15	-9.312	-8.224	11.783	1.00	1.00	TAG	C
ATOM	256	ND1	HIS	15	-9.302	-7.004	9.999	1.00	1.00	TAG	N
ATOM	257	CE1	HIS	15	-10.214	-8.009	9.898	1.00	1.00	TAG	C
ATOM	258	NE2	HIS	15	-10.262	-8.713	11.028	1.00	1.00	TAG	N
ATOM	259	H	HIS	15	-4.931	-5.654	11.588	1.00	1.00	TAG	H
ATOM	260	HA	HIS	15	-6.378	-8.138	12.481	1.00	1.00	TAG	H
ATOM	261	1HB	HIS	15	-7.800	-5.943	12.763	1.00	1.00	TAG	H
ATOM	262	2HB	HIS	15	-7.383	-5.444	11.118	1.00	1.00	TAG	H
ATOM	263	HD1	HIS	15	-9.131	-6.277	9.334	1.00	1.00	TAG	H
ATOM	264	HD2	HIS	15	-9.072	-8.615	12.783	1.00	1.00	TAG	H
ATOM	265	HE1	HIS	15	-10.827	-8.212	9.008	1.00	1.00	TAG	H
ATOM	266	N	GLU	16	-4.781	-8.395	10.176	1.00	0.00	TAG	N
ATOM	267	CA	GLU	16	-4.461	-9.077	8.926	1.00	0.00	TAG	C
ATOM	268	C	GLU	16	-5.285	-10.332	8.769	1.00	0.00	TAG	C
ATOM	269	O	GLU	16	-5.038	-11.119	7.849	1.00	0.00	TAG	O
ATOM	270	CB	GLU	16	-2.943	-9.416	8.885	1.00	0.00	TAG	C
ATOM	271	CG	GLU	16	-2.458	-10.479	9.923	1.00	0.00	TAG	C
ATOM	272	CD	GLU	16	-0.973	-10.779	10.008	1.00	0.00	TAG	C
ATOM	273	OE1	GLU	16	-0.153	-10.158	9.303	1.00	0.00	TAG	O
ATOM	274	OE2	GLU	16	-0.627	-11.659	10.823	1.00	0.00	TAG	O
ATOM	275	H	GLU	16	-4.077	-8.343	10.879	1.00	0.00	TAG	H
ATOM	276	HA	GLU	16	-4.703	-8.405	8.083	1.00	0.00	TAG	H
ATOM	277	2HB	GLU	16	-2.349	-8.490	9.029	1.00	0.00	TAG	H
ATOM	278	3HB	GLU	16	-2.661	-9.767	7.874	1.00	0.00	TAG	H
ATOM	279	2HG	GLU	16	-2.960	-11.447	9.767	1.00	0.00	TAG	H
ATOM	280	3HG	GLU	16	-2.709	-10.177	10.953	1.00	0.00	TAG	H
ATOM	281	H01	GLU	16	-0.432	-12.473	10.353	1.00	0.00	TAG	H
ATOM	282	N	LYS	17	-6.235	-10.560	9.650	1.00	1.00	TAG	N

ATOM	283	CA	LYS	17	-6.978	-11.813	9.729	1.00	1.00	TAG C
ATOM	284	C	LYS	17	-8.079	-11.819	8.688	1.00	1.00	TAG C
ATOM	285	O	LYS	17	-8.369	-12.859	8.088	1.00	1.00	TAG O
ATOM	286	CB	LYS	17	-7.569	-11.984	11.130	1.00	1.00	TAG C
ATOM	287	CG	LYS	17	-8.316	-13.281	11.353	1.00	1.00	TAG C
ATOM	288	CD	LYS	17	-8.333	-13.602	12.837	1.00	1.00	TAG C
ATOM	289	CE	LYS	17	-9.095	-14.876	13.146	1.00	1.00	TAG C
ATOM	290	NZ	LYS	17	-10.550	-14.626	13.118	1.00	1.00	TAG N1+
ATOM	291	H	LYS	17	-6.524	-9.884	10.328	1.00	1.00	TAG H
ATOM	292	HA	LYS	17	-6.296	-12.653	9.532	1.00	1.00	TAG H
ATOM	293	1HB	LYS	17	-6.755	-11.915	11.867	1.00	1.00	TAG H
ATOM	294	2HB	LYS	17	-8.253	-11.145	11.328	1.00	1.00	TAG H
ATOM	295	1HG	LYS	17	-9.345	-13.196	10.973	1.00	1.00	TAG H
ATOM	296	2HG	LYS	17	-7.834	-14.097	10.794	1.00	1.00	TAG H
ATOM	297	1HD	LYS	17	-7.299	-13.700	13.200	1.00	1.00	TAG H
ATOM	298	2HD	LYS	17	-8.788	-12.764	13.386	1.00	1.00	TAG H
ATOM	299	1HE	LYS	17	-8.836	-15.654	12.412	1.00	1.00	TAG H
ATOM	300	2HE	LYS	17	-8.801	-15.258	14.135	1.00	1.00	TAG H
ATOM	301	1HZ	LYS	17	-11.004	-15.213	13.789	1.00	1.00	TAG H
ATOM	302	2HZ	LYS	17	-10.729	-13.668	13.340	1.00	1.00	TAG H
ATOM	303	3HZ	LYS	17	-10.907	-14.828	12.205	1.00	1.00	TAG H
ATOM	304	N	HIS	18	-8.574	-10.671	8.316	1.00	1.00	TAG N
ATOM	305	CA	HIS	18	-9.668	-10.511	7.329	1.00	1.00	TAG C
ATOM	306	C	HIS	18	-9.215	-11.031	5.984	1.00	1.00	TAG C
ATOM	307	CB	HIS	18	-9.947	-8.905	7.252	1.00	1.00	TAG C
ATOM	308	CG	HIS	18	-10.976	-8.738	6.156	1.00	1.00	TAG C
ATOM	309	CD2	HIS	18	-10.761	-8.088	4.949	1.00	1.00	TAG C
ATOM	310	ND1	HIS	18	-12.281	-9.065	6.134	1.00	1.00	TAG N
ATOM	311	CE1	HIS	18	-12.884	-8.720	5.026	1.00	1.00	TAG C
ATOM	312	NE2	HIS	18	-11.934	-8.180	4.262	1.00	1.00	TAG N
ATOM	313	O01	HIS	18	-9.085	-9.893	5.128	1.00	1.00	TAG O
ATOM	314	H	HIS	18	-8.243	-9.800	8.678	1.00	1.00	TAG H
ATOM	315	HA	HIS	18	-10.573	-11.067	7.613	1.00	1.00	TAG H
ATOM	316	1HB	HIS	18	-10.321	-8.519	8.212	1.00	1.00	TAG H
ATOM	317	2HB	HIS	18	-9.025	-8.351	7.020	1.00	1.00	TAG H
ATOM	318	HD1	HIS	18	-12.744	-9.526	6.891	1.00	1.00	TAG H
ATOM	319	HD2	HIS	18	-9.834	-7.599	4.615	1.00	1.00	TAG H
ATOM	320	HE1	HIS	18	-13.948	-8.848	4.778	1.00	1.00	TAG H
ATOM	321	N	HIS	19	-8.098	-11.717	5.871	1.00	0.00	TAG N
ATOM	322	CA	HIS	19	-7.530	-12.232	4.628	1.00	0.00	TAG C
ATOM	323	C	HIS	19	-8.463	-11.992	3.466	1.00	0.00	TAG C
ATOM	324	O	HIS	19	-8.093	-11.943	2.245	1.00	0.00	TAG O
ATOM	325	CB	HIS	19	-7.316	-13.739	4.842	1.00	0.00	TAG C
ATOM	326	CG	HIS	19	-8.610	-14.479	5.021	1.00	0.00	TAG C
ATOM	327	CD2	HIS	19	-9.208	-15.202	3.998	1.00	0.00	TAG C
ATOM	328	ND1	HIS	19	-9.359	-14.540	6.194	1.00	0.00	TAG N
ATOM	329	CE1	HIS	19	-10.380	-15.311	5.775	1.00	0.00	TAG C
ATOM	330	NE2	HIS	19	-10.367	-15.748	4.486	1.00	0.00	TAG N
ATOM	331	H	HIS	19	-7.576	-11.908	6.737	1.00	0.00	TAG H
ATOM	332	HA	HIS	19	-6.611	-11.659	4.418	1.00	0.00	TAG H
ATOM	333	2HB	HIS	19	-6.688	-13.932	5.734	1.00	0.00	TAG H

ATOM	334	3HB	HIS	19	-6.775	-14.209	3.995	1.00	0.00	TAG H
ATOM	335	2HD	HIS	19	-8.804	-15.298	2.994	1.00	0.00	TAG H
ATOM	336	1HE	HIS	19	-11.158	-15.544	6.490	1.00	0.00	TAG H
ATOM	337	2HE	HIS	19	-11.051	-16.339	3.993	1.00	0.00	TAG H
ATOM	338	CA	SER	20	-10.787	-11.412	2.755	1.00	1.00	TAG C
ATOM	339	C	SER	20	-10.501	-10.090	2.059	1.00	1.00	TAG C
ATOM	340	O	SER	20	-10.550	-9.874	0.858	1.00	1.00	TAG O
ATOM	341	CB	SER	20	-12.174	-11.334	3.399	1.00	1.00	TAG C
ATOM	342	OG	SER	20	-13.123	-10.835	2.474	1.00	1.00	TAG O
ATOM	343	N01	SER	20	-9.717	-11.531	3.919	1.00	1.00	TAG N
ATOM	344	HA	SER	20	-10.736	-12.196	1.985	1.00	1.00	TAG H
ATOM	345	1HB	SER	20	-12.481	-12.332	3.745	1.00	1.00	TAG H
ATOM	346	2HB	SER	20	-12.138	-10.683	4.285	1.00	1.00	TAG H
ATOM	347	HG	SER	20	-12.892	-11.152	1.554	1.00	1.00	TAG H
ATOM	348	H01	SER	20	-9.912	-11.300	4.882	1.00	1.00	TAG H
ATOM	349	N	HIS	21	-10.115	-9.020	2.892	1.00	0.00	TAG N
ATOM	350	CA	HIS	21	-9.880	-7.689	2.337	1.00	0.00	TAG C
ATOM	351	C	HIS	21	-8.662	-7.682	1.445	1.00	0.00	TAG C
ATOM	352	O	HIS	21	-8.610	-7.110	0.307	1.00	0.00	TAG O
ATOM	353	CB	HIS	21	-9.672	-6.751	3.538	1.00	0.00	TAG C
ATOM	354	CG	HIS	21	-10.935	-6.534	4.317	1.00	0.00	TAG C
ATOM	355	CD2	HIS	21	-12.184	-6.914	3.843	1.00	0.00	TAG C
ATOM	356	ND1	HIS	21	-11.027	-5.945	5.577	1.00	0.00	TAG N
ATOM	357	CE1	HIS	21	-12.357	-6.012	5.767	1.00	0.00	TAG C
ATOM	358	NE2	HIS	21	-13.117	-6.575	4.789	1.00	0.00	TAG N
ATOM	359	H	HIS	21	-10.001	-9.173	3.870	1.00	0.00	TAG H
ATOM	360	HA	HIS	21	-10.742	-7.437	1.696	1.00	0.00	TAG H
ATOM	361	2HB	HIS	21	-9.298	-5.760	3.212	1.00	0.00	TAG H
ATOM	362	3HB	HIS	21	-8.905	-7.137	4.242	1.00	0.00	TAG H
ATOM	363	2HD	HIS	21	-12.358	-7.394	2.885	1.00	0.00	TAG H
ATOM	364	1HE	HIS	21	-12.751	-5.616	6.693	1.00	0.00	TAG H
ATOM	365	2HE	HIS	21	-14.138	-6.713	4.757	1.00	0.00	TAG H
ATOM	366	N	ARG	22	-7.530	-8.298	1.880	1.00	1.00	TAG N
ATOM	367	CA	ARG	22	-6.290	-8.346	1.124	1.00	1.00	TAG C
ATOM	368	C	ARG	22	-6.777	-8.305	-0.323	1.00	1.00	TAG C
ATOM	369	CB	ARG	22	-5.560	-9.656	1.442	1.00	1.00	TAG C
ATOM	370	CG	ARG	22	-4.211	-9.821	0.749	1.00	1.00	TAG C
ATOM	371	CD	ARG	22	-3.398	-10.948	1.373	1.00	1.00	TAG C
ATOM	372	NE	ARG	22	-4.227	-12.113	1.677	1.00	1.00	TAG N
ATOM	373	CZ	ARG	22	-4.219	-12.756	2.844	1.00	1.00	TAG C
ATOM	374	NH1	ARG	22	-3.418	-12.354	3.830	1.00	1.00	TAG N
ATOM	375	NH2	ARG	22	-5.032	-13.793	3.034	1.00	1.00	TAG N1+
ATOM	376	O01	ARG	22	-5.593	-8.216	-1.120	1.00	1.00	TAG O
ATOM	377	H	ARG	22	-7.489	-8.770	2.760	1.00	1.00	TAG H
ATOM	378	HA	ARG	22	-5.580	-7.537	1.348	1.00	1.00	TAG H
ATOM	379	1HB	ARG	22	-5.408	-9.719	2.530	1.00	1.00	TAG H
ATOM	380	2HB	ARG	22	-6.208	-10.498	1.158	1.00	1.00	TAG H
ATOM	381	1HG	ARG	22	-4.369	-10.029	-0.320	1.00	1.00	TAG H
ATOM	382	2HG	ARG	22	-3.645	-8.879	0.814	1.00	1.00	TAG H
ATOM	383	1HD	ARG	22	-2.590	-11.241	0.686	1.00	1.00	TAG H
ATOM	384	2HD	ARG	22	-2.920	-10.587	2.297	1.00	1.00	TAG H

ATOM	385	HE	ARG	22	-4.839	-12.450	0.962	1.00	1.00	TAG	H
ATOM	386	1HH1	ARG	22	-2.818	-11.566	3.696	1.00	1.00	TAG	H
ATOM	387	2HH1	ARG	22	-3.418	-12.841	4.703	1.00	1.00	TAG	H
ATOM	388	H01	ARG	22	-5.225	-13.894	4.020	1.00	1.00	TAG	H
ATOM	389	H02	ARG	22	-4.592	-14.634	2.688	1.00	1.00	TAG	H
ATOM	390	H03	ARG	22	-5.897	-13.637	2.537	1.00	1.00	TAG	H
ATOM	391	N	GLY	23	-7.457	-9.146	-0.854	1.00	1.00	TAG	N
ATOM	392	CA	GLY	23	-7.954	-9.169	-2.226	1.00	1.00	TAG	C
ATOM	393	C	GLY	23	-7.076	-8.328	-3.151	1.00	1.00	TAG	C
ATOM	394	O	GLY	23	-6.593	-8.821	-4.173	1.00	1.00	TAG	O
ATOM	395	H	GLY	23	-7.754	-9.955	-0.347	1.00	1.00	TAG	H
ATOM	396	1HA	GLY	23	-7.984	-10.207	-2.589	1.00	1.00	TAG	H
ATOM	397	2HA	GLY	23	-8.986	-8.790	-2.251	1.00	1.00	TAG	H
ATOM	398	N	TYR	24	-6.851	-7.092	-2.813	1.00	0.00	TAG	N
ATOM	399	CA	TYR	24	-6.007	-6.142	-3.531	1.00	0.00	TAG	C
ATOM	400	C	TYR	24	-4.974	-6.859	-4.366	1.00	0.00	TAG	C
ATOM	401	O	TYR	24	-4.416	-7.886	-4.038	1.00	0.00	TAG	O
ATOM	402	CB	TYR	24	-5.256	-5.206	-2.539	1.00	0.00	TAG	C
ATOM	403	CG	TYR	24	-4.437	-4.066	-3.154	1.00	0.00	TAG	C
ATOM	404	CD1	TYR	24	-4.706	-3.614	-4.450	1.00	0.00	TAG	C
ATOM	405	CD2	TYR	24	-3.417	-3.464	-2.411	1.00	0.00	TAG	C
ATOM	406	CE1	TYR	24	-3.964	-2.567	-4.992	1.00	0.00	TAG	C
ATOM	407	CE2	TYR	24	-2.677	-2.418	-2.955	1.00	0.00	TAG	C
ATOM	408	CZ	TYR	24	-2.951	-1.971	-4.246	1.00	0.00	TAG	C
ATOM	409	OH	TYR	24	-2.228	-0.943	-4.781	1.00	0.00	TAG	O
ATOM	410	OXT	TYR	24	-4.606	-6.310	-5.645	0.00	0.00	TAG	O
ATOM	411	H	TYR	24	-7.325	-6.743	-1.937	1.00	0.00	TAG	H
ATOM	412	HA	TYR	24	-6.640	-5.544	-4.214	1.00	0.00	TAG	H
ATOM	413	2HB	TYR	24	-4.571	-5.806	-1.908	1.00	0.00	TAG	H
ATOM	414	3HB	TYR	24	-5.980	-4.790	-1.808	1.00	0.00	TAG	H
ATOM	415	1HD	TYR	24	-5.494	-4.067	-5.035	1.00	0.00	TAG	H
ATOM	416	2HD	TYR	24	-3.206	-3.799	-1.405	1.00	0.00	TAG	H
ATOM	417	1HE	TYR	24	-4.174	-2.212	-5.990	1.00	0.00	TAG	H
ATOM	418	2HE	TYR	24	-1.896	-1.958	-2.369	1.00	0.00	TAG	H
ATOM	419	HH	TYR	24	-1.582	-0.656	-4.132	1.00	0.00	TAG	H
ATOM	420	H01	TYR	24	-4.688	-5.354	-5.619	0.00	0.00	TAG	H
END											

Histatin conformer 3:

ATOM	1	N	ASP	1	-0.753	-1.254	-0.000	1.00	1.00	TAG	N1+
ATOM	2	CA	ASP	1	0.000	0.000	0.000	1.00	1.00	TAG	C
ATOM	3	C	ASP	1	-0.977	1.162	0.126	1.00	1.00	TAG	C
ATOM	4	O	ASP	1	-0.996	1.864	1.147	1.00	1.00	TAG	O
ATOM	5	CB	ASP	1	0.960	0.223	-1.175	1.00	1.00	TAG	C
ATOM	6	CG	ASP	1	1.836	1.489	-1.014	1.00	1.00	TAG	C
ATOM	7	OD1	ASP	1	1.994	2.027	0.117	1.00	1.00	TAG	O
ATOM	8	OD2	ASP	1	2.382	1.952	-2.045	1.00	1.00	TAG	O1-
ATOM	9	1H	ASP	1	-0.117	-2.025	-0.000	1.00	1.00	TAG	H
ATOM	10	2H	ASP	1	-1.329	-1.298	0.816	1.00	1.00	TAG	H
ATOM	11	3H	ASP	1	-1.329	-1.298	-0.816	1.00	1.00	TAG	H

ATOM	12	HA	ASP	1	0.619	-0.066	0.906	1.00	1.00	TAG	H
ATOM	13	1HB	ASP	1	1.613	-0.656	-1.279	1.00	1.00	TAG	H
ATOM	14	2HB	ASP	1	0.379	0.303	-2.105	1.00	1.00	TAG	H
ATOM	15	H01	ASP	1	2.425	2.909	-1.983	1.00	1.00	TAG	H
ATOM	16	N	SER	2	-1.783	1.400	-0.850	1.00	1.00	TAG	N
ATOM	17	CA	SER	2	-2.804	2.448	-0.821	1.00	1.00	TAG	C
ATOM	18	C	SER	2	-3.967	2.161	0.116	1.00	1.00	TAG	C
ATOM	19	O	SER	2	-4.487	2.934	0.906	1.00	1.00	TAG	O
ATOM	20	CB	SER	2	-3.356	2.664	-2.232	1.00	1.00	TAG	C
ATOM	21	OG	SER	2	-4.446	3.566	-2.207	1.00	1.00	TAG	O
ATOM	22	H	SER	2	-1.770	0.881	-1.705	1.00	1.00	TAG	H
ATOM	23	HA	SER	2	-2.301	3.348	-0.437	1.00	1.00	TAG	H
ATOM	24	1HB	SER	2	-2.563	3.057	-2.886	1.00	1.00	TAG	H
ATOM	25	2HB	SER	2	-3.677	1.703	-2.658	1.00	1.00	TAG	H
ATOM	26	HG	SER	2	-4.793	3.697	-3.136	1.00	1.00	TAG	H
ATOM	27	N	HIS	3	-4.468	0.848	0.012	1.00	0.00	TAG	N
ATOM	28	CA	HIS	3	-5.469	0.326	0.939	1.00	0.00	TAG	C
ATOM	29	C	HIS	3	-4.957	0.347	2.358	1.00	0.00	TAG	C
ATOM	30	O	HIS	3	-5.590	-0.174	3.294	1.00	0.00	TAG	O
ATOM	31	CB	HIS	3	-5.759	-1.117	0.494	1.00	0.00	TAG	C
ATOM	32	CG	HIS	3	-6.501	-1.174	-0.809	1.00	0.00	TAG	C
ATOM	33	CD2	HIS	3	-5.940	-1.689	-1.970	1.00	0.00	TAG	C
ATOM	34	ND1	HIS	3	-7.806	-0.736	-1.025	1.00	0.00	TAG	N
ATOM	35	CE1	HIS	3	-7.932	-1.023	-2.334	1.00	0.00	TAG	C
ATOM	36	NE2	HIS	3	-6.872	-1.593	-2.970	1.00	0.00	TAG	N
ATOM	37	H	HIS	3	-4.131	0.260	-0.712	1.00	0.00	TAG	H
ATOM	38	HA	HIS	3	-6.339	1.004	0.907	1.00	0.00	TAG	H
ATOM	39	2HB	HIS	3	-6.361	-1.657	1.252	1.00	0.00	TAG	H
ATOM	40	3HB	HIS	3	-4.830	-1.714	0.378	1.00	0.00	TAG	H
ATOM	41	2HD	HIS	3	-4.933	-2.091	-2.041	1.00	0.00	TAG	H
ATOM	42	1HE	HIS	3	-8.874	-0.787	-2.810	1.00	0.00	TAG	H
ATOM	43	2HE	HIS	3	-6.784	-1.881	-3.956	1.00	0.00	TAG	H
ATOM	44	N	ALA	4	-3.773	0.942	2.578	1.00	1.00	TAG	N
ATOM	45	CA	ALA	4	-3.163	1.024	3.891	1.00	1.00	TAG	C
ATOM	46	C	ALA	4	-4.026	1.905	4.812	1.00	1.00	TAG	C
ATOM	47	O	ALA	4	-4.295	1.519	5.946	1.00	1.00	TAG	O
ATOM	48	CB	ALA	4	-1.759	1.612	3.765	1.00	1.00	TAG	C
ATOM	49	H	ALA	4	-3.227	1.362	1.853	1.00	1.00	TAG	H
ATOM	50	HA	ALA	4	-3.093	0.017	4.327	1.00	1.00	TAG	H
ATOM	51	1HB	ALA	4	-1.296	1.675	4.761	1.00	1.00	TAG	H
ATOM	52	2HB	ALA	4	-1.148	0.968	3.117	1.00	1.00	TAG	H
ATOM	53	3HB	ALA	4	-1.821	2.619	3.325	1.00	1.00	TAG	H
ATOM	54	N	LYS	5	-4.452	3.041	4.371	1.00	0.00	TAG	N
ATOM	55	CA	LYS	5	-5.239	3.947	5.204	1.00	0.00	TAG	C
ATOM	56	C	LYS	5	-6.317	3.197	5.950	1.00	0.00	TAG	C
ATOM	57	O	LYS	5	-6.608	3.513	7.086	1.00	0.00	TAG	O
ATOM	58	CB	LYS	5	-5.852	5.063	4.315	1.00	0.00	TAG	C
ATOM	59	CG	LYS	5	-4.799	6.047	3.746	1.00	0.00	TAG	C
ATOM	60	CD	LYS	5	-5.378	7.240	2.981	1.00	0.00	TAG	C
ATOM	61	CE	LYS	5	-5.955	6.753	1.645	1.00	0.00	TAG	C
ATOM	62	NZ	LYS	5	-4.863	6.241	0.799	1.00	0.00	TAG	N1+

