

# Glycerol Dehydration by the $B_{12}$ -independent Enzyme May Not Involve the Migration of a Hydroxyl Group – A Computational Study.

Supplementary materials

Mikolaj Feliks,<sup>1</sup> G. Matthias Ullmann<sup>1,†</sup>

<sup>1</sup>) Computational Biochemistry Group, University of Bayreuth, Universitätsstr. 30,  
BGI, 95447 Bayreuth, Germany

<sup>†</sup>) to whom correspondence should be addressed;

e-mail: Matthias.Ullmann@uni-bayreuth.de

Table 1: Geometries of the cluster model for all intermediates and transition states discussed in the text. The geometries are in the PDB format. The last two columns, occupancy and temperature factor, are Mulliken atomic charge and Mulliken atomic spin density, respectively. Atoms where the truncation has been done are "h" hydrogens. Charges and spin densities were obtained from single-point calculations at the B3LYP/6-311+G(2d,2p) level on top of geometries optimized at the B3LYP/6-31G(d) level.

Atoms frozen during the geometry optimizations: 4, 8, 21, 25, 33, 40, 50, 55, 62, 84, (88)

TITLE	Sub								
ATOM	1	h	VAL	162	22.635	18.910	25.050	0.098	0.00
ATOM	2	C	VAL	162	22.762	19.891	25.542	0.300	0.00
ATOM	3	O	VAL	162	23.715	20.616	25.290	-0.503	0.00
ATOM	4	N	GLY	163	21.765	20.175	26.409	-0.195	0.00
ATOM	5	H	GLY	163	21.034	19.507	26.605	0.175	0.00
ATOM	6	h	GLY	163	21.798	21.030	26.951	0.192	0.00
ATOM	7	h	HIP	164	22.593	23.227	23.375	0.112	0.00
ATOM	8	CB	HIP	164	23.623	23.237	22.997	-0.548	0.00
ATOM	9	HB2	HIP	164	23.900	22.203	22.762	0.121	0.00
ATOM	10	HB3	HIP	164	23.636	23.818	22.071	0.127	0.00
ATOM	11	CG	HIP	164	24.561	23.844	23.984	0.111	0.00
ATOM	12	ND1	HIP	164	24.889	23.235	25.190	-0.248	0.00
ATOM	13	HD1	HIP	164	24.555	22.312	25.471	0.387	0.00
ATOM	14	CE1	HIP	164	25.713	24.033	25.888	0.110	0.00
ATOM	15	HE1	HIP	164	26.188	23.788	26.833	0.228	0.00
ATOM	16	NE2	HIP	164	25.915	25.132	25.165	-0.263	0.00
ATOM	17	HE2	HIP	164	26.475	25.971	25.467	0.555	0.00
ATOM	18	CD2	HIP	164	25.223	25.039	23.978	-0.232	0.00
ATOM	19	HD2	HIP	164	25.275	25.821	23.238	0.207	0.00
ATOM	20	h	HIE	281	22.539	25.167	30.199	0.081	0.00
ATOM	21	CB	HIE	281	22.848	26.185	29.924	-0.553	0.00
ATOM	22	HB2	HIE	281	22.292	26.484	29.030	0.091	0.00
ATOM	23	HB3	HIE	281	22.544	26.842	30.749	0.096	0.00
ATOM	24	CG	HIE	281	24.333	26.270	29.661	-0.217	0.00
ATOM	25	ND1	HIE	281	25.331	25.972	30.589	-0.345	0.00