ATOM	63	H	LYS	5	-4.330	3.441	3.468	1.00	0.00	TAG	H
ATOM	64	HA	LYS	5	-4.567	4.401	5.956	1.00	0.00	TAG	H
ATOM	65	2HB	LYS	5	-6.616	5.623	4.894	1.00	0.00	TAG	H
ATOM	66	3HB	LYS	5	-6.412	4.606	3.475	1.00	0.00	TAG	H
ATOM	67	2HG	LYS	5	-4.086	5.495	3.102	1.00	0.00	TAG	H
ATOM	68	3HG	LYS	5	-4.188	6.469	4.566	1.00	0.00	TAG	H
ATOM	69	2HD	LYS	5	-4.584	7.994	2.803	1.00	0.00	TAG	H
ATOM	70	3HD	LYS	5	-6.150	7.741	3.597	1.00	0.00	TAG	H
ATOM	71	2HE	LYS	5	-6.483	7.572	1.115	1.00	0.00	TAG	H
ATOM	72	3HE	LYS	5	-6.716	5.962	1.816	1.00	0.00	TAG	H
ATOM	73	H01	LYS	5	-4.666	6.905	0.064	1.00	0.00	TAG	H
ATOM	74	H02	LYS	5	-5.138	5.359	0.391	1.00	0.00	TAG	H
ATOM	75	N	ARG	6	-6.907	2.204	5.321	1.00	1.00	TAG	N
ATOM	76	CA	ARG	6	-8.112	1.526	5.835	1.00	1.00	TAG	C
ATOM	77	C	ARG	6	-7.767	0.680	7.051	1.00	1.00	TAG	C
ATOM	78	O	ARG	6	-8.570	0.559	7.988	1.00	1.00	TAG	O
ATOM	79	CB	ARG	6	-8.795	0.652	4.775	1.00	1.00	TAG	C
ATOM	80	CG	ARG	6	-9.399	1.416	3.632	1.00	1.00	TAG	C
ATOM	81	CD	ARG	6	-10.553	2.279	4.082	1.00	1.00	TAG	C
ATOM	82	NE	ARG	6	-10.763	3.377	3.144	1.00	1.00	TAG	N
ATOM	83	CZ	ARG	6	-11.945	3.912	2.860	1.00	1.00	TAG	C
ATOM	84	NH1	ARG	6	-13.060	3.408	3.392	1.00	1.00	TAG	N1+
ATOM	85	NH2	ARG	6	-12.014	4.916	1.988	1.00	1.00	TAG	N1+
ATOM	86	H	ARG	6	-6.579	1.833	4.453	1.00	1.00	TAG	H
ATOM	87	HA	ARG	6	-8.822	2.316	6.119	1.00	1.00	TAG	H
ATOM	88	1HB	ARG	6	-8.058	-0.060	4.374	1.00	1.00	TAG	H
ATOM	89	2HB	ARG	6	-9.584	0.058	5.261	1.00	1.00	TAG	H
ATOM	90	1HG	ARG	6	-8.629	2.047	3.166	1.00	1.00	TAG	H
ATOM	91	2HG	ARG	6	-9.748	0.710	2.862	1.00	1.00	TAG	H
ATOM	92	1HD	ARG	6	-11.467	1.672	4.156	1.00	1.00	TAG	H
ATOM	93	2HD	ARG	6	-10.350	2.680	5.087	1.00	1.00	TAG	H
ATOM	94	HE	ARG	6	-9.959	3.753	2.682	1.00	1.00	TAG	H
ATOM	95	H01	ARG	6	-13.006	2.630	4.034	1.00	1.00	TAG	H
ATOM	96	H02	ARG	6	-13.958	3.804	3.152	1.00	1.00	TAG	H
ATOM	97	H03	ARG	6	-12.554	4.628	1.185	1.00	1.00	TAG	H
ATOM	98	H04	ARG	6	-11.082	5.172	1.694	1.00	1.00	TAG	H
ATOM	99	H05	ARG	6	-12.458	5.711	2.425	1.00	1.00	TAG	H
ATOM	100	N	HIS	7	-6.588	0.077	7.084	1.00	1.00	TAG	N
ATOM	101	CA	HIS	7	-6.124	-0.708	8.218	1.00	1.00	TAG	C
ATOM	102	C	HIS	7	-5.130	0.007	9.135	1.00	1.00	TAG	C
ATOM	103	O	HIS	7	-5.015	-0.297	10.332	1.00	1.00	TAG	O
ATOM	104	CB	HIS	7	-5.585	-2.058	7.758	1.00	1.00	TAG	C
ATOM	105	CG	HIS	7	-6.660	-3.059	7.484	1.00	1.00	TAG	C
ATOM	106	CD2	HIS	7	-7.189	-3.261	6.227	1.00	1.00	TAG	C
ATOM	107	ND1	HIS	7	-7.333	-3.899	8.311	1.00	1.00	TAG	N
ATOM	108	CE1	HIS	7	-8.246	-4.581	7.549	1.00	1.00	TAG	C
ATOM	109	NE2	HIS	7	-8.143	-4.181	6.291	1.00	1.00	TAG	N
ATOM	110	H	HIS	7	-5.933	0.119	6.330	1.00	1.00	TAG	H
ATOM	111	HA	HIS	7	-7.013	-0.867	8.845	1.00	1.00	TAG	H
ATOM	112	1HB	HIS	7	-4.986	-1.914	6.847	1.00	1.00	TAG	H
ATOM	113	2HB	HIS	7	-4.909	-2.457	8.528	1.00	1.00	TAG	H

ATOM	114	HD1	HIS	7	-7.189	-4.002	9.296	1.00	1.00	TAG	H
ATOM	115	HD2	HIS	7	-6.869	-2.740	5.312	1.00	1.00	TAG	H
ATOM	116	HE1	HIS	7	-8.951	-5.338	7.921	1.00	1.00	TAG	H
ATOM	117	N	HIS	8	-4.392	0.982	8.582	1.00	1.00	TAG	N
ATOM	118	CA	HIS	8	-3.472	1.790	9.369	1.00	1.00	TAG	C
ATOM	119	C	HIS	8	-4.053	3.105	9.891	1.00	1.00	TAG	C
ATOM	120	O	HIS	8	-3.327	3.927	10.464	1.00	1.00	TAG	O
ATOM	121	CB	HIS	8	-2.169	2.017	8.614	1.00	1.00	TAG	C
ATOM	122	CG	HIS	8	-1.233	0.853	8.686	1.00	1.00	TAG	C
ATOM	123	CD2	HIS	8	-0.327	0.490	9.628	1.00	1.00	TAG	C
ATOM	124	ND1	HIS	8	-1.189	-0.129	7.720	1.00	1.00	TAG	N
ATOM	125	CE1	HIS	8	-0.296	-1.048	8.062	1.00	1.00	TAG	C
ATOM	126	NE2	HIS	8	0.241	-0.689	9.220	1.00	1.00	TAG	N
ATOM	127	H	HIS	8	-4.420	1.217	7.610	1.00	1.00	TAG	H
ATOM	128	HA	HIS	8	-3.268	1.200	10.274	1.00	1.00	TAG	H
ATOM	129	1HB	HIS	8	-2.396	2.230	7.558	1.00	1.00	TAG	H
ATOM	130	2HB	HIS	8	-1.668	2.907	9.021	1.00	1.00	TAG	H
ATOM	131	HD2	HIS	8	-0.090	1.041	10.551	1.00	1.00	TAG	H
ATOM	132	HE1	HIS	8	-0.044	-1.950	7.487	1.00	1.00	TAG	H
ATOM	133	HE2	HIS	8	0.946	-1.196	9.716	1.00	1.00	TAG	H
ATOM	134	N	GLY	9	-5.433	3.160	9.790	1.00	1.00	TAG	N
ATOM	135	CA	GLY	9	-6.227	4.287	10.314	1.00	1.00	TAG	C
ATOM	136	C	GLY	9	-5.881	5.647	9.694	1.00	1.00	TAG	C
ATOM	137	O	GLY	9	-6.369	6.692	10.132	1.00	1.00	TAG	O
ATOM	138	H	GLY	9	-5.982	2.445	9.357	1.00	1.00	TAG	H
ATOM	139	1HA	GLY	9	-7.293	4.079	10.142	1.00	1.00	TAG	H
ATOM	140	2HA	GLY	9	-6.082	4.346	11.402	1.00	1.00	TAG	H
ATOM	141	N	TYR	10	-5.025	5.607	8.703	1.00	0.00	TAG	N
ATOM	142	CA	TYR	10	-4.565	6.828	8.048	1.00	0.00	TAG	C
ATOM	143	C	TYR	10	-5.284	7.042	6.738	1.00	0.00	TAG	C
ATOM	144	O	TYR	10	-4.672	7.352	5.737	1.00	0.00	TAG	O
ATOM	145	CB	TYR	10	-3.038	6.759	7.753	1.00	0.00	TAG	C
ATOM	146	CG	TYR	10	-2.102	6.761	8.967	1.00	0.00	TAG	C
ATOM	147	CD1	TYR	10	-2.570	7.144	10.228	1.00	0.00	TAG	C
ATOM	148	CD2	TYR	10	-0.769	6.368	8.817	1.00	0.00	TAG	C
ATOM	149	CE1	TYR	10	-1.714	7.127	11.325	1.00	0.00	TAG	C
ATOM	150	CE2	TYR	10	0.086	6.353	9.915	1.00	0.00	TAG	C
ATOM	151	CZ	TYR	10	-0.388	6.732	11.169	1.00	0.00	TAG	C
ATOM	152	OH	TYR	10	0.448	6.715	12.249	1.00	0.00	TAG	O
ATOM	153	H	TYR	10	-4.679	4.724	8.390	1.00	0.00	TAG	H
ATOM	154	HA	TYR	10	-4.788	7.692	8.702	1.00	0.00	TAG	H
ATOM	155	2HB	TYR	10	-2.746	7.609	7.105	1.00	0.00	TAG	H
ATOM	156	3HB	TYR	10	-2.826	5.870	7.123	1.00	0.00	TAG	H
ATOM	157	1HD	TYR	10	-3.600	7.446	10.360	1.00	0.00	TAG	H
ATOM	158	2HD	TYR	10	-0.397	6.061	7.848	1.00	0.00	TAG	H
ATOM	159	1HE	TYR	10	-2.075	7.416	12.301	1.00	0.00	TAG	H
ATOM	160	2HE	TYR	10	1.111	6.041	9.786	1.00	0.00	TAG	H
ATOM	161	HH	TYR	10	1.313	6.418	11.959	1.00	0.00	TAG	H
ATOM	162	N	LYS	11	-6.493	6.863	6.627	1.00	0.00	TAG	N
ATOM	163	CA	LYS	11	-7.236	6.950	5.373	1.00	0.00	TAG	C
ATOM	164	C	LYS	11	-7.582	8.384	5.047	1.00	0.00	TAG	C

ATOM	165	O	LYS	11	-7.981	8.665	3.916	1.00	0.00	TAG O
ATOM	166	CB	LYS	11	-8.518	6.078	5.470	1.00	0.00	TAG C
ATOM	167	CG	LYS	11	-9.590	6.663	6.423	1.00	0.00	TAG C
ATOM	168	CD	LYS	11	-10.877	5.840	6.528	1.00	0.00	TAG C
ATOM	169	CE	LYS	11	-11.875	6.574	7.434	1.00	0.00	TAG C
ATOM	170	NZ	LYS	11	-13.118	5.789	7.531	1.00	0.00	TAG N1+
ATOM	171	H	LYS	11	-7.006	6.643	7.455	1.00	0.00	TAG H
ATOM	172	HA	LYS	11	-6.592	6.570	4.558	1.00	0.00	TAG H
ATOM	173	2HB	LYS	11	-8.247	5.052	5.793	1.00	0.00	TAG H
ATOM	174	3HB	LYS	11	-8.960	5.951	4.462	1.00	0.00	TAG H
ATOM	175	2HG	LYS	11	-9.829	7.701	6.120	1.00	0.00	TAG H
ATOM	176	3HG	LYS	11	-9.186	6.742	7.450	1.00	0.00	TAG H
ATOM	177	2HD	LYS	11	-10.649	4.837	6.943	1.00	0.00	TAG H
ATOM	178	3HD	LYS	11	-11.297	5.671	5.517	1.00	0.00	TAG H
ATOM	179	2HE	LYS	11	-12.105	7.585	7.039	1.00	0.00	TAG H
ATOM	180	3HE	LYS	11	-11.438	6.734	8.442	1.00	0.00	TAG H
ATOM	181	H01	LYS	11	-13.396	5.716	8.499	1.00	0.00	TAG H
ATOM	182	H02	LYS	11	-12.963	4.865	7.154	1.00	0.00	TAG H
ATOM	183	N	ARG	12	-7.483	9.277	5.901	1.00	1.00	TAG N
ATOM	184	CA	ARG	12	-7.755	10.689	5.688	1.00	1.00	TAG C
ATOM	185	C	ARG	12	-6.827	11.040	4.528	1.00	1.00	TAG C
ATOM	186	O	ARG	12	-7.286	12.080	3.795	1.00	1.00	TAG O
ATOM	187	CB	ARG	12	-7.395	11.463	6.959	1.00	1.00	TAG C
ATOM	188	CG	ARG	12	-7.677	12.963	6.896	1.00	1.00	TAG C
ATOM	189	CD	ARG	12	-7.634	13.597	8.280	1.00	1.00	TAG C
ATOM	190	NE	ARG	12	-6.527	13.082	9.082	1.00	1.00	TAG N
ATOM	191	CZ	ARG	12	-6.646	12.651	10.337	1.00	1.00	TAG C
ATOM	192	NH1	ARG	12	-7.829	12.676	10.948	1.00	1.00	TAG N1+
ATOM	193	NH2	ARG	12	-5.582	12.173	10.977	1.00	1.00	TAG N1+
ATOM	194	H	ARG	12	-7.192	9.086	6.838	1.00	1.00	TAG H
ATOM	195	HA	ARG	12	-8.806	10.929	5.467	1.00	1.00	TAG H
ATOM	196	1HB	ARG	12	-7.955	11.035	7.804	1.00	1.00	TAG H
ATOM	197	2HB	ARG	12	-6.326	11.314	7.172	1.00	1.00	TAG H
ATOM	198	1HG	ARG	12	-6.936	13.450	6.245	1.00	1.00	TAG H
ATOM	199	2HG	ARG	12	-8.664	13.133	6.443	1.00	1.00	TAG H
ATOM	200	1HD	ARG	12	-7.536	14.689	8.180	1.00	1.00	TAG H
ATOM	201	2HD	ARG	12	-8.584	13.406	8.801	1.00	1.00	TAG H
ATOM	202	HE	ARG	12	-5.620	13.050	8.662	1.00	1.00	TAG H
ATOM	203	H01	ARG	12	-8.641	13.031	10.463	1.00	1.00	TAG H
ATOM	204	H02	ARG	12	-7.915	12.340	11.897	1.00	1.00	TAG H
ATOM	205	H03	ARG	12	-5.267	11.328	10.523	1.00	1.00	TAG H
ATOM	206	H04	ARG	12	-5.828	11.970	11.935	1.00	1.00	TAG H
ATOM	207	H05	ARG	12	-4.842	12.860	10.959	1.00	1.00	TAG H
ATOM	208	N	LYS	13	-5.729	10.669	4.320	1.00	1.00	TAG N
ATOM	209	CA	LYS	13	-4.870	11.043	3.204	1.00	1.00	TAG C
ATOM	210	C	LYS	13	-5.674	11.078	1.910	1.00	1.00	TAG C
ATOM	211	O	LYS	13	-5.181	11.590	0.894	1.00	1.00	TAG O
ATOM	212	CB	LYS	13	-3.703	10.059	3.072	1.00	1.00	TAG C
ATOM	213	CG	LYS	13	-2.662	10.221	4.152	1.00	1.00	TAG C
ATOM	214	CD	LYS	13	-1.550	9.204	4.009	1.00	1.00	TAG C
ATOM	215	CE	LYS	13	-0.545	9.385	5.143	1.00	1.00	TAG C

ATOM	216	NZ	LYS	13	0.449	8.285	5.217	1.00	1.00	TAG	N1+
ATOM	217	H	LYS	13	-5.276	10.025	4.938	1.00	1.00	TAG	H
ATOM	218	HA	LYS	13	-4.462	12.047	3.397	1.00	1.00	TAG	H
ATOM	219	1HB	LYS	13	-4.094	9.031	3.101	1.00	1.00	TAG	H
ATOM	220	2HB	LYS	13	-3.227	10.194	2.090	1.00	1.00	TAG	H
ATOM	221	1HG	LYS	13	-2.240	11.236	4.107	1.00	1.00	TAG	H
ATOM	222	2HG	LYS	13	-3.135	10.113	5.139	1.00	1.00	TAG	H
ATOM	223	1HD	LYS	13	-1.965	8.186	4.031	1.00	1.00	TAG	H
ATOM	224	2HD	LYS	13	-1.048	9.326	3.037	1.00	1.00	TAG	H
ATOM	225	1HE	LYS	13	-0.016	10.341	5.008	1.00	1.00	TAG	H
ATOM	226	2HE	LYS	13	-1.086	9.448	6.099	1.00	1.00	TAG	H
ATOM	227	H01	LYS	13	0.679	7.975	4.284	1.00	1.00	TAG	H
ATOM	228	H02	LYS	13	0.061	7.514	5.742	1.00	1.00	TAG	H
ATOM	229	N	PHE	14	-6.870	10.602	1.862	1.00	0.00	TAG	N
ATOM	230	CA	PHE	14	-7.671	10.603	0.641	1.00	0.00	TAG	C
ATOM	231	C	PHE	14	-8.212	11.983	0.349	1.00	0.00	TAG	C
ATOM	232	O	PHE	14	-8.529	12.282	-0.834	1.00	0.00	TAG	O
ATOM	233	CB	PHE	14	-8.868	9.615	0.786	1.00	0.00	TAG	C
ATOM	234	CG	PHE	14	-9.684	9.336	-0.486	1.00	0.00	TAG	C
ATOM	235	CD1	PHE	14	-9.148	8.515	-1.484	1.00	0.00	TAG	C
ATOM	236	CD2	PHE	14	-10.926	9.942	-0.686	1.00	0.00	TAG	C
ATOM	237	CE1	PHE	14	-9.838	8.318	-2.676	1.00	0.00	TAG	C
ATOM	238	CE2	PHE	14	-11.622	9.736	-1.875	1.00	0.00	TAG	C
ATOM	239	CZ	PHE	14	-11.076	8.926	-2.870	1.00	0.00	TAG	C
ATOM	240	H	PHE	14	-7.267	10.213	2.698	1.00	0.00	TAG	H
ATOM	241	HA	PHE	14	-7.031	10.299	-0.209	1.00	0.00	TAG	H
ATOM	242	2HB	PHE	14	-9.559	9.985	1.570	1.00	0.00	TAG	H
ATOM	243	3HB	PHE	14	-8.506	8.650	1.198	1.00	0.00	TAG	H
ATOM	244	1HD	PHE	14	-8.173	8.064	-1.353	1.00	0.00	TAG	H
ATOM	245	2HD	PHE	14	-11.346	10.589	0.072	1.00	0.00	TAG	H
ATOM	246	1HE	PHE	14	-9.402	7.707	-3.452	1.00	0.00	TAG	H
ATOM	247	2HE	PHE	14	-12.579	10.213	-2.029	1.00	0.00	TAG	H
ATOM	248	HZ	PHE	14	-11.607	8.776	-3.798	1.00	0.00	TAG	H
ATOM	249	N	HIS	15	-8.299	12.881	1.326	1.00	0.00	TAG	N
ATOM	250	CA	HIS	15	-8.707	14.273	1.155	1.00	0.00	TAG	C
ATOM	251	C	HIS	15	-7.691	15.213	1.758	1.00	0.00	TAG	C
ATOM	252	O	HIS	15	-7.035	16.024	1.046	1.00	0.00	TAG	O
ATOM	253	CB	HIS	15	-10.061	14.417	1.869	1.00	0.00	TAG	C
ATOM	254	CG	HIS	15	-10.670	15.774	1.668	1.00	0.00	TAG	C
ATOM	255	CD2	HIS	15	-10.078	16.752	0.881	1.00	0.00	TAG	C
ATOM	256	ND1	HIS	15	-11.867	16.221	2.223	1.00	0.00	TAG	N
ATOM	257	CE1	HIS	15	-11.903	17.469	1.718	1.00	0.00	TAG	C
ATOM	258	NE2	HIS	15	-10.882	17.863	0.910	1.00	0.00	TAG	N
ATOM	259	H	HIS	15	-8.059	12.580	2.261	1.00	0.00	TAG	H
ATOM	260	HA	HIS	15	-8.729	14.484	0.073	1.00	0.00	TAG	H
ATOM	261	2HB	HIS	15	-9.959	14.247	2.959	1.00	0.00	TAG	H
ATOM	262	3HB	HIS	15	-10.799	13.663	1.522	1.00	0.00	TAG	H
ATOM	263	2HD	HIS	15	-9.140	16.629	0.347	1.00	0.00	TAG	H
ATOM	264	1HE	HIS	15	-12.747	18.092	1.981	1.00	0.00	TAG	H
ATOM	265	2HE	HIS	15	-10.739	18.767	0.436	1.00	0.00	TAG	H
ATOM	266	N	GLU	16	-7.459	15.145	3.056	1.00	0.00	TAG	N

ATOM	267	CA	GLU	16	-6.630	16.106	3.779	1.00	0.00	TAG C
ATOM	268	C	GLU	16	-5.206	16.073	3.281	1.00	0.00	TAG C
ATOM	269	O	GLU	16	-4.505	17.082	3.345	1.00	0.00	TAG O
ATOM	270	CB	GLU	16	-6.681	15.800	5.303	1.00	0.00	TAG C
ATOM	271	CG	GLU	16	-5.908	16.802	6.221	1.00	0.00	TAG C
ATOM	272	CD	GLU	16	-6.017	16.634	7.725	1.00	0.00	TAG C
ATOM	273	OE1	GLU	16	-5.730	15.551	8.270	1.00	0.00	TAG O
ATOM	274	OE2	GLU	16	-6.391	17.634	8.373	1.00	0.00	TAG O1-
ATOM	275	H	GLU	16	-7.872	14.399	3.570	1.00	0.00	TAG H
ATOM	276	HA	GLU	16	-7.029	17.121	3.601	1.00	0.00	TAG H
ATOM	277	2HB	GLU	16	-6.291	14.779	5.493	1.00	0.00	TAG H
ATOM	278	3HB	GLU	16	-7.733	15.759	5.645	1.00	0.00	TAG H
ATOM	279	2HG	GLU	16	-6.196	17.844	6.005	1.00	0.00	TAG H
ATOM	280	3HG	GLU	16	-4.821	16.752	6.043	1.00	0.00	TAG H
ATOM	281	H01	GLU	16	-6.401	18.403	7.798	1.00	0.00	TAG H
ATOM	282	N	LYS	17	-4.757	14.928	2.800	1.00	0.00	TAG N
ATOM	283	CA	LYS	17	-3.432	14.789	2.201	1.00	0.00	TAG C
ATOM	284	C	LYS	17	-3.311	15.632	0.954	1.00	0.00	TAG C
ATOM	285	O	LYS	17	-2.293	16.274	0.725	1.00	0.00	TAG O
ATOM	286	CB	LYS	17	-3.161	13.292	1.889	1.00	0.00	TAG C
ATOM	287	CG	LYS	17	-1.735	13.024	1.347	1.00	0.00	TAG C
ATOM	288	CD	LYS	17	-0.610	13.217	2.369	1.00	0.00	TAG C
ATOM	289	CE	LYS	17	0.723	12.791	1.740	1.00	0.00	TAG C
ATOM	290	NZ	LYS	17	1.804	12.949	2.729	1.00	0.00	TAG N1+
ATOM	291	H	LYS	17	-5.346	14.127	2.847	1.00	0.00	TAG H
ATOM	292	HA	LYS	17	-2.682	15.157	2.925	1.00	0.00	TAG H
ATOM	293	2HB	LYS	17	-3.915	12.919	1.166	1.00	0.00	TAG H
ATOM	294	3HB	LYS	17	-3.321	12.686	2.803	1.00	0.00	TAG H
ATOM	295	2HG	LYS	17	-1.550	13.659	0.459	1.00	0.00	TAG H
ATOM	296	3HG	LYS	17	-1.653	11.982	0.986	1.00	0.00	TAG H
ATOM	297	2HD	LYS	17	-0.818	12.610	3.274	1.00	0.00	TAG H
ATOM	298	3HD	LYS	17	-0.582	14.273	2.701	1.00	0.00	TAG H
ATOM	299	2HE	LYS	17	0.952	13.397	0.839	1.00	0.00	TAG H
ATOM	300	3HE	LYS	17	0.668	11.738	1.391	1.00	0.00	TAG H
ATOM	301	1HZ	LYS	17	1.473	12.701	3.669	1.00	0.00	TAG H
ATOM	302	2HZ	LYS	17	2.588	12.321	2.528	1.00	0.00	TAG H
ATOM	303	3HZ	LYS	17	2.095	13.915	2.680	1.00	0.00	TAG H
ATOM	304	N	HIS	18	-4.401	15.777	0.216	1.00	0.00	TAG N
ATOM	305	CA	HIS	18	-4.444	16.400	-1.104	1.00	0.00	TAG C
ATOM	306	C	HIS	18	-4.447	17.905	-0.994	1.00	0.00	TAG C
ATOM	307	O	HIS	18	-4.036	18.640	-1.918	1.00	0.00	TAG O
ATOM	308	CB	HIS	18	-5.738	15.907	-1.773	1.00	0.00	TAG C
ATOM	309	CG	HIS	18	-5.698	14.439	-2.080	1.00	0.00	TAG C
ATOM	310	CD2	HIS	18	-4.524	13.698	-2.053	1.00	0.00	TAG C
ATOM	311	ND1	HIS	18	-6.792	13.647	-2.420	1.00	0.00	TAG N
ATOM	312	CE1	HIS	18	-6.177	12.461	-2.582	1.00	0.00	TAG C
ATOM	313	NE2	HIS	18	-4.832	12.403	-2.380	1.00	0.00	TAG N
ATOM	314	H	HIS	18	-5.258	15.435	0.590	1.00	0.00	TAG H
ATOM	315	HA	HIS	18	-3.515	16.124	-1.633	1.00	0.00	TAG H
ATOM	316	2HB	HIS	18	-5.930	16.448	-2.721	1.00	0.00	TAG H
ATOM	317	3HB	HIS	18	-6.632	16.095	-1.142	1.00	0.00	TAG H