ATOM	26	CE1	HIE	281	26.464	26.184	29.952	0.194	0.00
ATOM	27	HE1	HIE	281	27.454	26.046	30.367	0.108	0.00
ATOM	28	NE2	HIE	281	26.265	26.599	28.670	-0.270	0.00
ATOM	29	HE2	HIE	281	26.953	26.835	27.952	0.311	0.00
ATOM	30	CD2	HIE	281	24.903	26.657	28.472	0.266	0.00
ATOM	31	HD2	HIE	281	24.476	26.968	27.527	0.185	0.00
ATOM	32	h	SER	282	21.918	26.783	25.635	0.098	0.00
ATOM	33	CB	SER	282	22.623	27.103	24.858	-0.102	0.00
ATOM	34	HB2	SER	282	22.734	26.273	24.141	0.094	0.00
ATOM	35	HB3	SER	282	22.169	27.953	24.323	0.110	0.00
ATOM	36	OG	SER	282	23.831	27.445	25.494	-0.425	0.00
ATOM	37	HG	SER	282	24.488	27.768	24.832	0.316	0.00
ATOM	38	h	GLY	432	23.368	30.565	23.015	0.078	0.00
ATOM	39	C	GLY	432	23.751	31.604	22.951	0.249	0.00
ATOM	40	O	GLY	432	23.020	32.582	23.042	-0.458	0.00
ATOM	41	N	CYX	433	25.099	31.638	22.789	-0.220	0.00
ATOM	42	H	CYX	433	25.554	30.800	22.404	0.275	0.00
ATOM	43	CA	CYX	433	25.748	32.913	22.538	0.114	0.03
ATOM	44	HA	CYX	433	25.298	33.659	23.194	0.135	0.00
ATOM	45	CB	CYX	433	27.266	32.828	22.782	-0.069	-0.07
ATOM	46	HB2	CYX	433	27.677	31.940	22.280	0.121	0.03
ATOM	47	HB3	CYX	433	27.761	33.698	22.334	0.108	0.02
ATOM	48	SG	CYX	433	27.785	32.730	24.520	-0.208	0.97
ATOM	49	C	CYX	433	25.516	33.457	21.108	0.287	0.00
ATOM	50	O	CYX	433	25.274	34.645	20.933	-0.526	0.01
ATOM	51	N	VAL	434	25.656	32.549	20.108	-0.436	0.00
ATOM	52	H	VAL	434	25.932	31.574	20.269	0.293	0.00
ATOM	53	h	VAL	434	25.566	32.894	19.163	0.184	0.00
ATOM	54	h	GLU	435	26.140	29.015	18.506	0.083	0.00
ATOM	55	CG	GLU	435	26.884	28.523	19.144	-0.452	0.00
ATOM	56	HG2	GLU	435	26.932	27.460	18.898	0.102	0.00
ATOM	57	HG3	GLU	435	27.853	28.989	18.933	0.109	0.00

ATOM	58	CD	GLU	435	26.524	28.739	20.623	0.755	0.00
ATOM	59	OE1	GLU	435	26.345	27.718	21.346	-0.629	0.00
ATOM	60	OE2	GLU	435	26.439	29.941	21.017	-0.752	0.00
ATOM	61	h	ASP	447	29.210	25.176	22.757	0.117	0.00
ATOM	62	CB	ASP	447	28.913	25.620	23.710	-0.221	0.00
ATOM	63	HB2	ASP	447	28.159	26.387	23.510	0.128	0.00
ATOM	64	HB3	ASP	447	28.453	24.847	24.334	0.100	0.00
ATOM	65	CG	ASP	447	30.134	26.205	24.436	0.442	0.00
ATOM	66	OD1	ASP	447	31.256	26.169	23.913	-0.566	0.00
ATOM	67	OD2	ASP	447	29.899	26.697	25.614	-0.809	0.00
ATOM	68	O1	GOL	788	26.002	28.035	23.923	-0.410	0.00
ATOM	69	HO1	GOL	788	26.106	28.030	22.912	0.352	0.00
ATOM	70	C1	GOL	788	27.011	28.863	24.492	-0.164	-0.01
ATOM	71	H11	GOL	788	27.965	28.720	23.972	0.152	0.00
ATOM	72	H12	GOL	788	26.742	29.926	24.405	0.147	0.02
ATOM	73	C2	GOL	788	27.182	28.542	25.973	0.097	0.00
ATOM	74	O2	GOL	788	27.473	27.136	26.183	-0.597	0.00
ATOM	75	HO2	GOL	788	28.453	26.948	25.894	0.480	0.00
ATOM	76	H2	GOL	788	26.230	28.721	26.487	0.156	0.00
ATOM	77	C3	GOL	788	28.258	29.417	26.636	-0.416	0.00
ATOM	78	H31	GOL	788	27.891	30.449	26.670	0.127	0.00
ATOM	79	H32	GOL	788	28.376	29.076	27.680	0.086	0.00
ATOM	80	O3	GOL	788	29.492	29.457	25.950	-0.348	0.00
ATOM	81	HO3	GOL	788	29.855	28.546	25.893	0.274	0.00
ATOM	82	h	GLN	549	31.242	27.744	20.722	0.086	0.00
ATOM	83	CD	GLN	549	31.748	26.871	20.267	0.230	0.00
ATOM	84	OE1	GLN	549	32.132	26.869	19.103	-0.517	0.00
ATOM	85	NE2	GLN	549	31.860	25.845	21.141	-0.315	0.00
ATOM	86	HE21	GLN	549	32.364	25.024	20.831	0.155	0.00
ATOM	87	HE22	GLN	549	31.615	25.940	22.136	0.327	0.00
ATOM	88	CB	ASN	156	30.277	22.588	28.275	-0.526	0.00
ATOM	89	h	ASN	156	30.300	22.457	29.363	0.110	0.00

ATOM	90	HB2	ASN	156	31.208	23.070	27.963	0.093	0.00
ATOM	91	CG	ASN	156	29.036	23.392	27.906	0.463	0.00
ATOM	92	OD1	ASN	156	27.910	22.889	27.935	-0.466	0.00
ATOM	93	ND2	ASN	156	29.245	24.700	27.611	-0.239	0.00
ATOM	94	HD21	ASN	156	28.450	25.243	27.304	0.246	0.00
ATOM	95	HD22	ASN	156	30.130	25.075	27.293	0.204	0.00
ATOM	96	HB3	ASN	156	30.206	21.596	27.821	0.108	0.00

TITLE TS1

ATOM	1	h	VAL	162	22.623	18.946	25.010	0.100	0.00
ATOM	2	C	VAL	162	22.751	19.915	25.522	0.303	0.00
ATOM	3	O	VAL	162	23.696	20.652	25.273	-0.509	0.00
ATOM	4	N	GLY	163	21.765	20.175	26.409	-0.192	0.00
ATOM	5	H	GLY	163	21.044	19.496	26.605	0.175	0.00
ATOM	6	h	GLY	163	21.804	21.015	26.973	0.192	0.00
ATOM	7	h	HIP	164	22.597	23.202	23.384	0.115	0.00
ATOM	8	CB	HIP	164	23.623	23.237	22.997	-0.544	0.00
ATOM	9	HB2	HIP	164	23.925	22.211	22.762	0.122	0.00
ATOM	10	HB3	HIP	164	23.615	23.817	22.071	0.126	0.00
ATOM	11	CG	HIP	164	24.556	23.866	23.981	0.102	0.00
ATOM	12	ND1	HIP	164	24.895	23.253	25.181	-0.243	0.00
ATOM	13	HD1	HIP	164	24.564	22.326	25.459	0.388	0.00
ATOM	14	CE1	HIP	164	25.711	24.051	25.885	0.107	0.00
ATOM	15	HE1	HIP	164	26.185	23.798	26.829	0.224	0.00
ATOM	16	NE2	HIP	164	25.902	25.159	25.171	-0.187	0.00
ATOM	17	HE2	HIP	164	26.450	26.002	25.481	0.500	0.00
ATOM	18	CD2	HIP	164	25.205	25.069	23.985	-0.234	0.00
ATOM	19	HD2	HIP	164	25.247	25.858	23.249	0.201	0.00
ATOM	20	h	HIE	281	22.548	25.157	30.170	0.082	0.00
ATOM	21	CB	HIE	281	22.848	26.185	29.924	-0.553	0.00
ATOM	22	HB2	HIE	281	22.291	26.503	29.037	0.090	0.00
ATOM	23	HB3	HIE	281	22.537	26.817	30.765	0.098	0.00