ATOM	318	2HD	HIS	18	-3.546	14.104	-1.812	1.00	0.00	TAG	H
ATOM	319	1HE	HIS	18	-6.788	11.613	-2.861	1.00	0.00	TAG	H
ATOM	320	2HE	HIS	18	-4.198	11.595	-2.455	1.00	0.00	TAG	H
ATOM	321	N	HIS	19	-5.097	18.456	0.023	1.00	1.00	TAG	N
ATOM	322	CA	HIS	19	-5.235	19.895	0.197	1.00	1.00	TAG	C
ATOM	323	C	HIS	19	-5.060	20.392	1.633	1.00	1.00	TAG	C
ATOM	324	O	HIS	19	-4.194	21.163	2.064	1.00	1.00	TAG	O
ATOM	325	CB	HIS	19	-6.540	20.391	-0.411	1.00	1.00	TAG	C
ATOM	326	CG	HIS	19	-6.476	20.560	-1.894	1.00	1.00	TAG	C
ATOM	327	CD2	HIS	19	-6.872	19.576	-2.774	1.00	1.00	TAG	C
ATOM	328	ND1	HIS	19	-6.027	21.586	-2.661	1.00	1.00	TAG	N
ATOM	329	CE1	HIS	19	-6.159	21.209	-3.971	1.00	1.00	TAG	C
ATOM	330	NE2	HIS	19	-6.671	19.988	-4.019	1.00	1.00	TAG	N
ATOM	331	H	HIS	19	-5.553	17.920	0.734	1.00	1.00	TAG	H
ATOM	332	HA	HIS	19	-4.389	20.336	-0.351	1.00	1.00	TAG	H
ATOM	333	1HB	HIS	19	-7.344	19.682	-0.164	1.00	1.00	TAG	H
ATOM	334	2HB	HIS	19	-6.808	21.354	0.049	1.00	1.00	TAG	H
ATOM	335	HD2	HIS	19	-7.291	18.599	-2.488	1.00	1.00	TAG	H
ATOM	336	HE1	HIS	19	-5.884	21.820	-4.843	1.00	1.00	TAG	H
ATOM	337	HE2	HIS	19	-6.872	19.467	-4.849	1.00	1.00	TAG	H
ATOM	338	N	SER	20	-6.000	19.873	2.511	1.00	0.00	TAG	N
ATOM	339	CA	SER	20	-6.064	20.210	3.930	1.00	0.00	TAG	C
ATOM	340	C	SER	20	-4.694	20.139	4.565	1.00	0.00	TAG	C
ATOM	341	O	SER	20	-4.354	20.737	5.605	1.00	0.00	TAG	O
ATOM	342	CB	SER	20	-7.080	19.303	4.668	1.00	0.00	TAG	C
ATOM	343	OG	SER	20	-7.265	19.673	6.038	1.00	0.00	TAG	O
ATOM	344	H	SER	20	-6.699	19.208	2.138	1.00	0.00	TAG	H
ATOM	345	HA	SER	20	-6.403	21.259	4.017	1.00	0.00	TAG	H
ATOM	346	2HB	SER	20	-6.783	18.239	4.609	1.00	0.00	TAG	H
ATOM	347	3HB	SER	20	-8.062	19.353	4.158	1.00	0.00	TAG	H
ATOM	348	HG	SER	20	-6.423	19.555	6.484	1.00	0.00	TAG	H
ATOM	349	N	HIS	21	-3.765	19.238	4.013	1.00	0.00	TAG	N
ATOM	350	CA	HIS	21	-2.436	19.103	4.602	1.00	0.00	TAG	C
ATOM	351	C	HIS	21	-1.363	19.193	3.545	1.00	0.00	TAG	C
ATOM	352	O	HIS	21	-0.120	18.996	3.732	1.00	0.00	TAG	O
ATOM	353	CB	HIS	21	-2.403	17.725	5.284	1.00	0.00	TAG	C
ATOM	354	CG	HIS	21	-1.157	17.520	6.094	1.00	0.00	TAG	C
ATOM	355	CD2	HIS	21	-1.077	17.840	7.443	1.00	0.00	TAG	C
ATOM	356	ND1	HIS	21	0.046	16.998	5.623	1.00	0.00	TAG	N
ATOM	357	CE1	HIS	21	0.778	17.050	6.751	1.00	0.00	TAG	C
ATOM	358	NE2	HIS	21	0.186	17.534	7.877	1.00	0.00	TAG	N
ATOM	359	H	HIS	21	-4.011	18.699	3.231	1.00	0.00	TAG	H
ATOM	360	HA	HIS	21	-2.283	19.959	5.281	1.00	0.00	TAG	H
ATOM	361	2HB	HIS	21	-2.463	16.908	4.538	1.00	0.00	TAG	H
ATOM	362	3HB	HIS	21	-3.272	17.572	5.958	1.00	0.00	TAG	H
ATOM	363	2HD	HIS	21	-1.893	18.260	8.024	1.00	0.00	TAG	H
ATOM	364	1HE	HIS	21	1.800	16.700	6.702	1.00	0.00	TAG	H
ATOM	365	2HE	HIS	21	0.582	17.648	8.822	1.00	0.00	TAG	H
ATOM	366	N	ARG	22	-1.760	19.554	2.326	1.00	0.00	TAG	N
ATOM	367	CA	ARG	22	-0.847	19.917	1.247	1.00	0.00	TAG	C
ATOM	368	C	ARG	22	-0.559	21.400	1.259	1.00	0.00	TAG	C

ATOM	369	O	ARG	22	0.570	21.785	1.397	1.00	0.00	TAG O
ATOM	370	CB	ARG	22	-1.468	19.472	-0.107	1.00	0.00	TAG C
ATOM	371	CG	ARG	22	-0.619	19.788	-1.370	1.00	0.00	TAG C
ATOM	372	CD	ARG	22	0.696	18.991	-1.396	1.00	0.00	TAG C
ATOM	373	NE	ARG	22	0.398	17.534	-1.519	1.00	0.00	TAG N
ATOM	374	CZ	ARG	22	1.293	16.556	-1.427	1.00	0.00	TAG C
ATOM	375	NH1	ARG	22	2.563	16.757	-1.208	1.00	0.00	TAG N1+
ATOM	376	NH2	ARG	22	0.885	15.333	-1.563	1.00	0.00	TAG N1+
ATOM	377	H	ARG	22	-2.744	19.565	2.149	1.00	0.00	TAG H
ATOM	378	HA	ARG	22	0.111	19.390	1.417	1.00	0.00	TAG H
ATOM	379	2HB	ARG	22	-2.476	19.926	-0.203	1.00	0.00	TAG H
ATOM	380	3HB	ARG	22	-1.662	18.380	-0.076	1.00	0.00	TAG H
ATOM	381	2HG	ARG	22	-0.414	20.878	-1.407	1.00	0.00	TAG H
ATOM	382	3HG	ARG	22	-1.201	19.563	-2.287	1.00	0.00	TAG H
ATOM	383	2HD	ARG	22	1.272	19.202	-0.468	1.00	0.00	TAG H
ATOM	384	3HD	ARG	22	1.325	19.342	-2.243	1.00	0.00	TAG H
ATOM	385	HE	ARG	22	-0.557	17.204	-1.691	1.00	0.00	TAG H
ATOM	386	1HH1	ARG	22	2.818	17.742	-1.110	1.00	0.00	TAG H
ATOM	387	2HH1	ARG	22	3.187	15.951	-1.152	1.00	0.00	TAG H
ATOM	388	H01	ARG	22	0.763	14.915	-0.652	1.00	0.00	TAG H
ATOM	389	H02	ARG	22	1.569	14.806	-2.087	1.00	0.00	TAG H
ATOM	390	H03	ARG	22	0.004	15.326	-2.057	1.00	0.00	TAG H
ATOM	391	N	GLY	23	-1.471	22.214	1.294	1.00	1.00	TAG N
ATOM	392	CA	GLY	23	-1.339	23.657	1.119	1.00	1.00	TAG C
ATOM	393	C	GLY	23	-0.234	23.998	0.120	1.00	1.00	TAG C
ATOM	394	O	GLY	23	0.574	24.897	0.364	1.00	1.00	TAG O
ATOM	395	H	GLY	23	-2.427	21.949	1.413	1.00	1.00	TAG H
ATOM	396	1HA	GLY	23	-2.294	24.075	0.769	1.00	1.00	TAG H
ATOM	397	2HA	GLY	23	-1.118	24.127	2.088	1.00	1.00	TAG H
ATOM	398	N	TYR	24	-0.189	23.319	-0.988	1.00	0.00	TAG N
ATOM	399	CA	TYR	24	0.746	23.526	-2.090	1.00	0.00	TAG C
ATOM	400	C	TYR	24	1.383	24.892	-2.009	1.00	0.00	TAG C
ATOM	401	O	TYR	24	0.764	25.919	-1.779	1.00	0.00	TAG O
ATOM	402	CB	TYR	24	0.019	23.416	-3.463	1.00	0.00	TAG C
ATOM	403	CG	TYR	24	0.883	23.603	-4.716	1.00	0.00	TAG C
ATOM	404	CD1	TYR	24	1.711	22.572	-5.171	1.00	0.00	TAG C
ATOM	405	CD2	TYR	24	0.836	24.811	-5.418	1.00	0.00	TAG C
ATOM	406	CE1	TYR	24	2.480	22.749	-6.318	1.00	0.00	TAG C
ATOM	407	CE2	TYR	24	1.605	24.986	-6.564	1.00	0.00	TAG C
ATOM	408	CZ	TYR	24	2.427	23.954	-7.014	1.00	0.00	TAG C
ATOM	409	OH	TYR	24	3.180	24.122	-8.141	1.00	0.00	TAG O
ATOM	410	OXT	TYR	24	2.804	25.013	-2.212	0.00	0.00	TAG O1-
ATOM	411	H	TYR	24	-0.890	22.550	-1.100	1.00	0.00	TAG H
ATOM	412	HA	TYR	24	1.551	22.771	-2.025	1.00	0.00	TAG H
ATOM	413	2HB	TYR	24	-0.801	24.159	-3.510	1.00	0.00	TAG H
ATOM	414	3HB	TYR	24	-0.511	22.443	-3.520	1.00	0.00	TAG H
ATOM	415	1HD	TYR	24	1.755	21.631	-4.640	1.00	0.00	TAG H
ATOM	416	2HD	TYR	24	0.192	25.612	-5.081	1.00	0.00	TAG H
ATOM	417	1HE	TYR	24	3.115	21.952	-6.675	1.00	0.00	TAG H
ATOM	418	2HE	TYR	24	1.555	25.921	-7.101	1.00	0.00	TAG H
ATOM	419	HH	TYR	24	3.018	25.002	-8.486	1.00	0.00	TAG H

ATOM 420 H01 TYR 24 3.075 25.918 -2.046 0.00 0.00 TAG H
END

Histatin conformer 4:

ATOM	1	N	ASP	1	-0.753	-1.254	-0.000	1.00	1.00	TAG N1+
ATOM	2	CA	ASP	1	0.000	0.000	0.000	1.00	1.00	TAG C
ATOM	3	C	ASP	1	-0.977	1.169	-0.000	1.00	1.00	TAG C
ATOM	4	O	ASP	1	-0.980	1.990	0.930	1.00	1.00	TAG O
ATOM	5	CB	ASP	1	0.960	0.096	-1.192	1.00	1.00	TAG C
ATOM	6	CG	ASP	1	1.888	1.333	-1.129	1.00	1.00	TAG C
ATOM	7	OD1	ASP	1	2.076	1.945	-0.042	1.00	1.00	TAG O
ATOM	8	OD2	ASP	1	2.445	1.694	-2.194	1.00	1.00	TAG O
ATOM	9	1H	ASP	1	-0.117	-2.025	-0.000	1.00	1.00	TAG H
ATOM	10	2H	ASP	1	-1.329	-1.298	0.816	1.00	1.00	TAG H
ATOM	11	3H	ASP	1	-1.329	-1.298	-0.816	1.00	1.00	TAG H
ATOM	12	HA	ASP	1	0.619	0.032	0.908	1.00	1.00	TAG H
ATOM	13	1HB	ASP	1	1.576	-0.815	-1.233	1.00	1.00	TAG H
ATOM	14	2HB	ASP	1	0.376	0.131	-2.123	1.00	1.00	TAG H
ATOM	15	H01	ASP	1	2.490	2.653	-2.223	1.00	1.00	TAG H
ATOM	16	N	SER	2	-1.800	1.287	-0.984	1.00	1.00	TAG N
ATOM	17	CA	SER	2	-2.734	2.404	-1.129	1.00	1.00	TAG C
ATOM	18	C	SER	2	-3.968	2.304	-0.244	1.00	1.00	TAG C
ATOM	19	O	SER	2	-4.462	3.191	0.435	1.00	1.00	TAG O
ATOM	20	CB	SER	2	-3.187	2.505	-2.588	1.00	1.00	TAG C
ATOM	21	OG	SER	2	-4.203	3.480	-2.727	1.00	1.00	TAG O
ATOM	22	H	SER	2	-1.859	0.619	-1.726	1.00	1.00	TAG H
ATOM	23	HA	SER	2	-2.185	3.300	-0.809	1.00	1.00	TAG H
ATOM	24	1HB	SER	2	-2.331	2.765	-3.227	1.00	1.00	TAG H
ATOM	25	2HB	SER	2	-3.559	1.528	-2.932	1.00	1.00	TAG H
ATOM	26	HG	SER	2	-4.486	3.535	-3.685	1.00	1.00	TAG H
ATOM	27	N	HIS	3	-4.575	1.039	-0.256	1.00	0.00	TAG N
ATOM	28	CA	HIS	3	-5.668	0.686	0.647	1.00	0.00	TAG C
ATOM	29	C	HIS	3	-5.139	0.236	1.987	1.00	0.00	TAG C
ATOM	30	O	HIS	3	-5.872	-0.302	2.836	1.00	0.00	TAG O
ATOM	31	CB	HIS	3	-6.441	-0.454	-0.035	1.00	0.00	TAG C
ATOM	32	CG	HIS	3	-7.071	-0.022	-1.327	1.00	0.00	TAG C
ATOM	33	CD2	HIS	3	-6.654	-0.502	-2.562	1.00	0.00	TAG C
ATOM	34	ND1	HIS	3	-8.120	0.884	-1.461	1.00	0.00	TAG N
ATOM	35	CE1	HIS	3	-8.255	0.885	-2.800	1.00	0.00	TAG C
ATOM	36	NE2	HIS	3	-7.427	0.088	-3.528	1.00	0.00	TAG N
ATOM	37	H	HIS	3	-4.249	0.355	-0.904	1.00	0.00	TAG H
ATOM	38	HA	HIS	3	-6.257	1.601	0.832	1.00	0.00	TAG H
ATOM	39	2HB	HIS	3	-7.245	-0.842	0.622	1.00	0.00	TAG H
ATOM	40	3HB	HIS	3	-5.793	-1.328	-0.253	1.00	0.00	TAG H
ATOM	41	2HD	HIS	3	-5.852	-1.220	-2.704	1.00	0.00	TAG H
ATOM	42	1HE	HIS	3	-9.021	1.520	-3.226	1.00	0.00	TAG H
ATOM	43	2HE	HIS	3	-7.383	-0.043	-4.549	1.00	0.00	TAG H
ATOM	44	N	ALA	4	-3.830	0.419	2.228	1.00	1.00	TAG N
ATOM	45	CA	ALA	4	-3.190	0.008	3.463	1.00	1.00	TAG C
ATOM	46	C	ALA	4	-3.809	0.768	4.649	1.00	1.00	TAG C

ATOM	47	O	ALA	4	-4.177	0.150	5.644	1.00	1.00	TAG	O
ATOM	48	CB	ALA	4	-1.692	0.293	3.380	1.00	1.00	TAG	C
ATOM	49	H	ALA	4	-3.206	0.846	1.573	1.00	1.00	TAG	H
ATOM	50	HA	ALA	4	-3.344	-1.070	3.614	1.00	1.00	TAG	H
ATOM	51	1HB	ALA	4	-1.206	-0.019	4.318	1.00	1.00	TAG	H
ATOM	52	2HB	ALA	4	-1.258	-0.266	2.539	1.00	1.00	TAG	H
ATOM	53	3HB	ALA	4	-1.531	1.370	3.225	1.00	1.00	TAG	H
ATOM	54	N	LYS	5	-3.928	2.052	4.577	1.00	0.00	TAG	N
ATOM	55	CA	LYS	5	-4.539	2.837	5.645	1.00	0.00	TAG	C
ATOM	56	C	LYS	5	-5.987	2.453	5.839	1.00	0.00	TAG	C
ATOM	57	O	LYS	5	-6.497	2.520	6.939	1.00	0.00	TAG	O
ATOM	58	CB	LYS	5	-4.404	4.349	5.317	1.00	0.00	TAG	C
ATOM	59	CG	LYS	5	-5.264	4.796	4.109	1.00	0.00	TAG	C
ATOM	60	CD	LYS	5	-5.163	6.285	3.762	1.00	0.00	TAG	C
ATOM	61	CE	LYS	5	-6.093	6.593	2.581	1.00	0.00	TAG	C
ATOM	62	NZ	LYS	5	-5.966	8.015	2.216	1.00	0.00	TAG	N
ATOM	63	H	LYS	5	-3.592	2.522	3.765	1.00	0.00	TAG	H
ATOM	64	HA	LYS	5	-4.008	2.615	6.589	1.00	0.00	TAG	H
ATOM	65	2HB	LYS	5	-3.338	4.597	5.134	1.00	0.00	TAG	H
ATOM	66	3HB	LYS	5	-4.687	4.950	6.205	1.00	0.00	TAG	H
ATOM	67	2HG	LYS	5	-6.322	4.520	4.283	1.00	0.00	TAG	H
ATOM	68	3HG	LYS	5	-4.962	4.244	3.200	1.00	0.00	TAG	H
ATOM	69	2HD	LYS	5	-4.116	6.539	3.501	1.00	0.00	TAG	H
ATOM	70	3HD	LYS	5	-5.421	6.894	4.649	1.00	0.00	TAG	H
ATOM	71	2HE	LYS	5	-7.150	6.367	2.833	1.00	0.00	TAG	H
ATOM	72	3HE	LYS	5	-5.844	5.947	1.712	1.00	0.00	TAG	H
ATOM	73	H01	LYS	5	-6.081	8.586	3.041	1.00	0.00	TAG	H
ATOM	74	H02	LYS	5	-6.677	8.254	1.539	1.00	0.00	TAG	H
ATOM	75	N	ARG	6	-6.652	2.048	4.778	1.00	1.00	TAG	N
ATOM	76	CA	ARG	6	-8.032	1.534	4.840	1.00	1.00	TAG	C
ATOM	77	C	ARG	6	-8.060	0.166	5.503	1.00	1.00	TAG	C
ATOM	78	O	ARG	6	-8.881	-0.091	6.396	1.00	1.00	TAG	O
ATOM	79	CB	ARG	6	-8.695	1.451	3.458	1.00	1.00	TAG	C
ATOM	80	CG	ARG	6	-8.946	2.781	2.808	1.00	1.00	TAG	C
ATOM	81	CD	ARG	6	-9.965	3.594	3.568	1.00	1.00	TAG	C
ATOM	82	NE	ARG	6	-9.802	5.015	3.277	1.00	1.00	TAG	N
ATOM	83	CZ	ARG	6	-10.795	5.896	3.236	1.00	1.00	TAG	C
ATOM	84	NH1	ARG	6	-12.059	5.500	3.403	1.00	1.00	TAG	N
ATOM	85	NH2	ARG	6	-10.526	7.171	2.963	1.00	1.00	TAG	N1+
ATOM	86	H	ARG	6	-6.268	2.055	3.855	1.00	1.00	TAG	H
ATOM	87	HA	ARG	6	-8.609	2.252	5.441	1.00	1.00	TAG	H
ATOM	88	1HB	ARG	6	-8.057	0.848	2.795	1.00	1.00	TAG	H
ATOM	89	2HB	ARG	6	-9.652	0.918	3.556	1.00	1.00	TAG	H
ATOM	90	1HG	ARG	6	-8.002	3.342	2.744	1.00	1.00	TAG	H
ATOM	91	2HG	ARG	6	-9.298	2.625	1.776	1.00	1.00	TAG	H
ATOM	92	1HD	ARG	6	-10.980	3.272	3.295	1.00	1.00	TAG	H
ATOM	93	2HD	ARG	6	-9.851	3.420	4.649	1.00	1.00	TAG	H
ATOM	94	HE	ARG	6	-8.877	5.349	3.094	1.00	1.00	TAG	H
ATOM	95	1HH1	ARG	6	-12.263	4.533	3.559	1.00	1.00	TAG	H
ATOM	96	2HH1	ARG	6	-12.801	6.169	3.372	1.00	1.00	TAG	H
ATOM	97	H01	ARG	6	-10.510	7.703	3.821	1.00	1.00	TAG	H

ATOM	98	H02	ARG	6	-11.237	7.542	2.350	1.00	1.00	TAG	H
ATOM	99	H03	ARG	6	-9.625	7.235	2.511	1.00	1.00	TAG	H
ATOM	100	N	HIS	7	-7.185	-0.745	5.103	1.00	1.00	TAG	N
ATOM	101	CA	HIS	7	-7.144	-2.101	5.631	1.00	1.00	TAG	C
ATOM	102	C	HIS	7	-6.490	-2.238	7.007	1.00	1.00	TAG	C
ATOM	103	O	HIS	7	-6.984	-2.949	7.894	1.00	1.00	TAG	O
ATOM	104	CB	HIS	7	-6.522	-3.057	4.621	1.00	1.00	TAG	C
ATOM	105	CG	HIS	7	-7.474	-3.485	3.551	1.00	1.00	TAG	C
ATOM	106	CD2	HIS	7	-7.563	-2.847	2.332	1.00	1.00	TAG	C
ATOM	107	ND1	HIS	7	-8.407	-4.472	3.524	1.00	1.00	TAG	N
ATOM	108	CE1	HIS	7	-9.035	-4.409	2.307	1.00	1.00	TAG	C
ATOM	109	NE2	HIS	7	-8.510	-3.420	1.601	1.00	1.00	TAG	N
ATOM	110	H	HIS	7	-6.489	-0.565	4.408	1.00	1.00	TAG	H
ATOM	111	HA	HIS	7	-8.195	-2.380	5.796	1.00	1.00	TAG	H
ATOM	112	1HB	HIS	7	-5.652	-2.572	4.155	1.00	1.00	TAG	H
ATOM	113	2HB	HIS	7	-6.150	-3.948	5.149	1.00	1.00	TAG	H
ATOM	114	HD1	HIS	7	-8.599	-5.124	4.257	1.00	1.00	TAG	H
ATOM	115	HD2	HIS	7	-6.945	-1.994	2.015	1.00	1.00	TAG	H
ATOM	116	HE1	HIS	7	-9.845	-5.073	1.972	1.00	1.00	TAG	H
ATOM	117	N	HIS	8	-5.313	-1.535	7.217	1.00	0.00	TAG	N
ATOM	118	CA	HIS	8	-4.595	-1.726	8.474	1.00	0.00	TAG	C
ATOM	119	C	HIS	8	-4.178	-0.402	9.067	1.00	0.00	TAG	C
ATOM	120	O	HIS	8	-3.204	-0.361	9.879	1.00	0.00	TAG	O
ATOM	121	CB	HIS	8	-3.359	-2.578	8.140	1.00	0.00	TAG	C
ATOM	122	CG	HIS	8	-3.727	-3.930	7.602	1.00	0.00	TAG	C
ATOM	123	CD2	HIS	8	-3.556	-4.278	6.269	1.00	0.00	TAG	C
ATOM	124	ND1	HIS	8	-4.269	-4.981	8.337	1.00	0.00	TAG	N
ATOM	125	CE1	HIS	8	-4.391	-5.904	7.365	1.00	0.00	TAG	C
ATOM	126	NE2	HIS	8	-3.989	-5.569	6.109	1.00	0.00	TAG	N
ATOM	127	H	HIS	8	-4.969	-0.919	6.534	1.00	0.00	TAG	H
ATOM	128	HA	HIS	8	-5.295	-2.187	9.192	1.00	0.00	TAG	H
ATOM	129	2HB	HIS	8	-2.723	-2.730	9.035	1.00	0.00	TAG	H
ATOM	130	3HB	HIS	8	-2.702	-2.086	7.393	1.00	0.00	TAG	H
ATOM	131	2HD	HIS	8	-3.148	-3.618	5.508	1.00	0.00	TAG	H
ATOM	132	1HE	HIS	8	-4.801	-6.867	7.637	1.00	0.00	TAG	H
ATOM	133	2HE	HIS	8	-4.004	-6.136	5.249	1.00	0.00	TAG	H
ATOM	134	N	GLY	9	-5.081	0.623	8.884	1.00	1.00	TAG	N
ATOM	135	CA	GLY	9	-5.005	1.924	9.573	1.00	1.00	TAG	C
ATOM	136	C	GLY	9	-3.638	2.615	9.473	1.00	1.00	TAG	C
ATOM	137	O01	GLY	9	-3.828	3.956	9.933	1.00	1.00	TAG	O
ATOM	138	H	GLY	9	-5.848	0.547	8.246	1.00	1.00	TAG	H
ATOM	139	1HA	GLY	9	-5.771	2.592	9.153	1.00	1.00	TAG	H
ATOM	140	2HA	GLY	9	-5.251	1.778	10.635	1.00	1.00	TAG	H
ATOM	141	N	TYR	10	-3.150	2.707	8.232	1.00	0.00	TAG	N
ATOM	142	CA	TYR	10	-1.760	3.116	8.046	1.00	0.00	TAG	C
ATOM	143	C	TYR	10	-0.961	2.903	9.309	1.00	0.00	TAG	C
ATOM	144	O	TYR	10	0.161	3.347	9.417	1.00	0.00	TAG	O
ATOM	145	CB	TYR	10	-1.671	4.624	7.670	1.00	0.00	TAG	C
ATOM	146	CG	TYR	10	-2.177	5.625	8.715	1.00	0.00	TAG	C
ATOM	147	CD1	TYR	10	-1.311	6.144	9.683	1.00	0.00	TAG	C
ATOM	148	CD2	TYR	10	-3.514	6.033	8.697	1.00	0.00	TAG	C

ATOM	149	CE1	TYR	10	-1.779	7.064	10.617	1.00	0.00	TAG	C
ATOM	150	CE2	TYR	10	-3.980	6.952	9.632	1.00	0.00	TAG	C
ATOM	151	CZ	TYR	10	-3.111	7.467	10.592	1.00	0.00	TAG	C
ATOM	152	OH	TYR	10	-3.565	8.372	11.509	1.00	0.00	TAG	O
ATOM	153	H	TYR	10	-3.709	2.504	7.467	1.00	0.00	TAG	H
ATOM	154	HA	TYR	10	-1.308	2.497	7.249	1.00	0.00	TAG	H
ATOM	155	2HB	TYR	10	-2.234	4.808	6.733	1.00	0.00	TAG	H
ATOM	156	3HB	TYR	10	-0.625	4.872	7.395	1.00	0.00	TAG	H
ATOM	157	1HD	TYR	10	-0.273	5.841	9.707	1.00	0.00	TAG	H
ATOM	158	2HD	TYR	10	-4.191	5.646	7.947	1.00	0.00	TAG	H
ATOM	159	1HE	TYR	10	-1.110	7.470	11.362	1.00	0.00	TAG	H
ATOM	160	2HE	TYR	10	-5.013	7.264	9.603	1.00	0.00	TAG	H
ATOM	161	HH	TYR	10	-4.496	8.533	11.341	1.00	0.00	TAG	H
ATOM	162	N	LYS	11	-1.401	2.249	10.256	1.00	1.00	TAG	N
ATOM	163	CA	LYS	11	-0.665	1.953	11.480	1.00	1.00	TAG	C
ATOM	164	C	LYS	11	0.295	0.806	11.231	1.00	1.00	TAG	C
ATOM	165	O	LYS	11	1.415	0.834	11.763	1.00	1.00	TAG	O
ATOM	166	CB	LYS	11	-1.640	1.597	12.603	1.00	1.00	TAG	C
ATOM	167	CG	LYS	11	-0.995	1.325	13.947	1.00	1.00	TAG	C
ATOM	168	CD	LYS	11	-2.008	1.568	15.051	1.00	1.00	TAG	C
ATOM	169	CE	LYS	11	-1.443	1.284	16.429	1.00	1.00	TAG	C
ATOM	170	NZ	LYS	11	-1.417	-0.171	16.683	1.00	1.00	TAG	N
ATOM	171	HA	LYS	11	-0.090	2.840	11.783	1.00	1.00	TAG	H
ATOM	172	1HB	LYS	11	-2.360	2.421	12.719	1.00	1.00	TAG	H
ATOM	173	2HB	LYS	11	-2.213	0.707	12.303	1.00	1.00	TAG	H
ATOM	174	1HG	LYS	11	-0.630	0.289	13.989	1.00	1.00	TAG	H
ATOM	175	2HG	LYS	11	-0.121	1.979	14.086	1.00	1.00	TAG	H
ATOM	176	1HD	LYS	11	-2.351	2.612	15.007	1.00	1.00	TAG	H
ATOM	177	2HD	LYS	11	-2.890	0.932	14.881	1.00	1.00	TAG	H
ATOM	178	1HE	LYS	11	-0.427	1.696	16.507	1.00	1.00	TAG	H
ATOM	179	2HE	LYS	11	-2.053	1.787	17.193	1.00	1.00	TAG	H
ATOM	180	H01	LYS	11	-2.342	1.891	10.179	1.00	1.00	TAG	H
ATOM	181	H02	LYS	11	-1.009	-0.645	15.890	1.00	1.00	TAG	H
ATOM	182	H03	LYS	11	-2.359	-0.505	16.827	1.00	1.00	TAG	H
ATOM	183	N	ARG	12	-0.065	-0.171	10.549	1.00	0.00	TAG	N
ATOM	184	CA	ARG	12	0.890	-1.180	10.097	1.00	0.00	TAG	C
ATOM	185	C	ARG	12	2.144	-0.534	9.558	1.00	0.00	TAG	C
ATOM	186	O	ARG	12	2.997	-1.319	8.993	1.00	0.00	TAG	O
ATOM	187	CB	ARG	12	0.205	-2.073	9.024	1.00	0.00	TAG	C
ATOM	188	CG	ARG	12	-1.007	-2.909	9.523	1.00	0.00	TAG	C
ATOM	189	CD	ARG	12	-0.569	-4.232	10.171	1.00	0.00	TAG	C
ATOM	190	NE	ARG	12	-0.123	-3.980	11.573	1.00	0.00	TAG	N
ATOM	191	CZ	ARG	12	0.618	-4.808	12.305	1.00	0.00	TAG	C
ATOM	192	NH1	ARG	12	1.056	-5.957	11.873	1.00	0.00	TAG	N
ATOM	193	NH2	ARG	12	0.922	-4.455	13.514	1.00	0.00	TAG	N1+
ATOM	194	H	ARG	12	-0.989	-0.264	10.315	1.00	0.00	TAG	H
ATOM	195	HA	ARG	12	1.179	-1.793	10.972	1.00	0.00	TAG	H
ATOM	196	2HB	ARG	12	0.969	-2.741	8.576	1.00	0.00	TAG	H
ATOM	197	3HB	ARG	12	-0.129	-1.435	8.180	1.00	0.00	TAG	H
ATOM	198	2HG	ARG	12	-1.692	-3.101	8.671	1.00	0.00	TAG	H
ATOM	199	3HG	ARG	12	-1.599	-2.321	10.254	1.00	0.00	TAG	H

ATOM	200	2HD	ARG	12	0.250	-4.683	9.569	1.00	0.00	TAG H
ATOM	201	3HD	ARG	12	-1.412	-4.955	10.146	1.00	0.00	TAG H
ATOM	202	HE	ARG	12	-0.381	-3.117	12.062	1.00	0.00	TAG H
ATOM	203	1HH1	ARG	12	0.781	-6.174	10.912	1.00	0.00	TAG H
ATOM	204	2HH1	ARG	12	1.619	-6.537	12.497	1.00	0.00	TAG H
ATOM	205	H01	ARG	12	1.195	-5.271	14.044	1.00	0.00	TAG H
ATOM	206	H02	ARG	12	0.122	-4.021	13.950	1.00	0.00	TAG H
ATOM	207	H03	ARG	12	1.689	-3.799	13.489	1.00	0.00	TAG H
ATOM	208	N	LYS	13	2.255	0.671	9.441	1.00	0.00	TAG N
ATOM	209	CA	LYS	13	3.363	1.322	8.748	1.00	0.00	TAG C
ATOM	210	C	LYS	13	4.692	0.811	9.252	1.00	0.00	TAG C
ATOM	211	O	LYS	13	5.717	0.999	8.582	1.00	0.00	TAG O
ATOM	212	CB	LYS	13	3.254	2.860	8.931	1.00	0.00	TAG C
ATOM	213	CG	LYS	13	4.326	3.652	8.140	1.00	0.00	TAG C
ATOM	214	CD	LYS	13	4.173	5.175	8.196	1.00	0.00	TAG C
ATOM	215	CE	LYS	13	5.306	5.826	7.392	1.00	0.00	TAG C
ATOM	216	NZ	LYS	13	5.158	7.292	7.435	1.00	0.00	TAG N
ATOM	217	H	LYS	13	1.561	1.266	9.839	1.00	0.00	TAG H
ATOM	218	HA	LYS	13	3.297	1.072	7.672	1.00	0.00	TAG H
ATOM	219	2HB	LYS	13	3.318	3.113	10.009	1.00	0.00	TAG H
ATOM	220	3HB	LYS	13	2.248	3.203	8.618	1.00	0.00	TAG H
ATOM	221	2HG	LYS	13	4.336	3.312	7.086	1.00	0.00	TAG H
ATOM	222	3HG	LYS	13	5.335	3.426	8.533	1.00	0.00	TAG H
ATOM	223	2HD	LYS	13	4.207	5.517	9.251	1.00	0.00	TAG H
ATOM	224	3HD	LYS	13	3.180	5.467	7.805	1.00	0.00	TAG H
ATOM	225	2HE	LYS	13	5.297	5.483	6.336	1.00	0.00	TAG H
ATOM	226	3HE	LYS	13	6.294	5.525	7.799	1.00	0.00	TAG H
ATOM	227	H01	LYS	13	5.138	7.656	6.494	1.00	0.00	TAG H
ATOM	228	H02	LYS	13	5.936	7.695	7.937	1.00	0.00	TAG H
ATOM	229	N	PHE	14	4.769	0.196	10.377	1.00	1.00	TAG N
ATOM	230	CA	PHE	14	5.987	-0.446	10.867	1.00	1.00	TAG C
ATOM	231	C	PHE	14	6.509	-1.531	9.932	1.00	1.00	TAG C
ATOM	232	O	PHE	14	7.694	-1.873	9.976	1.00	1.00	TAG O
ATOM	233	CB	PHE	14	5.796	-0.980	12.287	1.00	1.00	TAG C
ATOM	234	CG	PHE	14	5.481	0.093	13.294	1.00	1.00	TAG C
ATOM	235	CD1	PHE	14	4.236	0.137	13.916	1.00	1.00	TAG C
ATOM	236	CD2	PHE	14	6.425	1.079	13.603	1.00	1.00	TAG C
ATOM	237	CE1	PHE	14	3.935	1.138	14.843	1.00	1.00	TAG C
ATOM	238	CE2	PHE	14	6.138	2.085	14.531	1.00	1.00	TAG C
ATOM	239	CZ	PHE	14	4.890	2.115	15.153	1.00	1.00	TAG C
ATOM	240	H	PHE	14	3.993	0.107	11.002	1.00	1.00	TAG H
ATOM	241	HA	PHE	14	6.762	0.335	10.892	1.00	1.00	TAG H
ATOM	242	1HB	PHE	14	4.983	-1.721	12.286	1.00	1.00	TAG H
ATOM	243	2HB	PHE	14	6.711	-1.507	12.599	1.00	1.00	TAG H
ATOM	244	HD1	PHE	14	3.481	-0.627	13.675	1.00	1.00	TAG H
ATOM	245	HD2	PHE	14	7.407	1.063	13.108	1.00	1.00	TAG H
ATOM	246	HE1	PHE	14	2.948	1.160	15.329	1.00	1.00	TAG H
ATOM	247	HE2	PHE	14	6.893	2.848	14.769	1.00	1.00	TAG H
ATOM	248	HZ	PHE	14	4.658	2.903	15.884	1.00	1.00	TAG H
ATOM	249	N	HIS	15	5.614	-2.075	9.077	1.00	0.00	TAG N
ATOM	250	CA	HIS	15	5.982	-3.068	8.071	1.00	0.00	TAG C

ATOM	251	C	HIS	15	7.011	-2.515	7.115	1.00	0.00	TAG C
ATOM	252	O	HIS	15	7.314	-3.107	6.063	1.00	0.00	TAG O
ATOM	253	CB	HIS	15	4.688	-3.422	7.320	1.00	0.00	TAG C
ATOM	254	CG	HIS	15	4.205	-2.296	6.454	1.00	0.00	TAG C
ATOM	255	CD2	HIS	15	4.487	-2.219	5.096	1.00	0.00	TAG C
ATOM	256	ND1	HIS	15	3.436	-1.213	6.876	1.00	0.00	TAG N
ATOM	257	CE1	HIS	15	3.315	-0.548	5.712	1.00	0.00	TAG C
ATOM	258	NE2	HIS	15	3.906	-1.078	4.607	1.00	0.00	TAG N
ATOM	259	H	HIS	15	4.652	-1.856	8.989	1.00	0.00	TAG H
ATOM	260	HA	HIS	15	6.460	-3.913	8.595	1.00	0.00	TAG H
ATOM	261	2HB	HIS	15	3.874	-3.682	8.026	1.00	0.00	TAG H
ATOM	262	3HB	HIS	15	4.812	-4.315	6.672	1.00	0.00	TAG H
ATOM	263	2HD	HIS	15	5.070	-2.953	4.547	1.00	0.00	TAG H
ATOM	264	1HE	HIS	15	2.749	0.374	5.718	1.00	0.00	TAG H
ATOM	265	2HE	HIS	15	3.921	-0.718	3.642	1.00	0.00	TAG H
ATOM	266	N	GLU	16	7.606	-1.350	7.408	1.00	1.00	TAG N
ATOM	267	CA	GLU	16	8.530	-0.659	6.513	1.00	1.00	TAG C
ATOM	268	C	GLU	16	9.885	-1.352	6.570	1.00	1.00	TAG C
ATOM	269	O	GLU	16	10.654	-1.271	5.598	1.00	1.00	TAG O
ATOM	270	CB	GLU	16	8.690	0.797	6.935	1.00	1.00	TAG C
ATOM	271	CG	GLU	16	9.566	1.617	6.003	1.00	1.00	TAG C
ATOM	272	CD	GLU	16	9.902	2.987	6.562	1.00	1.00	TAG C
ATOM	273	OE1	GLU	16	9.762	3.187	7.787	1.00	1.00	TAG O
ATOM	274	OE2	GLU	16	10.343	3.866	5.786	1.00	1.00	TAG O
ATOM	275	H	GLU	16	7.452	-0.865	8.268	1.00	1.00	TAG H
ATOM	276	HA	GLU	16	8.130	-0.688	5.489	1.00	1.00	TAG H
ATOM	277	1HB	GLU	16	7.695	1.263	6.991	1.00	1.00	TAG H
ATOM	278	2HB	GLU	16	9.118	0.830	7.948	1.00	1.00	TAG H
ATOM	279	1HG	GLU	16	10.499	1.068	5.807	1.00	1.00	TAG H
ATOM	280	2HG	GLU	16	9.055	1.737	5.037	1.00	1.00	TAG H
ATOM	281	H01	GLU	16	10.368	4.711	6.240	1.00	1.00	TAG H
ATOM	282	N	LYS	17	10.208	-2.029	7.651	1.00	1.00	TAG N
ATOM	283	CA	LYS	17	11.520	-2.627	7.874	1.00	1.00	TAG C
ATOM	284	C	LYS	17	11.584	-3.982	7.200	1.00	1.00	TAG C
ATOM	285	O	LYS	17	12.519	-4.263	6.442	1.00	1.00	TAG O
ATOM	286	CB	LYS	17	11.785	-2.766	9.374	1.00	1.00	TAG C
ATOM	287	CG	LYS	17	13.146	-3.321	9.734	1.00	1.00	TAG C
ATOM	288	CD	LYS	17	13.515	-2.877	11.138	1.00	1.00	TAG C
ATOM	289	CE	LYS	17	14.857	-3.424	11.584	1.00	1.00	TAG C
ATOM	290	NZ	LYS	17	14.728	-4.837	11.995	1.00	1.00	TAG N1+
ATOM	291	H	LYS	17	9.569	-2.183	8.405	1.00	1.00	TAG H
ATOM	292	HA	LYS	17	12.294	-1.976	7.440	1.00	1.00	TAG H
ATOM	293	1HB	LYS	17	11.672	-1.777	9.845	1.00	1.00	TAG H
ATOM	294	2HB	LYS	17	11.012	-3.418	9.808	1.00	1.00	TAG H
ATOM	295	1HG	LYS	17	13.134	-4.420	9.675	1.00	1.00	TAG H
ATOM	296	2HG	LYS	17	13.900	-2.969	9.015	1.00	1.00	TAG H
ATOM	297	1HD	LYS	17	13.538	-1.779	11.178	1.00	1.00	TAG H
ATOM	298	2HD	LYS	17	12.735	-3.208	11.841	1.00	1.00	TAG H
ATOM	299	1HE	LYS	17	15.586	-3.338	10.765	1.00	1.00	TAG H
ATOM	300	2HE	LYS	17	15.244	-2.825	12.423	1.00	1.00	TAG H
ATOM	301	1HZ	LYS	17	15.372	-5.030	12.736	1.00	1.00	TAG H

ATOM	302	2HZ	LYS	17	13.795	-5.008	12.312	1.00	1.00	TAG	H
ATOM	303	3HZ	LYS	17	14.929	-5.431	11.216	1.00	1.00	TAG	H
ATOM	304	N	HIS	18	10.541	-4.761	7.293	1.00	1.00	TAG	N
ATOM	305	CA	HIS	18	10.519	-6.183	6.878	1.00	1.00	TAG	C
ATOM	306	C	HIS	18	9.336	-6.425	5.968	1.00	1.00	TAG	C
ATOM	307	O	HIS	18	9.264	-7.482	5.292	1.00	1.00	TAG	O
ATOM	308	CB	HIS	18	10.354	-7.033	8.261	1.00	1.00	TAG	C
ATOM	309	CG	HIS	18	10.208	-8.473	7.822	1.00	1.00	TAG	C
ATOM	310	CD2	HIS	18	9.069	-9.248	7.989	1.00	1.00	TAG	C
ATOM	311	ND1	HIS	18	11.114	-9.316	7.298	1.00	1.00	TAG	N
ATOM	312	CE1	HIS	18	10.645	-10.518	7.087	1.00	1.00	TAG	C
ATOM	313	NE2	HIS	18	9.362	-10.463	7.447	1.00	1.00	TAG	N
ATOM	314	H	HIS	18	9.666	-4.445	7.659	1.00	1.00	TAG	H
ATOM	315	HA	HIS	18	11.426	-6.474	6.328	1.00	1.00	TAG	H
ATOM	316	1HB	HIS	18	11.228	-6.903	8.916	1.00	1.00	TAG	H
ATOM	317	2HB	HIS	18	9.473	-6.699	8.831	1.00	1.00	TAG	H
ATOM	318	HD1	HIS	18	12.055	-9.050	7.089	1.00	1.00	TAG	H
ATOM	319	HD2	HIS	18	8.123	-8.944	8.461	1.00	1.00	TAG	H
ATOM	320	HE1	HIS	18	11.192	-11.390	6.698	1.00	1.00	TAG	H
ATOM	321	N	HIS	19	8.278	-5.653	6.072	1.00	1.00	TAG	N
ATOM	322	CA	HIS	19	7.056	-5.872	5.313	1.00	1.00	TAG	C
ATOM	323	C	HIS	19	7.183	-5.651	3.805	1.00	1.00	TAG	C
ATOM	324	O	HIS	19	7.091	-6.499	2.908	1.00	1.00	TAG	O
ATOM	325	CB	HIS	19	5.903	-5.068	5.900	1.00	1.00	TAG	C
ATOM	326	CG	HIS	19	5.289	-5.705	7.104	1.00	1.00	TAG	C
ATOM	327	CD2	HIS	19	5.674	-5.392	8.390	1.00	1.00	TAG	C
ATOM	328	ND1	HIS	19	4.340	-6.668	7.223	1.00	1.00	TAG	N
ATOM	329	CE1	HIS	19	4.170	-6.915	8.560	1.00	1.00	TAG	C
ATOM	330	NE2	HIS	19	4.987	-6.134	9.250	1.00	1.00	TAG	N
ATOM	331	H	HIS	19	8.238	-4.859	6.679	1.00	1.00	TAG	H
ATOM	332	HA	HIS	19	6.838	-6.945	5.416	1.00	1.00	TAG	H
ATOM	333	1HB	HIS	19	6.265	-4.064	6.169	1.00	1.00	TAG	H
ATOM	334	2HB	HIS	19	5.129	-4.934	5.130	1.00	1.00	TAG	H
ATOM	335	HD2	HIS	19	6.432	-4.643	8.662	1.00	1.00	TAG	H
ATOM	336	HE1	HIS	19	3.469	-7.645	8.991	1.00	1.00	TAG	H
ATOM	337	HE2	HIS	19	5.072	-6.107	10.246	1.00	1.00	TAG	H
ATOM	338	N	SER	20	7.433	-4.306	3.487	1.00	1.00	TAG	N
ATOM	339	CA	SER	20	7.375	-3.833	2.103	1.00	1.00	TAG	C
ATOM	340	C	SER	20	7.152	-4.934	1.076	1.00	1.00	TAG	C
ATOM	341	O	SER	20	6.363	-4.912	0.145	1.00	1.00	TAG	O
ATOM	342	CB	SER	20	8.676	-3.102	1.759	1.00	1.00	TAG	C
ATOM	343	OG	SER	20	8.707	-2.765	0.384	1.00	1.00	TAG	O
ATOM	344	H	SER	20	7.659	-3.601	4.160	1.00	1.00	TAG	H
ATOM	345	HA	SER	20	6.503	-3.165	2.049	1.00	1.00	TAG	H
ATOM	346	1HB	SER	20	8.763	-2.191	2.369	1.00	1.00	TAG	H
ATOM	347	2HB	SER	20	9.538	-3.739	2.007	1.00	1.00	TAG	H
ATOM	348	HG	SER	20	7.782	-2.548	0.073	1.00	1.00	TAG	H
ATOM	349	N	HIS	21	7.931	-6.061	1.234	1.00	1.00	TAG	N
ATOM	350	CA	HIS	21	7.945	-7.144	0.262	1.00	1.00	TAG	C
ATOM	351	C	HIS	21	6.658	-7.970	0.198	1.00	1.00	TAG	C
ATOM	352	O	HIS	21	6.001	-8.269	-0.805	1.00	1.00	TAG	O