ATOM	24	CG	HIE	281	24.332	26.290	29.666	-0.179	0.00
ATOM	25	ND1	HIE	281	25.331	25.972	30.589	-0.342	0.00
ATOM	26	CE1	HIE	281	26.463	26.208	29.959	0.187	0.00
ATOM	27	HE1	HIE	281	27.454	26.063	30.369	0.112	0.00
ATOM	28	NE2	HIE	281	26.264	26.656	28.687	-0.272	0.00
ATOM	29	HE2	HIE	281	26.949	26.915	27.974	0.306	0.00
ATOM	30	CD2	HIE	281	24.901	26.713	28.490	0.270	0.00
ATOM	31	HD2	HIE	281	24.474	27.049	27.553	0.182	0.00
ATOM	32	h	SER	282	22.026	26.588	25.618	0.101	0.00
ATOM	33	CB	SER	282	22.623	27.103	24.858	-0.099	0.00
ATOM	34	HB2	SER	282	22.711	26.436	23.985	0.092	0.00
ATOM	35	HB3	SER	282	22.074	28.004	24.547	0.120	0.00
ATOM	36	OG	SER	282	23.873	27.406	25.443	-0.434	0.00
ATOM	37	HG	SER	282	24.436	27.917	24.825	0.312	0.00
ATOM	38	h	GLY	432	23.262	30.591	22.623	0.060	0.00
ATOM	39	C	GLY	432	23.691	31.611	22.721	0.280	0.00
ATOM	40	O	GLY	432	23.020	32.582	23.042	-0.460	0.00
ATOM	41	N	CYX	433	25.013	31.633	22.459	-0.247	0.00
ATOM	42	H	CYX	433	25.501	30.810	22.095	0.259	0.00
ATOM	43	CA	CYX	433	25.764	32.876	22.516	0.273	0.01
ATOM	44	HA	CYX	433	25.207	33.561	23.156	0.144	0.00
ATOM	45	CB	CYX	433	27.163	32.620	23.096	-0.358	-0.01
ATOM	46	HB2	CYX	433	27.707	31.887	22.495	0.120	0.01
ATOM	47	HB3	CYX	433	27.741	33.550	23.088	0.102	0.01
ATOM	48	SG	CYX	433	27.123	32.044	24.843	-0.226	0.33
ATOM	49	C	CYX	433	25.792	33.550	21.124	0.259	0.00
ATOM	50	O	CYX	433	25.274	34.645	20.933	-0.517	0.00
ATOM	51	N	VAL	434	26.435	32.840	20.149	-0.429	0.00
ATOM	52	H	VAL	434	26.639	31.844	20.266	0.280	0.00
ATOM	53	h	VAL	434	26.335	33.197	19.208	0.185	0.00
ATOM	54	h	GLU	435	26.163	29.083	18.538	0.090	0.00
ATOM	55	CG	GLU	435	26.884	28.523	19.144	-0.456	0.00

ATOM	56	HG2	GLU	435	26.779	27.454	18.945	0.097	0.00
ATOM	57	HG3	GLU	435	27.885	28.852	18.847	0.112	0.00
ATOM	58	CD	GLU	435	26.662	28.848	20.627	0.739	0.00
ATOM	59	OE1	GLU	435	26.386	27.895	21.421	-0.642	0.00
ATOM	60	OE2	GLU	435	26.763	30.059	20.964	-0.708	0.00
ATOM	61	h	ASP	447	29.206	25.179	22.754	0.117	0.00
ATOM	62	CB	ASP	447	28.913	25.620	23.710	-0.196	0.00
ATOM	63	HB2	ASP	447	28.227	26.448	23.505	0.133	0.00
ATOM	64	HB3	ASP	447	28.377	24.870	24.300	0.103	0.00
ATOM	65	CG	ASP	447	30.147	26.103	24.483	0.420	0.00
ATOM	66	OD1	ASP	447	31.270	26.071	23.964	-0.549	0.00
ATOM	67	OD2	ASP	447	29.910	26.519	25.691	-0.816	0.00
ATOM	68	O1	GOL	788	26.082	28.449	23.908	-0.315	0.14
ATOM	69	H01	GOL	788	26.220	28.337	22.881	0.349	0.00
ATOM	70	C1	GOL	788	27.183	28.997	24.500	-0.360	0.58
ATOM	71	H11	GOL	788	28.094	28.967	23.898	0.181	-0.02
ATOM	72	H12	GOL	788	27.079	30.530	24.601	0.284	-0.06
ATOM	73	C2	GOL	788	27.343	28.640	25.962	-0.053	-0.01
ATOM	74	O2	GOL	788	27.473	27.192	26.151	-0.491	0.03
ATOM	75	H02	GOL	788	28.437	26.915	25.917	0.445	0.00
ATOM	76	H2	GOL	788	26.421	28.906	26.493	0.159	0.00
ATOM	77	C3	GOL	788	28.528	29.354	26.638	-0.280	0.00
ATOM	78	H31	GOL	788	28.297	30.420	26.719	0.143	0.00
ATOM	79	H32	GOL	788	28.611	28.954	27.664	0.087	0.00
ATOM	80	O3	GOL	788	29.746	29.264	25.934	-0.371	0.00
ATOM	81	H03	GOL	788	30.035	28.324	25.919	0.281	0.00
ATOM	82	h	GLN	549	31.260	27.763	20.722	0.088	0.00
ATOM	83	CD	GLN	549	31.757	26.882	20.270	0.228	0.00
ATOM	84	OE1	GLN	549	32.132	26.869	19.103	-0.516	0.00
ATOM	85	NE2	GLN	549	31.872	25.862	21.151	-0.309	0.00
ATOM	86	HE21	GLN	549	32.366	25.036	20.841	0.155	0.00
ATOM	87	HE22	GLN	549	31.628	25.953	22.146	0.318	0.00