ATOM	353	CB	HIS	21	9.169	-8.030	0.457	1.00	1.00	TAG	C
ATOM	354	CG	HIS	21	10.413	-7.459	-0.140	1.00	1.00	TAG	C
ATOM	355	CD2	HIS	21	11.308	-6.701	0.585	1.00	1.00	TAG	C
ATOM	356	ND1	HIS	21	10.902	-7.501	-1.406	1.00	1.00	TAG	N
ATOM	357	CE1	HIS	21	12.066	-6.778	-1.421	1.00	1.00	TAG	C
ATOM	358	NE2	HIS	21	12.295	-6.301	-0.206	1.00	1.00	TAG	N
ATOM	359	H	HIS	21	8.534	-6.210	2.018	1.00	1.00	TAG	H
ATOM	360	HA	HIS	21	8.005	-6.654	-0.721	1.00	1.00	TAG	H
ATOM	361	1HB	HIS	21	9.328	-8.192	1.534	1.00	1.00	TAG	H
ATOM	362	2HB	HIS	21	8.974	-9.016	0.008	1.00	1.00	TAG	H
ATOM	363	HD1	HIS	21	10.488	-7.973	-2.185	1.00	1.00	TAG	H
ATOM	364	HD2	HIS	21	11.216	-6.464	1.656	1.00	1.00	TAG	H
ATOM	365	HE1	HIS	21	12.708	-6.619	-2.301	1.00	1.00	TAG	H
ATOM	366	N	ARG	22	6.222	-8.409	1.427	1.00	1.00	TAG	N
ATOM	367	CA	ARG	22	5.080	-9.296	1.579	1.00	1.00	TAG	C
ATOM	368	C	ARG	22	3.914	-8.424	1.118	1.00	1.00	TAG	C
ATOM	369	O	ARG	22	2.933	-9.000	0.625	1.00	1.00	TAG	O
ATOM	370	CB	ARG	22	4.946	-9.691	3.053	1.00	1.00	TAG	C
ATOM	371	CG	ARG	22	3.809	-10.664	3.353	1.00	1.00	TAG	C
ATOM	372	CD	ARG	22	3.954	-11.280	4.740	1.00	1.00	TAG	C
ATOM	373	NE	ARG	22	4.371	-10.292	5.733	1.00	1.00	TAG	N
ATOM	374	CZ	ARG	22	5.366	-10.474	6.601	1.00	1.00	TAG	C
ATOM	375	NH1	ARG	22	6.052	-11.615	6.609	1.00	1.00	TAG	N
ATOM	376	NH2	ARG	22	5.689	-9.502	7.451	1.00	1.00	TAG	N1+
ATOM	377	H	ARG	22	6.655	-8.152	2.290	1.00	1.00	TAG	H
ATOM	378	HA	ARG	22	5.146	-10.237	1.013	1.00	1.00	TAG	H
ATOM	379	1HB	ARG	22	5.893	-10.143	3.384	1.00	1.00	TAG	H
ATOM	380	2HB	ARG	22	4.797	-8.780	3.651	1.00	1.00	TAG	H
ATOM	381	1HG	ARG	22	2.845	-10.137	3.283	1.00	1.00	TAG	H
ATOM	382	2HG	ARG	22	3.796	-11.461	2.596	1.00	1.00	TAG	H
ATOM	383	1HD	ARG	22	2.995	-11.725	5.045	1.00	1.00	TAG	H
ATOM	384	2HD	ARG	22	4.690	-12.096	4.702	1.00	1.00	TAG	H
ATOM	385	HE	ARG	22	3.878	-9.423	5.764	1.00	1.00	TAG	H
ATOM	386	1HH1	ARG	22	5.823	-12.341	5.962	1.00	1.00	TAG	H
ATOM	387	2HH1	ARG	22	6.798	-11.745	7.263	1.00	1.00	TAG	H
ATOM	388	H01	ARG	22	5.904	-9.901	8.354	1.00	1.00	TAG	H
ATOM	389	H02	ARG	22	4.913	-8.862	7.541	1.00	1.00	TAG	H
ATOM	390	H03	ARG	22	6.496	-9.005	7.102	1.00	1.00	TAG	H
ATOM	391	N	GLY	23	3.870	-7.222	1.192	1.00	1.00	TAG	N
ATOM	392	CA	GLY	23	2.829	-6.326	0.699	1.00	1.00	TAG	C
ATOM	393	C	GLY	23	1.436	-6.828	1.078	1.00	1.00	TAG	C
ATOM	394	O	GLY	23	0.612	-7.105	0.204	1.00	1.00	TAG	O
ATOM	395	H	GLY	23	4.607	-6.713	1.635	1.00	1.00	TAG	H
ATOM	396	1HA	GLY	23	2.983	-5.319	1.113	1.00	1.00	TAG	H
ATOM	397	2HA	GLY	23	2.905	-6.239	-0.394	1.00	1.00	TAG	H
ATOM	398	N	TYR	24	1.157	-6.942	2.344	1.00	0.00	TAG	N
ATOM	399	CA	TYR	24	-0.141	-7.293	2.913	1.00	0.00	TAG	C
ATOM	400	C	TYR	24	-1.221	-7.255	1.859	1.00	0.00	TAG	C
ATOM	401	O	TYR	24	-1.407	-6.296	1.117	1.00	0.00	TAG	O
ATOM	402	CB	TYR	24	-0.538	-6.299	4.044	1.00	0.00	TAG	C
ATOM	403	CG	TYR	24	0.312	-6.333	5.319	1.00	0.00	TAG	C

ATOM	404	CD1	TYR	24	1.146	-7.423	5.592	1.00	0.00	TAG	C
ATOM	405	CD2	TYR	24	0.263	-5.262	6.216	1.00	0.00	TAG	C
ATOM	406	CE1	TYR	24	1.924	-7.435	6.746	1.00	0.00	TAG	C
ATOM	407	CE2	TYR	24	1.042	-5.276	7.369	1.00	0.00	TAG	C
ATOM	408	CZ	TYR	24	1.872	-6.363	7.633	1.00	0.00	TAG	C
ATOM	409	OH	TYR	24	2.639	-6.379	8.763	1.00	0.00	TAG	O
ATOM	410	OXT	TYR	24	-2.087	-8.395	1.705	0.00	0.00	TAG	O
ATOM	411	H	TYR	24	1.937	-6.766	3.017	1.00	0.00	TAG	H
ATOM	412	HA	TYR	24	-0.091	-8.323	3.312	1.00	0.00	TAG	H
ATOM	413	2HB	TYR	24	-1.591	-6.475	4.341	1.00	0.00	TAG	H
ATOM	414	3HB	TYR	24	-0.554	-5.267	3.637	1.00	0.00	TAG	H
ATOM	415	1HD	TYR	24	1.197	-8.257	4.905	1.00	0.00	TAG	H
ATOM	416	2HD	TYR	24	-0.371	-4.410	6.011	1.00	0.00	TAG	H
ATOM	417	1HE	TYR	24	2.573	-8.273	6.955	1.00	0.00	TAG	H
ATOM	418	2HE	TYR	24	0.999	-4.440	8.050	1.00	0.00	TAG	H
ATOM	419	HH	TYR	24	2.479	-5.567	9.250	1.00	0.00	TAG	H
ATOM	420	H01	TYR	24	-2.289	-8.763	2.569	0.00	0.00	TAG	H
END											

Histatin conformer 5:

ATOM	1	N	ASP	1	-0.753	-1.254	-0.000	1.00	1.00	TAG	N1+
ATOM	2	CA	ASP	1	0.000	0.000	0.000	1.00	1.00	TAG	C
ATOM	3	C	ASP	1	-0.977	1.169	-0.000	1.00	1.00	TAG	C
ATOM	4	O	ASP	1	-1.016	1.960	0.954	1.00	1.00	TAG	O
ATOM	5	CB	ASP	1	0.960	0.096	-1.192	1.00	1.00	TAG	C
ATOM	6	CG	ASP	1	1.888	1.333	-1.129	1.00	1.00	TAG	C
ATOM	7	OD1	ASP	1	2.076	1.945	-0.042	1.00	1.00	TAG	O
ATOM	8	OD2	ASP	1	2.445	1.694	-2.194	1.00	1.00	TAG	O
ATOM	9	1H	ASP	1	-0.117	-2.025	-0.000	1.00	1.00	TAG	H
ATOM	10	2H	ASP	1	-1.329	-1.298	0.816	1.00	1.00	TAG	H
ATOM	11	3H	ASP	1	-1.329	-1.298	-0.816	1.00	1.00	TAG	H
ATOM	12	HA	ASP	1	0.619	0.032	0.908	1.00	1.00	TAG	H
ATOM	13	1HB	ASP	1	1.576	-0.815	-1.233	1.00	1.00	TAG	H
ATOM	14	2HB	ASP	1	0.376	0.131	-2.123	1.00	1.00	TAG	H
ATOM	15	H01	ASP	1	2.490	2.653	-2.223	1.00	1.00	TAG	H
ATOM	16	N	SER	2	-1.762	1.319	-1.010	1.00	1.00	TAG	N
ATOM	17	CA	SER	2	-2.774	2.372	-1.101	1.00	1.00	TAG	C
ATOM	18	C	SER	2	-4.177	1.865	-1.398	1.00	1.00	TAG	C
ATOM	19	O	SER	2	-5.207	2.155	-0.808	1.00	1.00	TAG	O
ATOM	20	CB	SER	2	-2.375	3.371	-2.190	1.00	1.00	TAG	C
ATOM	21	OG	SER	2	-3.408	4.315	-2.400	1.00	1.00	TAG	O
ATOM	22	H	SER	2	-1.736	0.721	-1.812	1.00	1.00	TAG	H
ATOM	23	HA	SER	2	-2.809	2.842	-0.108	1.00	1.00	TAG	H
ATOM	24	1HB	SER	2	-1.450	3.890	-1.900	1.00	1.00	TAG	H
ATOM	25	2HB	SER	2	-2.163	2.836	-3.127	1.00	1.00	TAG	H
ATOM	26	HG	SER	2	-3.131	4.961	-3.113	1.00	1.00	TAG	H
ATOM	27	N	HIS	3	-4.246	0.984	-2.485	1.00	0.00	TAG	N
ATOM	28	CA	HIS	3	-5.465	0.260	-2.834	1.00	0.00	TAG	C

ATOM	29	C	HIS	3	-5.501	-1.094	-2.167	1.00	0.00	TAG	C
ATOM	30	O	HIS	3	-6.551	-1.559	-1.660	1.00	0.00	TAG	O
ATOM	31	CB	HIS	3	-5.452	0.104	-4.364	1.00	0.00	TAG	C
ATOM	32	CG	HIS	3	-5.491	1.427	-5.072	1.00	0.00	TAG	C
ATOM	33	CD2	HIS	3	-4.386	1.964	-5.718	1.00	0.00	TAG	C
ATOM	34	ND1	HIS	3	-6.598	2.266	-5.174	1.00	0.00	TAG	N
ATOM	35	CE1	HIS	3	-6.060	3.272	-5.889	1.00	0.00	TAG	C
ATOM	36	NE2	HIS	3	-4.754	3.171	-6.255	1.00	0.00	TAG	N
ATOM	37	H	HIS	3	-3.429	0.846	-3.044	1.00	0.00	TAG	H
ATOM	38	HA	HIS	3	-6.319	0.831	-2.434	1.00	0.00	TAG	H
ATOM	39	2HB	HIS	3	-6.318	-0.494	-4.713	1.00	0.00	TAG	H
ATOM	40	3HB	HIS	3	-4.555	-0.442	-4.721	1.00	0.00	TAG	H
ATOM	41	2HD	HIS	3	-3.412	1.486	-5.772	1.00	0.00	TAG	H
ATOM	42	1HE	HIS	3	-6.700	4.108	-6.136	1.00	0.00	TAG	H
ATOM	43	2HE	HIS	3	-4.178	3.831	-6.797	1.00	0.00	TAG	H
ATOM	44	N	ALA	4	-4.356	-1.773	-2.106	1.00	1.00	TAG	N
ATOM	45	CA	ALA	4	-4.234	-3.067	-1.464	1.00	1.00	TAG	C
ATOM	46	C	ALA	4	-5.188	-3.144	-0.259	1.00	1.00	TAG	C
ATOM	47	O	ALA	4	-5.949	-4.101	-0.145	1.00	1.00	TAG	O
ATOM	48	CB	ALA	4	-2.791	-3.274	-1.006	1.00	1.00	TAG	C
ATOM	49	H	ALA	4	-3.505	-1.443	-2.515	1.00	1.00	TAG	H
ATOM	50	HA	ALA	4	-4.501	-3.859	-2.179	1.00	1.00	TAG	H
ATOM	51	1HB	ALA	4	-2.698	-4.256	-0.518	1.00	1.00	TAG	H
ATOM	52	2HB	ALA	4	-2.120	-3.232	-1.876	1.00	1.00	TAG	H
ATOM	53	3HB	ALA	4	-2.515	-2.483	-0.293	1.00	1.00	TAG	H
ATOM	54	N	LYS	5	-5.168	-2.196	0.616	1.00	0.00	TAG	N
ATOM	55	CA	LYS	5	-6.038	-2.204	1.789	1.00	0.00	TAG	C
ATOM	56	C	LYS	5	-7.492	-2.149	1.385	1.00	0.00	TAG	C
ATOM	57	O	LYS	5	-8.318	-2.812	1.979	1.00	0.00	TAG	O
ATOM	58	CB	LYS	5	-5.672	-1.009	2.711	1.00	0.00	TAG	C
ATOM	59	CG	LYS	5	-4.318	-1.186	3.442	1.00	0.00	TAG	C
ATOM	60	CD	LYS	5	-3.987	-0.090	4.460	1.00	0.00	TAG	C
ATOM	61	CE	LYS	5	-3.604	1.194	3.713	1.00	0.00	TAG	C
ATOM	62	NZ	LYS	5	-3.199	2.224	4.686	1.00	0.00	TAG	N
ATOM	63	H	LYS	5	-4.539	-1.434	0.487	1.00	0.00	TAG	H
ATOM	64	HA	LYS	5	-5.880	-3.153	2.335	1.00	0.00	TAG	H
ATOM	65	2HB	LYS	5	-6.483	-0.848	3.452	1.00	0.00	TAG	H
ATOM	66	3HB	LYS	5	-5.643	-0.074	2.116	1.00	0.00	TAG	H
ATOM	67	2HG	LYS	5	-3.502	-1.269	2.698	1.00	0.00	TAG	H
ATOM	68	3HG	LYS	5	-4.307	-2.141	3.999	1.00	0.00	TAG	H
ATOM	69	2HD	LYS	5	-3.149	-0.420	5.108	1.00	0.00	TAG	H
ATOM	70	3HD	LYS	5	-4.853	0.074	5.129	1.00	0.00	TAG	H
ATOM	71	2HE	LYS	5	-4.452	1.572	3.104	1.00	0.00	TAG	H
ATOM	72	3HE	LYS	5	-2.781	0.995	2.994	1.00	0.00	TAG	H
ATOM	73	H01	LYS	5	-2.984	1.786	5.570	1.00	0.00	TAG	H
ATOM	74	H02	LYS	5	-3.953	2.885	4.811	1.00	0.00	TAG	H
ATOM	75	N	ARG	6	-7.809	-1.368	0.375	1.00	1.00	TAG	N
ATOM	76	CA	ARG	6	-9.183	-1.244	-0.148	1.00	1.00	TAG	C
ATOM	77	C	ARG	6	-9.589	-2.514	-0.879	1.00	1.00	TAG	C
ATOM	78	O	ARG	6	-10.676	-3.063	-0.643	1.00	1.00	TAG	O
ATOM	79	CB	ARG	6	-9.354	-0.036	-1.078	1.00	1.00	TAG	C

ATOM	80	CG	ARG	6	-9.218	1.297	-0.399	1.00	1.00	TAG	C
ATOM	81	CD	ARG	6	-10.329	1.537	0.594	1.00	1.00	TAG	C
ATOM	82	NE	ARG	6	-9.913	2.514	1.596	1.00	1.00	TAG	N
ATOM	83	CZ	ARG	6	-10.726	3.383	2.186	1.00	1.00	TAG	C
ATOM	84	NH1	ARG	6	-12.011	3.456	1.831	1.00	1.00	TAG	N
ATOM	85	NH2	ARG	6	-10.234	4.227	3.090	1.00	1.00	TAG	N1+
ATOM	86	H	ARG	6	-7.143	-0.805	-0.114	1.00	1.00	TAG	H
ATOM	87	HA	ARG	6	-9.838	-1.088	0.722	1.00	1.00	TAG	H
ATOM	88	1HB	ARG	6	-8.608	-0.101	-1.884	1.00	1.00	TAG	H
ATOM	89	2HB	ARG	6	-10.346	-0.092	-1.552	1.00	1.00	TAG	H
ATOM	90	1HG	ARG	6	-8.248	1.348	0.116	1.00	1.00	TAG	H
ATOM	91	2HG	ARG	6	-9.224	2.096	-1.156	1.00	1.00	TAG	H
ATOM	92	1HD	ARG	6	-11.227	1.898	0.072	1.00	1.00	TAG	H
ATOM	93	2HD	ARG	6	-10.601	0.591	1.086	1.00	1.00	TAG	H
ATOM	94	HE	ARG	6	-8.948	2.530	1.856	1.00	1.00	TAG	H
ATOM	95	1HH1	ARG	6	-12.367	2.854	1.116	1.00	1.00	TAG	H
ATOM	96	2HH1	ARG	6	-12.616	4.113	2.280	1.00	1.00	TAG	H
ATOM	97	H01	ARG	6	-10.012	3.723	3.937	1.00	1.00	TAG	H
ATOM	98	H02	ARG	6	-10.919	4.941	3.292	1.00	1.00	TAG	H
ATOM	99	H03	ARG	6	-9.396	4.658	2.726	1.00	1.00	TAG	H
ATOM	100	N	HIS	7	-8.752	-3.020	-1.773	1.00	1.00	TAG	N
ATOM	101	CA	HIS	7	-9.107	-4.107	-2.674	1.00	1.00	TAG	C
ATOM	102	C	HIS	7	-8.403	-5.435	-2.390	1.00	1.00	TAG	C
ATOM	103	O	HIS	7	-8.922	-6.522	-2.685	1.00	1.00	TAG	O
ATOM	104	CB	HIS	7	-8.934	-3.684	-4.127	1.00	1.00	TAG	C
ATOM	105	CG	HIS	7	-10.073	-2.864	-4.642	1.00	1.00	TAG	C
ATOM	106	CD2	HIS	7	-10.066	-1.486	-4.629	1.00	1.00	TAG	C
ATOM	107	ND1	HIS	7	-11.275	-3.227	-5.159	1.00	1.00	TAG	N
ATOM	108	CE1	HIS	7	-11.963	-2.075	-5.442	1.00	1.00	TAG	C
ATOM	109	NE2	HIS	7	-11.215	-1.034	-5.114	1.00	1.00	TAG	N
ATOM	110	H	HIS	7	-7.816	-2.690	-1.892	1.00	1.00	TAG	H
ATOM	111	HA	HIS	7	-10.170	-4.310	-2.479	1.00	1.00	TAG	H
ATOM	112	1HB	HIS	7	-8.002	-3.108	-4.226	1.00	1.00	TAG	H
ATOM	113	2HB	HIS	7	-8.825	-4.582	-4.753	1.00	1.00	TAG	H
ATOM	114	HD1	HIS	7	-11.599	-4.161	-5.307	1.00	1.00	TAG	H
ATOM	115	HD2	HIS	7	-9.236	-0.858	-4.272	1.00	1.00	TAG	H
ATOM	116	HE1	HIS	7	-12.974	-2.024	-5.871	1.00	1.00	TAG	H
ATOM	117	N	HIS	8	-7.198	-5.367	-1.805	1.00	1.00	TAG	N
ATOM	118	CA	HIS	8	-6.371	-6.549	-1.607	1.00	1.00	TAG	C
ATOM	119	C	HIS	8	-6.299	-7.052	-0.165	1.00	1.00	TAG	C
ATOM	120	O	HIS	8	-5.475	-7.918	0.156	1.00	1.00	TAG	O
ATOM	121	CB	HIS	8	-4.981	-6.342	-2.196	1.00	1.00	TAG	C
ATOM	122	CG	HIS	8	-4.932	-6.536	-3.677	1.00	1.00	TAG	C
ATOM	123	CD2	HIS	8	-4.805	-7.658	-4.430	1.00	1.00	TAG	C
ATOM	124	ND1	HIS	8	-5.059	-5.494	-4.570	1.00	1.00	TAG	N
ATOM	125	CE1	HIS	8	-5.013	-5.964	-5.810	1.00	1.00	TAG	C
ATOM	126	NE2	HIS	8	-4.858	-7.279	-5.746	1.00	1.00	TAG	N
ATOM	127	H	HIS	8	-6.789	-4.517	-1.470	1.00	1.00	TAG	H
ATOM	128	HA	HIS	8	-6.880	-7.355	-2.155	1.00	1.00	TAG	H
ATOM	129	1HB	HIS	8	-4.635	-5.326	-1.955	1.00	1.00	TAG	H
ATOM	130	2HB	HIS	8	-4.281	-7.042	-1.718	1.00	1.00	TAG	H

ATOM	131	HD2	HIS	8	-4.683	-8.685	-4.053	1.00	1.00	TAG	H
ATOM	132	HE1	HIS	8	-5.090	-5.367	-6.730	1.00	1.00	TAG	H
ATOM	133	HE2	HIS	8	-4.789	-7.895	-6.530	1.00	1.00	TAG	H
ATOM	134	N	GLY	9	-7.324	-6.562	0.627	1.00	1.00	TAG	N
ATOM	135	CA	GLY	9	-7.444	-6.878	2.062	1.00	1.00	TAG	C
ATOM	136	C	GLY	9	-6.174	-6.609	2.879	1.00	1.00	TAG	C
ATOM	137	O	GLY	9	-5.974	-7.173	3.958	1.00	1.00	TAG	O
ATOM	138	H	GLY	9	-8.047	-5.963	0.282	1.00	1.00	TAG	H
ATOM	139	1HA	GLY	9	-8.270	-6.288	2.486	1.00	1.00	TAG	H
ATOM	140	2HA	GLY	9	-7.717	-7.938	2.170	1.00	1.00	TAG	H
ATOM	141	N	TYR	10	-5.328	-5.766	2.329	1.00	0.00	TAG	N
ATOM	142	CA	TYR	10	-4.009	-5.542	2.914	1.00	0.00	TAG	C
ATOM	143	C	TYR	10	-4.050	-4.422	3.925	1.00	0.00	TAG	C
ATOM	144	O	TYR	10	-3.111	-3.667	4.057	1.00	0.00	TAG	O
ATOM	145	CB	TYR	10	-2.973	-5.161	1.816	1.00	0.00	TAG	C
ATOM	146	CG	TYR	10	-2.644	-6.238	0.776	1.00	0.00	TAG	C
ATOM	147	CD1	TYR	10	-2.994	-7.573	0.998	1.00	0.00	TAG	C
ATOM	148	CD2	TYR	10	-1.997	-5.883	-0.411	1.00	0.00	TAG	C
ATOM	149	CE1	TYR	10	-2.704	-8.540	0.039	1.00	0.00	TAG	C
ATOM	150	CE2	TYR	10	-1.707	-6.850	-1.368	1.00	0.00	TAG	C
ATOM	151	CZ	TYR	10	-2.061	-8.179	-1.143	1.00	0.00	TAG	C
ATOM	152	OH	TYR	10	-1.781	-9.130	-2.082	1.00	0.00	TAG	O
ATOM	153	H	TYR	10	-5.590	-5.275	1.504	1.00	0.00	TAG	H
ATOM	154	HA	TYR	10	-3.688	-6.462	3.437	1.00	0.00	TAG	H
ATOM	155	2HB	TYR	10	-2.020	-4.857	2.294	1.00	0.00	TAG	H
ATOM	156	3HB	TYR	10	-3.307	-4.237	1.300	1.00	0.00	TAG	H
ATOM	157	1HD	TYR	10	-3.499	-7.862	1.909	1.00	0.00	TAG	H
ATOM	158	2HD	TYR	10	-1.729	-4.851	-0.598	1.00	0.00	TAG	H
ATOM	159	1HE	TYR	10	-2.979	-9.571	0.205	1.00	0.00	TAG	H
ATOM	160	2HE	TYR	10	-1.213	-6.562	-2.284	1.00	0.00	TAG	H
ATOM	161	HH	TYR	10	-1.343	-8.705	-2.823	1.00	0.00	TAG	H
ATOM	162	N	LYS	11	-5.036	-4.223	4.636	1.00	1.00	TAG	N
ATOM	163	CA	LYS	11	-5.153	-3.155	5.622	1.00	1.00	TAG	C
ATOM	164	C	LYS	11	-3.960	-3.193	6.558	1.00	1.00	TAG	C
ATOM	165	O	LYS	11	-3.654	-2.167	7.183	1.00	1.00	TAG	O
ATOM	166	CB	LYS	11	-6.454	-3.311	6.412	1.00	1.00	TAG	C
ATOM	167	CG	LYS	11	-6.718	-2.222	7.430	1.00	1.00	TAG	C
ATOM	168	CD	LYS	11	-8.209	-2.138	7.703	1.00	1.00	TAG	C
ATOM	169	CE	LYS	11	-8.550	-1.088	8.742	1.00	1.00	TAG	C
ATOM	170	NZ	LYS	11	-8.263	-1.596	10.100	1.00	1.00	TAG	N
ATOM	171	H	LYS	11	-5.854	-4.797	4.595	1.00	1.00	TAG	H
ATOM	172	HA	LYS	11	-5.170	-2.184	5.106	1.00	1.00	TAG	H
ATOM	173	1HB	LYS	11	-7.294	-3.341	5.702	1.00	1.00	TAG	H
ATOM	174	2HB	LYS	11	-6.435	-4.281	6.930	1.00	1.00	TAG	H
ATOM	175	1HG	LYS	11	-6.174	-2.435	8.362	1.00	1.00	TAG	H
ATOM	176	2HG	LYS	11	-6.347	-1.256	7.056	1.00	1.00	TAG	H
ATOM	177	1HD	LYS	11	-8.738	-1.908	6.766	1.00	1.00	TAG	H
ATOM	178	2HD	LYS	11	-8.571	-3.119	8.045	1.00	1.00	TAG	H
ATOM	179	1HE	LYS	11	-7.967	-0.174	8.554	1.00	1.00	TAG	H
ATOM	180	2HE	LYS	11	-9.612	-0.813	8.661	1.00	1.00	TAG	H
ATOM	181	H01	LYS	11	-7.978	-2.563	10.045	1.00	1.00	TAG	H

ATOM	182	H02	LYS	11	-9.093	-1.521	10.671	1.00	1.00	TAG	H
ATOM	183	N	ARG	12	-3.338	-4.258	6.731	1.00	0.00	TAG	N
ATOM	184	CA	ARG	12	-2.061	-4.287	7.438	1.00	0.00	TAG	C
ATOM	185	C	ARG	12	-1.173	-3.148	6.997	1.00	0.00	TAG	C
ATOM	186	O	ARG	12	-0.401	-2.642	7.909	1.00	0.00	TAG	O
ATOM	187	CB	ARG	12	-1.382	-5.664	7.189	1.00	0.00	TAG	C
ATOM	188	CG	ARG	12	-2.076	-6.883	7.858	1.00	0.00	TAG	C
ATOM	189	CD	ARG	12	-1.270	-8.180	7.676	1.00	0.00	TAG	C
ATOM	190	NE	ARG	12	-2.010	-9.322	8.288	1.00	0.00	TAG	N
ATOM	191	CZ	ARG	12	-2.830	-10.143	7.640	1.00	0.00	TAG	C
ATOM	192	NH1	ARG	12	-3.086	-10.049	6.365	1.00	0.00	TAG	N
ATOM	193	NH2	ARG	12	-3.410	-11.089	8.309	1.00	0.00	TAG	N1+
ATOM	194	H	ARG	12	-3.706	-5.075	6.393	1.00	0.00	TAG	H
ATOM	195	HA	ARG	12	-2.265	-4.155	8.518	1.00	0.00	TAG	H
ATOM	196	2HB	ARG	12	-0.323	-5.603	7.515	1.00	0.00	TAG	H
ATOM	197	3HB	ARG	12	-1.322	-5.847	6.097	1.00	0.00	TAG	H
ATOM	198	2HG	ARG	12	-3.096	-6.998	7.437	1.00	0.00	TAG	H
ATOM	199	3HG	ARG	12	-2.221	-6.692	8.941	1.00	0.00	TAG	H
ATOM	200	2HD	ARG	12	-0.268	-8.059	8.144	1.00	0.00	TAG	H
ATOM	201	3HD	ARG	12	-1.091	-8.356	6.593	1.00	0.00	TAG	H
ATOM	202	HE	ARG	12	-1.918	-9.535	9.287	1.00	0.00	TAG	H
ATOM	203	1HH1	ARG	12	-2.596	-9.283	5.896	1.00	0.00	TAG	H
ATOM	204	2HH1	ARG	12	-3.729	-10.719	5.940	1.00	0.00	TAG	H
ATOM	205	H01	ARG	12	-3.502	-10.811	9.276	1.00	0.00	TAG	H
ATOM	206	H02	ARG	12	-2.855	-11.931	8.252	1.00	0.00	TAG	H
ATOM	207	H03	ARG	12	-4.326	-11.263	7.920	1.00	0.00	TAG	H
ATOM	208	N	LYS	13	-1.088	-2.779	5.854	1.00	0.00	TAG	N
ATOM	209	CA	LYS	13	-0.076	-1.842	5.376	1.00	0.00	TAG	C
ATOM	210	C	LYS	13	0.122	-0.712	6.358	1.00	0.00	TAG	C
ATOM	211	O	LYS	13	1.254	-0.250	6.545	1.00	0.00	TAG	O
ATOM	212	CB	LYS	13	-0.492	-1.299	3.982	1.00	0.00	TAG	C
ATOM	213	CG	LYS	13	0.562	-0.358	3.347	1.00	0.00	TAG	C
ATOM	214	CD	LYS	13	1.850	-1.049	2.891	1.00	0.00	TAG	C
ATOM	215	CE	LYS	13	2.733	-0.035	2.152	1.00	0.00	TAG	C
ATOM	216	NZ	LYS	13	3.980	-0.692	1.722	1.00	0.00	TAG	N
ATOM	217	H	LYS	13	-1.746	-3.135	5.197	1.00	0.00	TAG	H
ATOM	218	HA	LYS	13	0.886	-2.380	5.290	1.00	0.00	TAG	H
ATOM	219	2HB	LYS	13	-1.467	-0.774	4.062	1.00	0.00	TAG	H
ATOM	220	3HB	LYS	13	-0.683	-2.147	3.293	1.00	0.00	TAG	H
ATOM	221	2HG	LYS	13	0.802	0.461	4.053	1.00	0.00	TAG	H
ATOM	222	3HG	LYS	13	0.141	0.138	2.452	1.00	0.00	TAG	H
ATOM	223	2HD	LYS	13	1.605	-1.900	2.224	1.00	0.00	TAG	H
ATOM	224	3HD	LYS	13	2.374	-1.480	3.766	1.00	0.00	TAG	H
ATOM	225	2HE	LYS	13	2.976	0.833	2.800	1.00	0.00	TAG	H
ATOM	226	3HE	LYS	13	2.194	0.384	1.276	1.00	0.00	TAG	H
ATOM	227	H01	LYS	13	4.237	-0.360	0.803	1.00	0.00	TAG	H
ATOM	228	H02	LYS	13	3.841	-1.692	1.692	1.00	0.00	TAG	H
ATOM	229	N	PHE	14	-0.878	-0.227	7.012	1.00	0.00	TAG	N
ATOM	230	CA	PHE	14	-0.736	0.853	7.984	1.00	0.00	TAG	C
ATOM	231	C	PHE	14	-0.064	0.364	9.244	1.00	0.00	TAG	C
ATOM	232	O	PHE	14	0.673	1.159	9.892	1.00	0.00	TAG	O

ATOM	233	CB	PHE	14	-2.137	1.429	8.352	1.00	0.00	TAG	C
ATOM	234	CG	PHE	14	-2.150	2.678	9.247	1.00	0.00	TAG	C
ATOM	235	CD1	PHE	14	-1.777	3.916	8.711	1.00	0.00	TAG	C
ATOM	236	CD2	PHE	14	-2.469	2.584	10.603	1.00	0.00	TAG	C
ATOM	237	CE1	PHE	14	-1.706	5.041	9.525	1.00	0.00	TAG	C
ATOM	238	CE2	PHE	14	-2.409	3.713	11.417	1.00	0.00	TAG	C
ATOM	239	CZ	PHE	14	-2.024	4.939	10.878	1.00	0.00	TAG	C
ATOM	240	H	PHE	14	-1.860	-0.636	6.833	1.00	0.00	TAG	H
ATOM	241	HA	PHE	14	-0.104	1.650	7.546	1.00	0.00	TAG	H
ATOM	242	2HB	PHE	14	-2.740	0.641	8.845	1.00	0.00	TAG	H
ATOM	243	3HB	PHE	14	-2.705	1.647	7.425	1.00	0.00	TAG	H
ATOM	244	1HD	PHE	14	-1.499	3.995	7.668	1.00	0.00	TAG	H
ATOM	245	2HD	PHE	14	-2.748	1.631	11.033	1.00	0.00	TAG	H
ATOM	246	1HE	PHE	14	-1.388	5.985	9.108	1.00	0.00	TAG	H
ATOM	247	2HE	PHE	14	-2.649	3.633	12.467	1.00	0.00	TAG	H
ATOM	248	HZ	PHE	14	-1.963	5.813	11.509	1.00	0.00	TAG	H
ATOM	249	N	HIS	15	-0.221	-0.910	9.632	1.00	0.00	TAG	N
ATOM	250	CA	HIS	15	0.471	-1.524	10.762	1.00	0.00	TAG	C
ATOM	251	C	HIS	15	1.861	-1.966	10.370	1.00	0.00	TAG	C
ATOM	252	O	HIS	15	2.672	-2.413	11.205	1.00	0.00	TAG	O
ATOM	253	CB	HIS	15	-0.378	-2.736	11.182	1.00	0.00	TAG	C
ATOM	254	CG	HIS	15	-1.720	-2.332	11.717	1.00	0.00	TAG	C
ATOM	255	CD2	HIS	15	-1.950	-2.093	13.066	1.00	0.00	TAG	C
ATOM	256	ND1	HIS	15	-2.878	-2.148	10.964	1.00	0.00	TAG	N
ATOM	257	CE1	HIS	15	-3.738	-1.809	11.941	1.00	0.00	TAG	C
ATOM	258	NE2	HIS	15	-3.268	-1.750	13.217	1.00	0.00	TAG	N
ATOM	259	H	HIS	15	-0.855	-1.477	9.113	1.00	0.00	TAG	H
ATOM	260	HA	HIS	15	0.593	-0.752	11.539	1.00	0.00	TAG	H
ATOM	261	2HB	HIS	15	0.135	-3.333	11.963	1.00	0.00	TAG	H
ATOM	262	3HB	HIS	15	-0.549	-3.439	10.340	1.00	0.00	TAG	H
ATOM	263	2HD	HIS	15	-1.194	-2.173	13.842	1.00	0.00	TAG	H
ATOM	264	1HE	HIS	15	-4.761	-1.598	11.658	1.00	0.00	TAG	H
ATOM	265	2HE	HIS	15	-3.770	-1.511	14.084	1.00	0.00	TAG	H
ATOM	266	N	GLU	16	2.230	-1.863	9.088	1.00	1.00	TAG	N
ATOM	267	CA	GLU	16	3.558	-2.208	8.589	1.00	1.00	TAG	C
ATOM	268	C	GLU	16	4.185	-3.234	9.525	1.00	1.00	TAG	C
ATOM	269	O	GLU	16	5.412	-3.426	9.484	1.00	1.00	TAG	O
ATOM	270	CB	GLU	16	4.443	-0.969	8.533	1.00	1.00	TAG	C
ATOM	271	CG	GLU	16	5.820	-1.221	7.938	1.00	1.00	TAG	C
ATOM	272	CD	GLU	16	6.760	-0.042	8.106	1.00	1.00	TAG	C
ATOM	273	OE1	GLU	16	6.489	0.825	8.964	1.00	1.00	TAG	O
ATOM	274	OE2	GLU	16	7.797	0.010	7.406	1.00	1.00	TAG	O
ATOM	275	H	GLU	16	1.608	-1.547	8.372	1.00	1.00	TAG	H
ATOM	276	HA	GLU	16	3.465	-2.623	7.575	1.00	1.00	TAG	H
ATOM	277	1HB	GLU	16	3.935	-0.194	7.940	1.00	1.00	TAG	H
ATOM	278	2HB	GLU	16	4.563	-0.568	9.551	1.00	1.00	TAG	H
ATOM	279	1HG	GLU	16	6.263	-2.107	8.415	1.00	1.00	TAG	H
ATOM	280	2HG	GLU	16	5.715	-1.450	6.868	1.00	1.00	TAG	H
ATOM	281	H01	GLU	16	8.008	0.926	7.213	1.00	1.00	TAG	H
ATOM	282	N	LYS	17	3.409	-3.899	10.352	1.00	1.00	TAG	N
ATOM	283	CA	LYS	17	3.880	-4.969	11.225	1.00	1.00	TAG	C

ATOM	284	C	LYS	17	3.924	-6.273	10.455	1.00	1.00	TAG C
ATOM	285	O	LYS	17	4.998	-6.853	10.263	1.00	1.00	TAG O
ATOM	286	CB	LYS	17	2.957	-5.099	12.439	1.00	1.00	TAG C
ATOM	287	CG	LYS	17	3.378	-6.142	13.452	1.00	1.00	TAG C
ATOM	288	CD	LYS	17	2.789	-5.793	14.807	1.00	1.00	TAG C
ATOM	289	CE	LYS	17	3.141	-6.813	15.872	1.00	1.00	TAG C
ATOM	290	NZ	LYS	17	2.289	-8.012	15.738	1.00	1.00	TAG N1+
ATOM	291	H	LYS	17	2.430	-3.716	10.442	1.00	1.00	TAG H
ATOM	292	HA	LYS	17	4.893	-4.730	11.579	1.00	1.00	TAG H
ATOM	293	1HB	LYS	17	2.898	-4.123	12.942	1.00	1.00	TAG H
ATOM	294	2HB	LYS	17	1.943	-5.341	12.085	1.00	1.00	TAG H
ATOM	295	1HG	LYS	17	3.036	-7.138	13.135	1.00	1.00	TAG H
ATOM	296	2HG	LYS	17	4.476	-6.185	13.516	1.00	1.00	TAG H
ATOM	297	1HD	LYS	17	3.152	-4.803	15.117	1.00	1.00	TAG H
ATOM	298	2HD	LYS	17	1.694	-5.720	14.720	1.00	1.00	TAG H
ATOM	299	1HE	LYS	17	4.200	-7.095	15.783	1.00	1.00	TAG H
ATOM	300	2HE	LYS	17	3.009	-6.371	16.871	1.00	1.00	TAG H
ATOM	301	1HZ	LYS	17	2.116	-8.402	16.643	1.00	1.00	TAG H
ATOM	302	2HZ	LYS	17	1.420	-7.759	15.314	1.00	1.00	TAG H
ATOM	303	3HZ	LYS	17	2.754	-8.690	15.168	1.00	1.00	TAG H
ATOM	304	N	HIS	18	2.816	-6.677	9.853	1.00	0.00	TAG N
ATOM	305	CA	HIS	18	2.629	-7.976	9.213	1.00	0.00	TAG C
ATOM	306	C	HIS	18	3.400	-8.058	7.918	1.00	0.00	TAG C
ATOM	307	O	HIS	18	4.121	-9.049	7.635	1.00	0.00	TAG O
ATOM	308	CB	HIS	18	1.120	-8.113	8.948	1.00	0.00	TAG C
ATOM	309	CG	HIS	18	0.326	-8.216	10.218	1.00	0.00	TAG C
ATOM	310	CD2	HIS	18	-0.076	-9.432	10.755	1.00	0.00	TAG C
ATOM	311	ND1	HIS	18	-0.101	-7.147	11.002	1.00	0.00	TAG N
ATOM	312	CE1	HIS	18	-0.747	-7.817	11.974	1.00	0.00	TAG C
ATOM	313	NE2	HIS	18	-0.778	-9.176	11.904	1.00	0.00	TAG N
ATOM	314	H	HIS	18	2.051	-6.045	9.835	1.00	0.00	TAG H
ATOM	315	HA	HIS	18	3.053	-8.743	9.883	1.00	0.00	TAG H
ATOM	316	2HB	HIS	18	0.901	-9.010	8.336	1.00	0.00	TAG H
ATOM	317	3HB	HIS	18	0.717	-7.256	8.369	1.00	0.00	TAG H
ATOM	318	2HD	HIS	18	0.144	-10.401	10.316	1.00	0.00	TAG H
ATOM	319	1HE	HIS	18	-1.208	-7.237	12.763	1.00	0.00	TAG H
ATOM	320	2HE	HIS	18	-1.217	-9.850	12.547	1.00	0.00	TAG H
ATOM	321	N	HIS	19	3.157	-7.158	6.984	1.00	1.00	TAG N
ATOM	322	CA	HIS	19	3.721	-7.223	5.644	1.00	1.00	TAG C
ATOM	323	C	HIS	19	4.792	-6.173	5.342	1.00	1.00	TAG C
ATOM	324	O	HIS	19	5.902	-6.355	4.828	1.00	1.00	TAG O
ATOM	325	CB	HIS	19	2.619	-7.215	4.593	1.00	1.00	TAG C
ATOM	326	CG	HIS	19	1.972	-8.549	4.403	1.00	1.00	TAG C
ATOM	327	CD2	HIS	19	0.824	-8.922	5.067	1.00	1.00	TAG C
ATOM	328	ND1	HIS	19	2.331	-9.620	3.649	1.00	1.00	TAG N
ATOM	329	CE1	HIS	19	1.405	-10.606	3.869	1.00	1.00	TAG C
ATOM	330	NE2	HIS	19	0.502	-10.165	4.732	1.00	1.00	TAG N
ATOM	331	H	HIS	19	2.551	-6.376	7.128	1.00	1.00	TAG H
ATOM	332	HA	HIS	19	4.257	-8.182	5.600	1.00	1.00	TAG H
ATOM	333	1HB	HIS	19	1.852	-6.481	4.881	1.00	1.00	TAG H
ATOM	334	2HB	HIS	19	3.040	-6.880	3.633	1.00	1.00	TAG H

ATOM	335	HD2	HIS	19	0.261	-8.288	5.768	1.00	1.00	TAG	H
ATOM	336	HE1	HIS	19	1.411	-11.603	3.405	1.00	1.00	TAG	H
ATOM	337	HE2	HIS	19	-0.286	-10.678	5.071	1.00	1.00	TAG	H
ATOM	338	N	SER	20	4.388	-4.883	5.723	1.00	1.00	TAG	N
ATOM	339	CA	SER	20	5.217	-3.714	5.426	1.00	1.00	TAG	C
ATOM	340	C	SER	20	6.615	-3.770	6.026	1.00	1.00	TAG	C
ATOM	341	O	SER	20	7.671	-3.703	5.418	1.00	1.00	TAG	O
ATOM	342	CB	SER	20	4.519	-2.450	5.935	1.00	1.00	TAG	C
ATOM	343	OG	SER	20	5.364	-1.323	5.792	1.00	1.00	TAG	O
ATOM	344	H	SER	20	3.538	-4.679	6.208	1.00	1.00	TAG	H
ATOM	345	HA	SER	20	5.340	-3.702	4.332	1.00	1.00	TAG	H
ATOM	346	1HB	SER	20	3.586	-2.289	5.375	1.00	1.00	TAG	H
ATOM	347	2HB	SER	20	4.242	-2.577	6.992	1.00	1.00	TAG	H
ATOM	348	HG	SER	20	5.921	-1.426	4.967	1.00	1.00	TAG	H
ATOM	349	N	HIS	21	6.679	-3.939	7.431	1.00	0.00	TAG	N
ATOM	350	CA	HIS	21	7.976	-4.035	8.094	1.00	0.00	TAG	C
ATOM	351	C	HIS	21	8.503	-5.449	8.053	1.00	0.00	TAG	C
ATOM	352	O	HIS	21	9.487	-5.899	8.719	1.00	0.00	TAG	O
ATOM	353	CB	HIS	21	7.752	-3.589	9.548	1.00	0.00	TAG	C
ATOM	354	CG	HIS	21	9.034	-3.212	10.233	1.00	0.00	TAG	C
ATOM	355	CD2	HIS	21	9.397	-1.893	10.472	1.00	0.00	TAG	C
ATOM	356	ND1	HIS	21	9.999	-4.099	10.705	1.00	0.00	TAG	N
ATOM	357	CE1	HIS	21	10.894	-3.224	11.200	1.00	0.00	TAG	C
ATOM	358	NE2	HIS	21	10.612	-1.896	11.105	1.00	0.00	TAG	N
ATOM	359	H	HIS	21	5.846	-3.993	7.962	1.00	0.00	TAG	H
ATOM	360	HA	HIS	21	8.689	-3.416	7.524	1.00	0.00	TAG	H
ATOM	361	2HB	HIS	21	7.272	-4.390	10.144	1.00	0.00	TAG	H
ATOM	362	3HB	HIS	21	7.066	-2.719	9.618	1.00	0.00	TAG	H
ATOM	363	2HD	HIS	21	8.799	-1.030	10.193	1.00	0.00	TAG	H
ATOM	364	1HE	HIS	21	11.791	-3.627	11.651	1.00	0.00	TAG	H
ATOM	365	2HE	HIS	21	11.168	-1.089	11.424	1.00	0.00	TAG	H
ATOM	366	N	ARG	22	7.908	-6.270	7.196	1.00	0.00	TAG	N
ATOM	367	CA	ARG	22	8.372	-7.618	6.882	1.00	0.00	TAG	C
ATOM	368	C	ARG	22	9.167	-7.631	5.598	1.00	0.00	TAG	C
ATOM	369	O	ARG	22	9.918	-8.505	5.345	1.00	0.00	TAG	O
ATOM	370	CB	ARG	22	7.140	-8.564	6.795	1.00	0.00	TAG	C
ATOM	371	CG	ARG	22	6.311	-8.704	8.103	1.00	0.00	TAG	C
ATOM	372	CD	ARG	22	7.072	-9.482	9.189	1.00	0.00	TAG	C
ATOM	373	NE	ARG	22	6.189	-9.682	10.375	1.00	0.00	TAG	N
ATOM	374	CZ	ARG	22	6.513	-10.367	11.468	1.00	0.00	TAG	C
ATOM	375	NH1	ARG	22	7.665	-10.952	11.638	1.00	0.00	TAG	N
ATOM	376	NH2	ARG	22	5.636	-10.461	12.418	1.00	0.00	TAG	N1+
ATOM	377	H	ARG	22	7.079	-5.939	6.730	1.00	0.00	TAG	H
ATOM	378	HA	ARG	22	9.045	-7.947	7.696	1.00	0.00	TAG	H
ATOM	379	2HB	ARG	22	7.481	-9.562	6.451	1.00	0.00	TAG	H
ATOM	380	3HB	ARG	22	6.468	-8.211	5.987	1.00	0.00	TAG	H
ATOM	381	2HG	ARG	22	5.347	-9.203	7.871	1.00	0.00	TAG	H
ATOM	382	3HG	ARG	22	6.041	-7.701	8.492	1.00	0.00	TAG	H
ATOM	383	2HD	ARG	22	7.991	-8.920	9.468	1.00	0.00	TAG	H
ATOM	384	3HD	ARG	22	7.412	-10.457	8.778	1.00	0.00	TAG	H
ATOM	385	HE	ARG	22	5.245	-9.283	10.403	1.00	0.00	TAG	H