ATOM	88	CB	ASN	156	30.277	22.588	28.275	-0.511	0.00
ATOM	89	h	ASN	156	30.393	22.531	29.363	0.111	0.00
ATOM	90	HB2	ASN	156	31.167	23.071	27.860	0.098	0.00
ATOM	91	CG	ASN	156	28.993	23.348	27.959	0.452	0.00
ATOM	92	OD1	ASN	156	27.887	22.802	27.996	-0.470	0.00
ATOM	93	ND2	ASN	156	29.141	24.676	27.715	-0.247	0.00
ATOM	94	HD21	ASN	156	28.300	25.178	27.463	0.227	0.00
ATOM	95	HD22	ASN	156	29.976	25.088	27.308	0.218	0.00
ATOM	96	HB3	ASN	156	30.194	21.569	27.890	0.108	0.00

TITLE In1

ATOM	1	h	VAL	162	22.536	18.887	25.013	0.099	0.00
ATOM	2	C	VAL	162	22.718	19.858	25.506	0.304	0.00
ATOM	3	O	VAL	162	23.690	20.547	25.224	-0.505	0.00
ATOM	4	N	GLY	163	21.765	20.175	26.409	-0.195	0.00
ATOM	5	H	GLY	163	21.016	19.535	26.628	0.175	0.00
ATOM	6	h	GLY	163	21.851	21.022	26.957	0.192	0.00
ATOM	7	h	HIP	164	22.593	23.209	23.373	0.114	0.00
ATOM	8	CB	HIP	164	23.623	23.237	22.997	-0.562	0.00
ATOM	9	HB2	HIP	164	23.904	22.214	22.722	0.122	0.00
ATOM	10	HB3	HIP	164	23.636	23.853	22.094	0.128	0.00
ATOM	11	CG	HIP	164	24.560	23.807	24.009	0.108	0.00
ATOM	12	ND1	HIP	164	24.891	23.146	25.187	-0.265	0.00
ATOM	13	HD1	HIP	164	24.551	22.213	25.431	0.391	0.00
ATOM	14	CE1	HIP	164	25.720	23.908	25.916	0.128	0.00
ATOM	15	HE1	HIP	164	26.197	23.621	26.850	0.224	0.00
ATOM	16	NE2	HIP	164	25.923	25.038	25.242	-0.203	0.00
ATOM	17	HE2	HIP	164	26.496	25.862	25.572	0.519	0.00
ATOM	18	CD2	HIP	164	25.224	24.999	24.056	-0.246	0.00
ATOM	19	HD2	HIP	164	25.276	25.814	23.351	0.194	0.00
ATOM	20	h	HIE	281	22.546	25.162	30.187	0.082	0.00
ATOM	21	CB	HIE	281	22.848	26.185	29.924	-0.553	0.00