ATOM	386	1HH1	ARG	22	8.311	-10.839	10.853	1.00	0.00	TAG H
ATOM	387	2HH1	ARG	22	7.837	-11.461	12.507	1.00	0.00	TAG H
ATOM	388	H01	ARG	22	5.477	-9.549	12.822	1.00	0.00	TAG H
ATOM	389	H02	ARG	22	5.977	-11.090	13.131	1.00	0.00	TAG H
ATOM	390	H03	ARG	22	4.769	-10.818	12.041	1.00	0.00	TAG H
ATOM	391	N	GLY	23	9.069	-6.672	4.818	1.00	1.00	TAG N
ATOM	392	CA	GLY	23	9.552	-6.640	3.441	1.00	1.00	TAG C
ATOM	393	C	GLY	23	9.266	-7.956	2.720	1.00	1.00	TAG C
ATOM	394	O	GLY	23	9.916	-8.278	1.723	1.00	1.00	TAG O
ATOM	395	H	GLY	23	8.632	-5.808	5.068	1.00	1.00	TAG H
ATOM	396	1HA	GLY	23	9.072	-5.812	2.901	1.00	1.00	TAG H
ATOM	397	2HA	GLY	23	10.634	-6.444	3.435	1.00	1.00	TAG H
ATOM	398	N	TYR	24	8.310	-8.706	3.187	1.00	0.00	TAG N
ATOM	399	CA	TYR	24	7.828	-9.953	2.600	1.00	0.00	TAG C
ATOM	400	C	TYR	24	8.143	-10.014	1.125	1.00	0.00	TAG C
ATOM	401	O	TYR	24	7.683	-9.205	0.314	1.00	0.00	TAG O
ATOM	402	CB	TYR	24	6.286	-10.086	2.768	1.00	0.00	TAG C
ATOM	403	CG	TYR	24	5.639	-11.357	2.205	1.00	0.00	TAG C
ATOM	404	CD1	TYR	24	5.731	-12.570	2.896	1.00	0.00	TAG C
ATOM	405	CD2	TYR	24	4.943	-11.305	0.994	1.00	0.00	TAG C
ATOM	406	CE1	TYR	24	5.127	-13.714	2.382	1.00	0.00	TAG C
ATOM	407	CE2	TYR	24	4.340	-12.449	0.482	1.00	0.00	TAG C
ATOM	408	CZ	TYR	24	4.433	-13.654	1.176	1.00	0.00	TAG C
ATOM	409	OH	TYR	24	3.839	-14.778	0.677	1.00	0.00	TAG O
ATOM	410	OXT	TYR	24	9.013	-11.054	0.639	0.00	0.00	TAG O
ATOM	411	H	TYR	24	7.843	-8.385	4.066	1.00	0.00	TAG H
ATOM	412	HA	TYR	24	8.339	-10.802	3.092	1.00	0.00	TAG H
ATOM	413	2HB	TYR	24	5.784	-9.219	2.294	1.00	0.00	TAG H
ATOM	414	3HB	TYR	24	6.023	-9.981	3.841	1.00	0.00	TAG H
ATOM	415	1HD	TYR	24	6.263	-12.625	3.835	1.00	0.00	TAG H
ATOM	416	2HD	TYR	24	4.857	-10.371	0.455	1.00	0.00	TAG H
ATOM	417	1HE	TYR	24	5.191	-14.650	2.917	1.00	0.00	TAG H
ATOM	418	2HE	TYR	24	3.799	-12.394	-0.451	1.00	0.00	TAG H
ATOM	419	HH	TYR	24	3.409	-14.552	-0.151	1.00	0.00	TAG H
ATOM	420	H01	TYR	24	9.176	-10.923	-0.297	0.00	0.00	TAG H
END										

Histatin conformer 6:

ATOM	1	N	ASP	1	-0.753	-1.254	-0.000	1.00	1.00	TAG N1+
ATOM	2	CA	ASP	1	0.000	0.000	0.000	1.00	1.00	TAG C
ATOM	3	C	ASP	1	-0.977	1.163	0.124	1.00	1.00	TAG C
ATOM	4	O	ASP	1	-0.987	1.874	1.139	1.00	1.00	TAG O
ATOM	5	CB	ASP	1	0.960	0.222	-1.175	1.00	1.00	TAG C
ATOM	6	CG	ASP	1	1.836	1.487	-1.016	1.00	1.00	TAG C
ATOM	7	OD1	ASP	1	1.995	2.026	0.114	1.00	1.00	TAG O
ATOM	8	OD2	ASP	1	2.382	1.948	-2.048	1.00	1.00	TAG O
ATOM	9	1H	ASP	1	-0.117	-2.025	-0.000	1.00	1.00	TAG H
ATOM	10	2H	ASP	1	-1.329	-1.298	0.816	1.00	1.00	TAG H
ATOM	11	3H	ASP	1	-1.329	-1.298	-0.816	1.00	1.00	TAG H
ATOM	12	HA	ASP	1	0.619	-0.065	0.906	1.00	1.00	TAG H

ATOM	13	1HB	ASP	1	1.613	-0.658	-1.278	1.00	1.00	TAG	H
ATOM	14	2HB	ASP	1	0.379	0.301	-2.105	1.00	1.00	TAG	H
ATOM	15	H01	ASP	1	2.425	2.905	-1.988	1.00	1.00	TAG	H
ATOM	16	N	SER	2	-1.793	1.390	-0.846	1.00	1.00	TAG	N
ATOM	17	CA	SER	2	-2.716	2.526	-0.879	1.00	1.00	TAG	C
ATOM	18	C	SER	2	-4.177	2.137	-1.044	1.00	1.00	TAG	C
ATOM	19	O	SER	2	-5.131	2.569	-0.414	1.00	1.00	TAG	O
ATOM	20	CB	SER	2	-2.329	3.466	-2.024	1.00	1.00	TAG	C
ATOM	21	OG	SER	2	-3.292	4.492	-2.171	1.00	1.00	TAG	O
ATOM	22	H	SER	2	-1.855	0.803	-1.653	1.00	1.00	TAG	H
ATOM	23	HA	SER	2	-2.625	3.016	0.101	1.00	1.00	TAG	H
ATOM	24	1HB	SER	2	-1.341	3.908	-1.826	1.00	1.00	TAG	H
ATOM	25	2HB	SER	2	-2.244	2.897	-2.961	1.00	1.00	TAG	H
ATOM	26	HG	SER	2	-3.023	5.098	-2.920	1.00	1.00	TAG	H
ATOM	27	N	HIS	3	-4.390	1.184	-2.030	1.00	1.00	TAG	N
ATOM	28	CA	HIS	3	-5.717	0.551	-2.216	1.00	1.00	TAG	C
ATOM	29	C	HIS	3	-5.676	-0.869	-1.702	1.00	1.00	TAG	C
ATOM	30	O	HIS	3	-6.685	-1.368	-1.141	1.00	1.00	TAG	O
ATOM	31	CB	HIS	3	-5.979	0.564	-3.827	1.00	1.00	TAG	C
ATOM	32	CG	HIS	3	-7.275	-0.191	-4.018	1.00	1.00	TAG	C
ATOM	33	CD2	HIS	3	-8.539	0.160	-3.712	1.00	1.00	TAG	C
ATOM	34	ND1	HIS	3	-7.403	-1.406	-4.678	1.00	1.00	TAG	N
ATOM	35	CE1	HIS	3	-8.725	-1.729	-4.610	1.00	1.00	TAG	C
ATOM	36	NE2	HIS	3	-9.425	-0.729	-4.077	1.00	1.00	TAG	N
ATOM	37	H	HIS	3	-3.685	0.867	-2.665	1.00	1.00	TAG	H
ATOM	38	HA	HIS	3	-6.514	1.079	-1.672	1.00	1.00	TAG	H
ATOM	39	1HB	HIS	3	-6.058	1.593	-4.210	1.00	1.00	TAG	H
ATOM	40	2HB	HIS	3	-5.153	0.081	-4.370	1.00	1.00	TAG	H
ATOM	41	HD2	HIS	3	-8.799	1.102	-3.207	1.00	1.00	TAG	H
ATOM	42	HE1	HIS	3	-9.155	-2.684	-4.948	1.00	1.00	TAG	H
ATOM	43	HE2	HIS	3	-10.418	-0.671	-3.977	1.00	1.00	TAG	H
ATOM	44	N	ALA	4	-4.565	-1.562	-1.869	1.00	1.00	TAG	N
ATOM	45	CA	ALA	4	-4.424	-2.943	-1.447	1.00	1.00	TAG	C
ATOM	46	C	ALA	4	-4.400	-3.018	0.089	1.00	1.00	TAG	C
ATOM	47	O	ALA	4	-5.147	-3.798	0.673	1.00	1.00	TAG	O
ATOM	48	CB	ALA	4	-3.134	-3.523	-2.024	1.00	1.00	TAG	C
ATOM	49	H	ALA	4	-3.744	-1.185	-2.297	1.00	1.00	TAG	H
ATOM	50	HA	ALA	4	-5.279	-3.528	-1.818	1.00	1.00	TAG	H
ATOM	51	1HB	ALA	4	-3.027	-4.570	-1.704	1.00	1.00	TAG	H
ATOM	52	2HB	ALA	4	-3.169	-3.477	-3.122	1.00	1.00	TAG	H
ATOM	53	3HB	ALA	4	-2.275	-2.939	-1.661	1.00	1.00	TAG	H
ATOM	54	N	LYS	5	-3.589	-2.259	0.740	1.00	1.00	TAG	N
ATOM	55	CA	LYS	5	-3.540	-2.223	2.197	1.00	1.00	TAG	C
ATOM	56	C	LYS	5	-4.882	-1.766	2.756	1.00	1.00	TAG	C
ATOM	57	O	LYS	5	-5.304	-2.239	3.796	1.00	1.00	TAG	O
ATOM	58	CB	LYS	5	-2.425	-1.286	2.672	1.00	1.00	TAG	C
ATOM	59	CG	LYS	5	-1.043	-1.853	2.469	1.00	1.00	TAG	C
ATOM	60	CD	LYS	5	0.029	-0.881	2.912	1.00	1.00	TAG	C
ATOM	61	CE	LYS	5	1.405	-1.485	2.653	1.00	1.00	TAG	C
ATOM	62	NZ	LYS	5	2.511	-0.510	2.838	1.00	1.00	TAG	N
ATOM	63	H	LYS	5	-2.938	-1.643	0.298	1.00	1.00	TAG	H

ATOM	64	HA	LYS	5	-3.328	-3.238	2.564	1.00	1.00	TAG H
ATOM	65	1HB	LYS	5	-2.505	-0.330	2.134	1.00	1.00	TAG H
ATOM	66	2HB	LYS	5	-2.571	-1.067	3.741	1.00	1.00	TAG H
ATOM	67	1HG	LYS	5	-0.944	-2.792	3.033	1.00	1.00	TAG H
ATOM	68	2HG	LYS	5	-0.899	-2.100	1.407	1.00	1.00	TAG H
ATOM	69	1HD	LYS	5	-0.075	0.069	2.368	1.00	1.00	TAG H
ATOM	70	2HD	LYS	5	-0.088	-0.654	3.983	1.00	1.00	TAG H
ATOM	71	1HE	LYS	5	1.559	-2.338	3.330	1.00	1.00	TAG H
ATOM	72	2HE	LYS	5	1.439	-1.880	1.627	1.00	1.00	TAG H
ATOM	73	H01	LYS	5	2.775	-0.480	3.812	1.00	1.00	TAG H
ATOM	74	H02	LYS	5	2.205	0.406	2.543	1.00	1.00	TAG H
ATOM	75	N	ARG	6	-5.577	-0.845	2.057	1.00	0.00	TAG N
ATOM	76	CA	ARG	6	-6.902	-0.399	2.479	1.00	0.00	TAG C
ATOM	77	C	ARG	6	-7.940	-1.465	2.217	1.00	0.00	TAG C
ATOM	78	O	ARG	6	-8.874	-1.621	3.012	1.00	0.00	TAG O
ATOM	79	CB	ARG	6	-7.246	0.923	1.735	1.00	0.00	TAG C
ATOM	80	CG	ARG	6	-8.605	1.573	2.120	1.00	0.00	TAG C
ATOM	81	CD	ARG	6	-8.810	2.933	1.433	1.00	0.00	TAG C
ATOM	82	NE	ARG	6	-10.126	3.507	1.839	1.00	0.00	TAG N
ATOM	83	CZ	ARG	6	-10.644	4.643	1.380	1.00	0.00	TAG C
ATOM	84	NH1	ARG	6	-10.054	5.401	0.500	1.00	0.00	TAG N
ATOM	85	NH2	ARG	6	-11.798	5.020	1.832	1.00	0.00	TAG N1+
ATOM	86	H	ARG	6	-5.180	-0.462	1.238	1.00	0.00	TAG H
ATOM	87	HA	ARG	6	-6.872	-0.223	3.571	1.00	0.00	TAG H
ATOM	88	2HB	ARG	6	-7.210	0.735	0.642	1.00	0.00	TAG H
ATOM	89	3HB	ARG	6	-6.438	1.661	1.913	1.00	0.00	TAG H
ATOM	90	2HG	ARG	6	-8.656	1.683	3.223	1.00	0.00	TAG H
ATOM	91	3HG	ARG	6	-9.441	0.896	1.849	1.00	0.00	TAG H
ATOM	92	2HD	ARG	6	-8.759	2.799	0.330	1.00	0.00	TAG H
ATOM	93	3HD	ARG	6	-7.977	3.616	1.706	1.00	0.00	TAG H
ATOM	94	HE	ARG	6	-10.720	3.032	2.526	1.00	0.00	TAG H
ATOM	95	1HH1	ARG	6	-9.148	5.047	0.183	1.00	0.00	TAG H
ATOM	96	2HH1	ARG	6	-10.517	6.260	0.198	1.00	0.00	TAG H
ATOM	97	H01	ARG	6	-12.055	5.901	1.410	1.00	0.00	TAG H
ATOM	98	H02	ARG	6	-11.748	5.129	2.835	1.00	0.00	TAG H
ATOM	99	H03	ARG	6	-12.492	4.323	1.604	1.00	0.00	TAG H
ATOM	100	N	HIS	7	-7.843	-2.183	1.115	1.00	1.00	TAG N
ATOM	101	CA	HIS	7	-8.765	-3.261	0.789	1.00	1.00	TAG C
ATOM	102	C	HIS	7	-8.423	-4.614	1.416	1.00	1.00	TAG C
ATOM	103	O	HIS	7	-9.291	-5.479	1.609	1.00	1.00	TAG O
ATOM	104	CB	HIS	7	-8.950	-3.377	-0.719	1.00	1.00	TAG C
ATOM	105	CG	HIS	7	-9.905	-2.370	-1.275	1.00	1.00	TAG C
ATOM	106	CD2	HIS	7	-9.496	-1.160	-1.793	1.00	1.00	TAG C
ATOM	107	ND1	HIS	7	-11.260	-2.376	-1.366	1.00	1.00	TAG N
ATOM	108	CE1	HIS	7	-11.638	-1.184	-1.928	1.00	1.00	TAG C
ATOM	109	NE2	HIS	7	-10.556	-0.463	-2.179	1.00	1.00	TAG N
ATOM	110	H	HIS	7	-7.124	-2.050	0.433	1.00	1.00	TAG H
ATOM	111	HA	HIS	7	-9.720	-2.975	1.251	1.00	1.00	TAG H
ATOM	112	1HB	HIS	7	-7.975	-3.257	-1.212	1.00	1.00	TAG H
ATOM	113	2HB	HIS	7	-9.311	-4.387	-0.961	1.00	1.00	TAG H
ATOM	114	HD1	HIS	7	-11.870	-3.115	-1.078	1.00	1.00	TAG H

ATOM	115	HD2	HIS	7	-8.451	-0.825	-1.874	1.00	1.00	TAG	H
ATOM	116	HE1	HIS	7	-12.673	-0.876	-2.136	1.00	1.00	TAG	H
ATOM	117	N	HIS	8	-7.140	-4.818	1.749	1.00	1.00	TAG	N
ATOM	118	CA	HIS	8	-6.701	-6.043	2.403	1.00	1.00	TAG	C
ATOM	119	C	HIS	8	-6.202	-5.865	3.838	1.00	1.00	TAG	C
ATOM	120	O	HIS	8	-5.499	-6.734	4.369	1.00	1.00	TAG	O
ATOM	121	CB	HIS	8	-5.680	-6.779	1.545	1.00	1.00	TAG	C
ATOM	122	CG	HIS	8	-6.300	-7.572	0.439	1.00	1.00	TAG	C
ATOM	123	CD2	HIS	8	-6.834	-8.819	0.423	1.00	1.00	TAG	C
ATOM	124	ND1	HIS	8	-6.461	-7.075	-0.836	1.00	1.00	TAG	N
ATOM	125	CE1	HIS	8	-7.067	-7.981	-1.592	1.00	1.00	TAG	C
ATOM	126	NE2	HIS	8	-7.302	-9.050	-0.845	1.00	1.00	TAG	N
ATOM	127	H	HIS	8	-6.408	-4.159	1.576	1.00	1.00	TAG	H
ATOM	128	HA	HIS	8	-7.605	-6.660	2.501	1.00	1.00	TAG	H
ATOM	129	1HB	HIS	8	-4.979	-6.049	1.114	1.00	1.00	TAG	H
ATOM	130	2HB	HIS	8	-5.091	-7.452	2.184	1.00	1.00	TAG	H
ATOM	131	HD2	HIS	8	-6.883	-9.518	1.272	1.00	1.00	TAG	H
ATOM	132	HE1	HIS	8	-7.330	-7.865	-2.654	1.00	1.00	TAG	H
ATOM	133	HE2	HIS	8	-7.747	-9.889	-1.155	1.00	1.00	TAG	H
ATOM	134	N	GLY	9	-6.750	-4.758	4.464	1.00	1.00	TAG	N
ATOM	135	CA	GLY	9	-6.546	-4.469	5.895	1.00	1.00	TAG	C
ATOM	136	C	GLY	9	-5.080	-4.514	6.347	1.00	1.00	TAG	C
ATOM	137	O	GLY	9	-4.779	-4.508	7.543	1.00	1.00	TAG	O
ATOM	138	H	GLY	9	-7.319	-4.084	3.992	1.00	1.00	TAG	H
ATOM	139	1HA	GLY	9	-6.954	-3.472	6.117	1.00	1.00	TAG	H
ATOM	140	2HA	GLY	9	-7.122	-5.192	6.489	1.00	1.00	TAG	H
ATOM	141	N	TYR	10	-4.197	-4.589	5.378	1.00	0.00	TAG	N
ATOM	142	CA	TYR	10	-2.767	-4.487	5.657	1.00	0.00	TAG	C
ATOM	143	C	TYR	10	-2.299	-3.055	5.561	1.00	0.00	TAG	C
ATOM	144	O	TYR	10	-1.190	-2.788	5.154	1.00	0.00	TAG	O
ATOM	145	CB	TYR	10	-1.941	-5.331	4.644	1.00	0.00	TAG	C
ATOM	146	CG	TYR	10	-2.133	-6.852	4.696	1.00	0.00	TAG	C
ATOM	147	CD1	TYR	10	-2.748	-7.454	5.799	1.00	0.00	TAG	C
ATOM	148	CD2	TYR	10	-1.701	-7.644	3.629	1.00	0.00	TAG	C
ATOM	149	CE1	TYR	10	-2.930	-8.834	5.828	1.00	0.00	TAG	C
ATOM	150	CE2	TYR	10	-1.884	-9.023	3.660	1.00	0.00	TAG	C
ATOM	151	CZ	TYR	10	-2.498	-9.617	4.760	1.00	0.00	TAG	C
ATOM	152	OH	TYR	10	-2.682	-10.970	4.792	1.00	0.00	TAG	O
ATOM	153	H	TYR	10	-4.506	-4.718	4.440	1.00	0.00	TAG	H
ATOM	154	HA	TYR	10	-2.577	-4.838	6.689	1.00	0.00	TAG	H
ATOM	155	2HB	TYR	10	-0.861	-5.127	4.783	1.00	0.00	TAG	H
ATOM	156	3HB	TYR	10	-2.141	-4.968	3.614	1.00	0.00	TAG	H
ATOM	157	1HD	TYR	10	-3.091	-6.854	6.629	1.00	0.00	TAG	H
ATOM	158	2HD	TYR	10	-1.233	-7.188	2.767	1.00	0.00	TAG	H
ATOM	159	1HE	TYR	10	-3.410	-9.301	6.675	1.00	0.00	TAG	H
ATOM	160	2HE	TYR	10	-1.550	-9.623	2.827	1.00	0.00	TAG	H
ATOM	161	HH	TYR	10	-2.330	-11.344	3.981	1.00	0.00	TAG	H
ATOM	162	N	LYS	11	-3.027	-2.110	5.873	1.00	1.00	TAG	N
ATOM	163	CA	LYS	11	-2.650	-0.704	5.792	1.00	1.00	TAG	C
ATOM	164	C	LYS	11	-2.427	-0.156	7.188	1.00	1.00	TAG	C
ATOM	165	O	LYS	11	-1.573	0.727	7.357	1.00	1.00	TAG	O

ATOM	166	CB	LYS	11	-3.743	0.091	5.077	1.00	1.00	TAG	C
ATOM	167	CG	LYS	11	-3.438	1.561	4.878	1.00	1.00	TAG	C
ATOM	168	CD	LYS	11	-4.246	2.090	3.707	1.00	1.00	TAG	C
ATOM	169	CE	LYS	11	-4.018	3.569	3.466	1.00	1.00	TAG	C
ATOM	170	NZ	LYS	11	-4.784	4.373	4.441	1.00	1.00	TAG	N
ATOM	171	H	LYS	11	-3.956	-2.238	6.220	1.00	1.00	TAG	H
ATOM	172	HA	LYS	11	-1.716	-0.610	5.219	1.00	1.00	TAG	H
ATOM	173	1HB	LYS	11	-3.925	-0.367	4.093	1.00	1.00	TAG	H
ATOM	174	2HB	LYS	11	-4.677	0.000	5.652	1.00	1.00	TAG	H
ATOM	175	1HG	LYS	11	-3.681	2.125	5.790	1.00	1.00	TAG	H
ATOM	176	2HG	LYS	11	-2.363	1.703	4.690	1.00	1.00	TAG	H
ATOM	177	1HD	LYS	11	-3.981	1.528	2.799	1.00	1.00	TAG	H
ATOM	178	2HD	LYS	11	-5.316	1.912	3.894	1.00	1.00	TAG	H
ATOM	179	1HE	LYS	11	-2.946	3.800	3.550	1.00	1.00	TAG	H
ATOM	180	2HE	LYS	11	-4.323	3.832	2.443	1.00	1.00	TAG	H
ATOM	181	H01	LYS	11	-4.885	5.316	4.095	1.00	1.00	TAG	H
ATOM	182	H02	LYS	11	-4.294	4.389	5.324	1.00	1.00	TAG	H
ATOM	183	N	ARG	12	-3.072	-0.562	8.165	1.00	1.00	TAG	N
ATOM	184	CA	ARG	12	-2.958	-0.077	9.530	1.00	1.00	TAG	C
ATOM	185	C	ARG	12	-1.449	-0.075	9.762	1.00	1.00	TAG	C
ATOM	186	O	ARG	12	-1.038	0.995	10.481	1.00	1.00	TAG	O
ATOM	187	CB	ARG	12	-3.677	-1.051	10.468	1.00	1.00	TAG	C
ATOM	188	CG	ARG	12	-3.679	-0.640	11.938	1.00	1.00	TAG	C
ATOM	189	CD	ARG	12	-4.692	-1.446	12.741	1.00	1.00	TAG	C
ATOM	190	NE	ARG	12	-4.688	-2.858	12.363	1.00	1.00	TAG	N
ATOM	191	CZ	ARG	12	-5.784	-3.565	12.089	1.00	1.00	TAG	C
ATOM	192	NH1	ARG	12	-6.985	-2.995	12.153	1.00	1.00	TAG	N
ATOM	193	NH2	ARG	12	-5.675	-4.840	11.727	1.00	1.00	TAG	N1+
ATOM	194	H	ARG	12	-3.752	-1.290	8.078	1.00	1.00	TAG	H
ATOM	195	HA	ARG	12	-3.407	0.911	9.708	1.00	1.00	TAG	H
ATOM	196	1HB	ARG	12	-4.719	-1.161	10.131	1.00	1.00	TAG	H
ATOM	197	2HB	ARG	12	-3.203	-2.040	10.378	1.00	1.00	TAG	H
ATOM	198	1HG	ARG	12	-2.675	-0.784	12.363	1.00	1.00	TAG	H
ATOM	199	2HG	ARG	12	-3.912	0.431	12.020	1.00	1.00	TAG	H
ATOM	200	1HD	ARG	12	-4.466	-1.353	13.814	1.00	1.00	TAG	H
ATOM	201	2HD	ARG	12	-5.698	-1.029	12.587	1.00	1.00	TAG	H
ATOM	202	HE	ARG	12	-3.805	-3.324	12.307	1.00	1.00	TAG	H
ATOM	203	1HH1	ARG	12	-7.069	-2.032	12.409	1.00	1.00	TAG	H
ATOM	204	2HH1	ARG	12	-7.805	-3.531	11.946	1.00	1.00	TAG	H
ATOM	205	H01	ARG	12	-5.797	-4.918	10.727	1.00	1.00	TAG	H
ATOM	206	H02	ARG	12	-6.383	-5.386	12.197	1.00	1.00	TAG	H
ATOM	207	H03	ARG	12	-4.761	-5.185	11.982	1.00	1.00	TAG	H
ATOM	208	N	LYS	13	-0.671	-0.938	9.575	1.00	1.00	TAG	N
ATOM	209	CA	LYS	13	0.716	-0.986	10.023	1.00	1.00	TAG	C
ATOM	210	C	LYS	13	1.311	0.416	10.040	1.00	1.00	TAG	C
ATOM	211	O	LYS	13	2.068	0.751	10.964	1.00	1.00	TAG	O
ATOM	212	CB	LYS	13	1.542	-1.898	9.111	1.00	1.00	TAG	C
ATOM	213	CG	LYS	13	1.248	-3.364	9.309	1.00	1.00	TAG	C
ATOM	214	CD	LYS	13	2.054	-4.226	8.361	1.00	1.00	TAG	C
ATOM	215	CE	LYS	13	1.693	-5.694	8.575	1.00	1.00	TAG	C
ATOM	216	NZ	LYS	13	2.258	-6.587	7.532	1.00	1.00	TAG	N

ATOM	217	H	LYS	13	-0.922	-1.757	9.058	1.00	1.00	TAG H
ATOM	218	HA	LYS	13	0.739	-1.395	11.043	1.00	1.00	TAG H
ATOM	219	1HB	LYS	13	1.347	-1.631	8.062	1.00	1.00	TAG H
ATOM	220	2HB	LYS	13	2.612	-1.718	9.295	1.00	1.00	TAG H
ATOM	221	1HG	LYS	13	1.474	-3.648	10.347	1.00	1.00	TAG H
ATOM	222	2HG	LYS	13	0.174	-3.549	9.152	1.00	1.00	TAG H
ATOM	223	1HD	LYS	13	1.851	-3.935	7.321	1.00	1.00	TAG H
ATOM	224	2HD	LYS	13	3.130	-4.073	8.533	1.00	1.00	TAG H
ATOM	225	1HE	LYS	13	2.057	-6.015	9.562	1.00	1.00	TAG H
ATOM	226	2HE	LYS	13	0.598	-5.798	8.585	1.00	1.00	TAG H
ATOM	227	H01	LYS	13	2.295	-6.095	6.651	1.00	1.00	TAG H
ATOM	228	H02	LYS	13	1.674	-7.406	7.437	1.00	1.00	TAG H
ATOM	229	N	PHE	14	1.037	1.255	9.107	1.00	1.00	TAG N
ATOM	230	CA	PHE	14	1.564	2.618	9.060	1.00	1.00	TAG C
ATOM	231	C	PHE	14	0.557	3.665	9.522	1.00	1.00	TAG C
ATOM	232	O	PHE	14	0.934	4.644	10.172	1.00	1.00	TAG O
ATOM	233	CB	PHE	14	2.114	2.949	7.672	1.00	1.00	TAG C
ATOM	234	CG	PHE	14	3.258	2.066	7.254	1.00	1.00	TAG C
ATOM	235	CD1	PHE	14	3.115	1.175	6.193	1.00	1.00	TAG C
ATOM	236	CD2	PHE	14	4.478	2.108	7.940	1.00	1.00	TAG C
ATOM	237	CE1	PHE	14	4.172	0.345	5.809	1.00	1.00	TAG C
ATOM	238	CE2	PHE	14	5.545	1.287	7.563	1.00	1.00	TAG C
ATOM	239	CZ	PHE	14	5.392	0.403	6.495	1.00	1.00	TAG C
ATOM	240	H	PHE	14	0.438	1.034	8.337	1.00	1.00	TAG H
ATOM	241	HA	PHE	14	2.397	2.654	9.779	1.00	1.00	TAG H
ATOM	242	1HB	PHE	14	1.303	2.859	6.934	1.00	1.00	TAG H
ATOM	243	2HB	PHE	14	2.446	3.998	7.658	1.00	1.00	TAG H
ATOM	244	HD1	PHE	14	2.159	1.125	5.652	1.00	1.00	TAG H
ATOM	245	HD2	PHE	14	4.599	2.799	8.787	1.00	1.00	TAG H
ATOM	246	HE1	PHE	14	4.046	-0.352	4.967	1.00	1.00	TAG H
ATOM	247	HE2	PHE	14	6.499	1.337	8.107	1.00	1.00	TAG H
ATOM	248	HZ	PHE	14	6.226	-0.247	6.194	1.00	1.00	TAG H
ATOM	249	N	HIS	15	-0.735	3.453	9.186	1.00	0.00	TAG N
ATOM	250	CA	HIS	15	-1.827	4.291	9.674	1.00	0.00	TAG C
ATOM	251	C	HIS	15	-1.856	4.319	11.183	1.00	0.00	TAG C
ATOM	252	O	HIS	15	-2.341	5.281	11.819	1.00	0.00	TAG O
ATOM	253	CB	HIS	15	-3.124	3.673	9.124	1.00	0.00	TAG C
ATOM	254	CG	HIS	15	-4.313	4.564	9.335	1.00	0.00	TAG C
ATOM	255	CD2	HIS	15	-4.811	5.399	8.344	1.00	0.00	TAG C
ATOM	256	ND1	HIS	15	-5.053	4.672	10.511	1.00	0.00	TAG N
ATOM	257	CE1	HIS	15	-5.960	5.589	10.129	1.00	0.00	TAG C
ATOM	258	NE2	HIS	15	-5.890	6.071	8.858	1.00	0.00	TAG N
ATOM	259	H	HIS	15	-0.969	2.628	8.529	1.00	0.00	TAG H
ATOM	260	HA	HIS	15	-1.629	5.324	9.342	1.00	0.00	TAG H
ATOM	261	2HB	HIS	15	-3.339	2.698	9.605	1.00	0.00	TAG H
ATOM	262	3HB	HIS	15	-3.056	3.456	8.037	1.00	0.00	TAG H
ATOM	263	2HD	HIS	15	-4.396	5.482	7.344	1.00	0.00	TAG H
ATOM	264	1HE	HIS	15	-6.702	5.894	10.856	1.00	0.00	TAG H
ATOM	265	2HE	HIS	15	-6.490	6.767	8.392	1.00	0.00	TAG H
ATOM	266	N	GLU	16	-1.321	3.297	11.850	1.00	1.00	TAG N
ATOM	267	CA	GLU	16	-1.253	3.214	13.307	1.00	1.00	TAG C

ATOM	268	C	GLU	16	-0.840	4.572	13.859	1.00	1.00	TAG C
ATOM	269	O	GLU	16	-1.663	5.246	14.501	1.00	1.00	TAG O
ATOM	270	CB	GLU	16	-0.233	2.164	13.732	1.00	1.00	TAG C
ATOM	271	CG	GLU	16	-0.161	1.948	15.235	1.00	1.00	TAG C
ATOM	272	CD	GLU	16	1.013	1.081	15.651	1.00	1.00	TAG C
ATOM	273	OE1	GLU	16	1.960	0.929	14.851	1.00	1.00	TAG O
ATOM	274	OE2	GLU	16	1.014	0.573	16.796	1.00	1.00	TAG O
ATOM	275	H	GLU	16	-0.937	2.496	11.391	1.00	1.00	TAG H
ATOM	276	HA	GLU	16	-2.240	2.928	13.699	1.00	1.00	TAG H
ATOM	277	1HB	GLU	16	-0.480	1.209	13.245	1.00	1.00	TAG H
ATOM	278	2HB	GLU	16	0.761	2.464	13.368	1.00	1.00	TAG H
ATOM	279	1HG	GLU	16	-0.086	2.923	15.738	1.00	1.00	TAG H
ATOM	280	2HG	GLU	16	-1.095	1.480	15.578	1.00	1.00	TAG H
ATOM	281	H01	GLU	16	1.919	0.429	17.082	1.00	1.00	TAG H
ATOM	282	N	LYS	17	0.383	5.004	13.637	1.00	1.00	TAG N
ATOM	283	CA	LYS	17	0.910	6.258	14.165	1.00	1.00	TAG C
ATOM	284	C	LYS	17	1.368	7.140	13.022	1.00	1.00	TAG C
ATOM	285	O	LYS	17	1.042	8.332	12.979	1.00	1.00	TAG O
ATOM	286	CB	LYS	17	2.073	5.977	15.119	1.00	1.00	TAG C
ATOM	287	CG	LYS	17	2.667	7.202	15.780	1.00	1.00	TAG C
ATOM	288	CD	LYS	17	3.351	6.794	17.072	1.00	1.00	TAG C
ATOM	289	CE	LYS	17	4.001	7.967	17.779	1.00	1.00	TAG C
ATOM	290	NZ	LYS	17	5.285	8.311	17.133	1.00	1.00	TAG N1+
ATOM	291	H	LYS	17	1.044	4.497	13.085	1.00	1.00	TAG H
ATOM	292	HA	LYS	17	0.117	6.779	14.723	1.00	1.00	TAG H
ATOM	293	1HB	LYS	17	1.726	5.287	15.903	1.00	1.00	TAG H
ATOM	294	2HB	LYS	17	2.866	5.457	14.562	1.00	1.00	TAG H
ATOM	295	1HG	LYS	17	3.390	7.683	15.105	1.00	1.00	TAG H
ATOM	296	2HG	LYS	17	1.878	7.941	15.985	1.00	1.00	TAG H
ATOM	297	1HD	LYS	17	2.614	6.329	17.743	1.00	1.00	TAG H
ATOM	298	2HD	LYS	17	4.114	6.031	16.855	1.00	1.00	TAG H
ATOM	299	1HE	LYS	17	3.328	8.837	17.757	1.00	1.00	TAG H
ATOM	300	2HE	LYS	17	4.171	7.719	18.837	1.00	1.00	TAG H
ATOM	301	1HZ	LYS	17	5.926	8.648	17.822	1.00	1.00	TAG H
ATOM	302	2HZ	LYS	17	5.666	7.498	16.694	1.00	1.00	TAG H
ATOM	303	3HZ	LYS	17	5.132	9.021	16.444	1.00	1.00	TAG H
ATOM	304	N	HIS	18	1.949	6.568	12.003	1.00	1.00	TAG N
ATOM	305	CA	HIS	18	2.356	7.275	10.766	1.00	1.00	TAG C
ATOM	306	C	HIS	18	1.149	7.935	10.141	1.00	1.00	TAG C
ATOM	307	O	HIS	18	1.248	9.078	9.626	1.00	1.00	TAG O
ATOM	308	CB	HIS	18	2.943	6.114	9.780	1.00	1.00	TAG C
ATOM	309	CG	HIS	18	3.242	6.821	8.477	1.00	1.00	TAG C
ATOM	310	CD2	HIS	18	2.592	6.586	7.273	1.00	1.00	TAG C
ATOM	311	ND1	HIS	18	4.208	7.705	8.171	1.00	1.00	TAG N
ATOM	312	CE1	HIS	18	4.199	8.070	6.916	1.00	1.00	TAG C
ATOM	313	NE2	HIS	18	3.159	7.437	6.373	1.00	1.00	TAG N
ATOM	314	H	HIS	18	2.164	5.592	11.986	1.00	1.00	TAG H
ATOM	315	HA	HIS	18	3.102	8.060	10.958	1.00	1.00	TAG H
ATOM	316	1HB	HIS	18	3.849	5.654	10.202	1.00	1.00	TAG H
ATOM	317	2HB	HIS	18	2.210	5.306	9.636	1.00	1.00	TAG H
ATOM	318	HD1	HIS	18	4.868	8.049	8.839	1.00	1.00	TAG H

ATOM	319	HD2	HIS	18	1.785	5.863	7.085	1.00	1.00	TAG	H
ATOM	320	HE1	HIS	18	4.900	8.754	6.415	1.00	1.00	TAG	H
ATOM	321	N	HIS	19	0.070	7.219	9.918	1.00	1.00	TAG	N
ATOM	322	CA	HIS	19	-1.160	7.780	9.377	1.00	1.00	TAG	C
ATOM	323	C	HIS	19	-1.754	8.934	10.186	1.00	1.00	TAG	C
ATOM	324	O	HIS	19	-2.264	9.975	9.753	1.00	1.00	TAG	O
ATOM	325	CB	HIS	19	-2.189	6.686	9.126	1.00	1.00	TAG	C
ATOM	326	CG	HIS	19	-1.955	5.933	7.856	1.00	1.00	TAG	C
ATOM	327	CD2	HIS	19	-1.240	4.756	7.808	1.00	1.00	TAG	C
ATOM	328	ND1	HIS	19	-2.309	6.206	6.574	1.00	1.00	TAG	N
ATOM	329	CE1	HIS	19	-1.809	5.202	5.787	1.00	1.00	TAG	C
ATOM	330	NE2	HIS	19	-1.164	4.335	6.553	1.00	1.00	TAG	N
ATOM	331	H	HIS	19	0.016	6.238	10.104	1.00	1.00	TAG	H
ATOM	332	HA	HIS	19	-0.874	8.236	8.418	1.00	1.00	TAG	H
ATOM	333	1HB	HIS	19	-2.177	5.980	9.969	1.00	1.00	TAG	H
ATOM	334	2HB	HIS	19	-3.192	7.136	9.097	1.00	1.00	TAG	H
ATOM	335	HD2	HIS	19	-0.800	4.245	8.677	1.00	1.00	TAG	H
ATOM	336	HE1	HIS	19	-1.924	5.128	4.696	1.00	1.00	TAG	H
ATOM	337	HE2	HIS	19	-0.700	3.506	6.239	1.00	1.00	TAG	H
ATOM	338	N	SER	20	-1.670	8.706	11.570	1.00	1.00	TAG	N
ATOM	339	CA	SER	20	-2.008	9.759	12.530	1.00	1.00	TAG	C
ATOM	340	C	SER	20	-1.131	10.999	12.432	1.00	1.00	TAG	C
ATOM	341	CB	SER	20	-1.907	9.202	13.953	1.00	1.00	TAG	C
ATOM	342	OG	SER	20	-2.083	10.236	14.904	1.00	1.00	TAG	O
ATOM	343	O01	SER	20	-1.378	11.806	13.586	1.00	1.00	TAG	O
ATOM	344	H	SER	20	-1.384	7.841	11.982	1.00	1.00	TAG	H
ATOM	345	HA	SER	20	-3.034	10.072	12.285	1.00	1.00	TAG	H
ATOM	346	1HB	SER	20	-2.668	8.423	14.103	1.00	1.00	TAG	H
ATOM	347	2HB	SER	20	-0.926	8.726	14.098	1.00	1.00	TAG	H
ATOM	348	HG	SER	20	-2.740	10.904	14.553	1.00	1.00	TAG	H
ATOM	349	N	HIS	21	0.225	10.764	12.360	1.00	1.00	TAG	N
ATOM	350	CA	HIS	21	1.191	11.827	12.119	1.00	1.00	TAG	C
ATOM	351	C	HIS	21	0.582	13.177	11.736	1.00	1.00	TAG	C
ATOM	352	O	HIS	21	0.840	14.286	12.217	1.00	1.00	TAG	O
ATOM	353	CB	HIS	21	2.244	11.381	11.112	1.00	1.00	TAG	C
ATOM	354	CG	HIS	21	3.312	10.526	11.712	1.00	1.00	TAG	C
ATOM	355	CD2	HIS	21	3.257	9.149	11.702	1.00	1.00	TAG	C
ATOM	356	ND1	HIS	21	4.451	10.848	12.376	1.00	1.00	TAG	N
ATOM	357	CE1	HIS	21	5.055	9.676	12.750	1.00	1.00	TAG	C
ATOM	358	NE2	HIS	21	4.316	8.657	12.332	1.00	1.00	TAG	N
ATOM	359	H	HIS	21	0.635	9.858	12.467	1.00	1.00	TAG	H
ATOM	360	HA	HIS	21	1.673	12.009	13.091	1.00	1.00	TAG	H
ATOM	361	1HB	HIS	21	1.752	10.826	10.300	1.00	1.00	TAG	H
ATOM	362	2HB	HIS	21	2.708	12.271	10.660	1.00	1.00	TAG	H
ATOM	363	HD1	HIS	21	4.789	11.772	12.559	1.00	1.00	TAG	H
ATOM	364	HD2	HIS	21	2.457	8.549	11.243	1.00	1.00	TAG	H
ATOM	365	HE1	HIS	21	6.001	9.593	13.306	1.00	1.00	TAG	H
ATOM	366	N	ARG	22	-0.356	13.095	10.733	1.00	1.00	TAG	N
ATOM	367	CA	ARG	22	-1.205	14.216	10.365	1.00	1.00	TAG	C
ATOM	368	C	ARG	22	-1.900	14.557	11.681	1.00	1.00	TAG	C
ATOM	369	O	ARG	22	-2.179	15.748	11.886	1.00	1.00	TAG	O

ATOM	370	CB	ARG	22	-2.203	13.759	9.296	1.00	1.00	TAG	C
ATOM	371	CG	ARG	22	-3.132	14.853	8.779	1.00	1.00	TAG	C
ATOM	372	CD	ARG	22	-3.835	14.427	7.496	1.00	1.00	TAG	C
ATOM	373	NE	ARG	22	-4.282	13.037	7.556	1.00	1.00	TAG	N
ATOM	374	CZ	ARG	22	-4.065	12.136	6.599	1.00	1.00	TAG	C
ATOM	375	NH1	ARG	22	-3.407	12.475	5.492	1.00	1.00	TAG	N
ATOM	376	NH2	ARG	22	-4.489	10.885	6.758	1.00	1.00	TAG	N1+
ATOM	377	H	ARG	22	-0.517	12.269	10.195	1.00	1.00	TAG	H
ATOM	378	HA	ARG	22	-0.672	15.080	9.939	1.00	1.00	TAG	H
ATOM	379	1HB	ARG	22	-1.642	13.342	8.446	1.00	1.00	TAG	H
ATOM	380	2HB	ARG	22	-2.814	12.944	9.710	1.00	1.00	TAG	H
ATOM	381	1HG	ARG	22	-3.883	15.093	9.547	1.00	1.00	TAG	H
ATOM	382	2HG	ARG	22	-2.555	15.771	8.595	1.00	1.00	TAG	H
ATOM	383	1HD	ARG	22	-4.700	15.084	7.316	1.00	1.00	TAG	H
ATOM	384	2HD	ARG	22	-3.151	14.556	6.643	1.00	1.00	TAG	H
ATOM	385	HE	ARG	22	-4.785	12.743	8.369	1.00	1.00	TAG	H
ATOM	386	1HH1	ARG	22	-3.072	13.410	5.375	1.00	1.00	TAG	H
ATOM	387	2HH1	ARG	22	-3.247	11.794	4.777	1.00	1.00	TAG	H
ATOM	388	H01	ARG	22	-4.579	10.682	7.743	1.00	1.00	TAG	H
ATOM	389	H02	ARG	22	-3.825	10.248	6.342	1.00	1.00	TAG	H
ATOM	390	H03	ARG	22	-5.387	10.775	6.309	1.00	1.00	TAG	H
ATOM	391	N	GLY	23	-2.200	13.765	12.538	1.00	1.00	TAG	N
ATOM	392	CA	GLY	23	-2.753	14.033	13.861	1.00	1.00	TAG	C
ATOM	393	C	GLY	23	-1.981	15.144	14.573	1.00	1.00	TAG	C
ATOM	394	O	GLY	23	-2.573	16.131	15.016	1.00	1.00	TAG	O
ATOM	395	1HA	GLY	23	-3.810	14.320	13.768	1.00	1.00	TAG	H
ATOM	396	2HA	GLY	23	-2.720	13.116	14.467	1.00	1.00	TAG	H
ATOM	397	H01	GLY	23	-2.050	12.792	12.312	1.00	1.00	TAG	H
ATOM	398	N	TYR	24	-0.690	15.014	14.678	1.00	0.00	TAG	N
ATOM	399	CA	TYR	24	0.202	15.874	15.451	1.00	0.00	TAG	C
ATOM	400	C	TYR	24	-0.332	17.284	15.519	1.00	0.00	TAG	C
ATOM	401	O	TYR	24	-0.844	17.868	14.582	1.00	0.00	TAG	O
ATOM	402	CB	TYR	24	1.618	15.927	14.807	1.00	0.00	TAG	C
ATOM	403	CG	TYR	24	2.667	16.789	15.520	1.00	0.00	TAG	C
ATOM	404	CD1	TYR	24	3.305	16.325	16.674	1.00	0.00	TAG	C
ATOM	405	CD2	TYR	24	2.997	18.047	15.008	1.00	0.00	TAG	C
ATOM	406	CE1	TYR	24	4.266	17.110	17.304	1.00	0.00	TAG	C
ATOM	407	CE2	TYR	24	3.958	18.831	15.639	1.00	0.00	TAG	C
ATOM	408	CZ	TYR	24	4.592	18.362	16.787	1.00	0.00	TAG	C
ATOM	409	OH	TYR	24	5.538	19.128	17.407	1.00	0.00	TAG	O
ATOM	410	OXT	TYR	24	-0.241	18.006	16.762	0.00	0.00	TAG	O
ATOM	411	H	TYR	24	-0.251	14.220	14.161	1.00	0.00	TAG	H
ATOM	412	HA	TYR	24	0.268	15.486	16.485	1.00	0.00	TAG	H
ATOM	413	2HB	TYR	24	1.539	16.294	13.764	1.00	0.00	TAG	H
ATOM	414	3HB	TYR	24	2.006	14.894	14.688	1.00	0.00	TAG	H
ATOM	415	1HD	TYR	24	3.063	15.352	17.080	1.00	0.00	TAG	H
ATOM	416	2HD	TYR	24	2.516	18.413	14.110	1.00	0.00	TAG	H
ATOM	417	1HE	TYR	24	4.765	16.751	18.192	1.00	0.00	TAG	H
ATOM	418	2HE	TYR	24	4.208	19.798	15.230	1.00	0.00	TAG	H
ATOM	419	HH	TYR	24	5.634	19.947	16.917	1.00	0.00	TAG	H
ATOM	420	H01	TYR	24	0.298	17.509	17.382	0.00	0.00	TAG	H

END