ATOM	22	HB2	HIE	281	22.292	26.489	29.031	0.090	0.00
ATOM	23	HB3	HIE	281	22.537	26.832	30.755	0.097	0.00
ATOM	24	CG	HIE	281	24.333	26.283	29.665	-0.159	0.01
ATOM	25	ND1	HIE	281	25.331	25.972	30.589	-0.344	0.00
ATOM	26	CE1	HIE	281	26.464	26.200	29.959	0.180	0.00
ATOM	27	HE1	HIE	281	27.454	26.056	30.373	0.111	0.00
ATOM	28	NE2	HIE	281	26.267	26.639	28.686	-0.276	0.00
ATOM	29	HE2	HIE	281	26.955	26.867	27.965	0.307	0.00
ATOM	30	CD2	HIE	281	24.904	26.694	28.485	0.267	0.00
ATOM	31	HD2	HIE	281	24.479	27.017	27.544	0.181	0.00
ATOM	32	h	SER	282	21.962	26.716	25.641	0.102	0.00
ATOM	33	CB	SER	282	22.623	27.103	24.858	-0.103	0.00
ATOM	34	HB2	SER	282	22.708	26.332	24.074	0.092	0.00
ATOM	35	HB3	SER	282	22.140	27.987	24.415	0.116	0.00
ATOM	36	OG	SER	282	23.860	27.407	25.462	-0.436	0.00
ATOM	37	HG	SER	282	24.475	27.797	24.804	0.334	0.00
ATOM	38	h	GLY	432	23.377	30.566	23.056	0.070	0.00
ATOM	39	C	GLY	432	23.756	31.606	22.972	0.229	0.00
ATOM	40	O	GLY	432	23.020	32.582	23.042	-0.461	0.00
ATOM	41	N	CYX	433	25.103	31.645	22.815	-0.226	0.00
ATOM	42	H	CYX	433	25.569	30.804	22.459	0.265	0.00
ATOM	43	CA	CYX	433	25.740	32.923	22.541	0.218	0.00
ATOM	44	HA	CYX	433	25.300	33.668	23.203	0.134	0.00
ATOM	45	CB	CYX	433	27.258	32.858	22.761	-0.179	0.00
ATOM	46	HB2	CYX	433	27.704	32.076	22.140	0.126	0.00
ATOM	47	HB3	CYX	433	27.692	33.817	22.465	0.108	0.00
ATOM	48	SG	CYX	433	27.781	32.608	24.506	-0.226	0.01
ATOM	49	C	CYX	433	25.480	33.452	21.114	0.287	0.01
ATOM	50	O	CYX	433	25.274	34.645	20.933	-0.520	-0.01
ATOM	51	N	VAL	434	25.547	32.533	20.115	-0.447	0.00
ATOM	52	H	VAL	434	25.857	31.569	20.270	0.291	0.00
ATOM	53	h	VAL	434	25.473	32.886	19.172	0.183	0.00

ATOM	54	h	GLU	435	26.111	28.983	18.518	0.087	0.00
ATOM	55	CG	GLU	435	26.884	28.523	19.144	-0.466	0.00
ATOM	56	HG2	GLU	435	26.954	27.457	18.917	0.103	0.00
ATOM	57	HG3	GLU	435	27.834	29.010	18.900	0.112	0.00
ATOM	58	CD	GLU	435	26.558	28.762	20.624	0.745	0.00
ATOM	59	OE1	GLU	435	26.423	27.746	21.376	-0.608	0.00
ATOM	60	OE2	GLU	435	26.451	29.960	21.003	-0.734	0.00
ATOM	61	h	ASP	447	29.202	25.173	22.756	0.117	0.00
ATOM	62	CB	ASP	447	28.913	25.620	23.710	-0.208	0.00
ATOM	63	HB2	ASP	447	28.224	26.444	23.504	0.132	0.00
ATOM	64	HB3	ASP	447	28.384	24.872	24.308	0.098	0.00
ATOM	65	CG	ASP	447	30.152	26.113	24.470	0.437	0.00
ATOM	66	OD1	ASP	447	31.271	26.081	23.941	-0.556	0.00
ATOM	67	OD2	ASP	447	29.930	26.537	25.678	-0.830	0.00
ATOM	68	O1	GOL	788	26.014	28.182	23.837	-0.346	0.12
ATOM	69	HO1	GOL	788	26.169	28.107	22.799	0.365	0.01
ATOM	70	C1	GOL	788	27.094	28.732	24.454	-0.218	0.87
ATOM	71	H11	GOL	788	27.961	28.951	23.838	0.182	-0.05
ATOM	72	H12	GOL	788	27.381	31.318	24.591	0.111	0.00
ATOM	73	C2	GOL	788	27.235	28.483	25.910	0.056	0.00
ATOM	74	O2	GOL	788	27.482	27.046	26.209	-0.488	0.03
ATOM	75	HO2	GOL	788	28.456	26.827	25.944	0.454	0.00
ATOM	76	H2	GOL	788	26.284	28.687	26.418	0.161	0.01
ATOM	77	C3	GOL	788	28.343	29.319	26.571	-0.444	-0.01
ATOM	78	H31	GOL	788	28.020	30.365	26.605	0.121	0.00
ATOM	79	H32	GOL	788	28.440	28.978	27.617	0.091	0.00
ATOM	80	O3	GOL	788	29.578	29.300	25.892	-0.365	0.00
ATOM	81	HO3	GOL	788	29.920	28.379	25.882	0.282	0.00
ATOM	82	h	GLN	549	31.249	27.746	20.726	0.087	0.00
ATOM	83	CD	GLN	549	31.754	26.871	20.269	0.230	0.00
ATOM	84	OE1	GLN	549	32.132	26.869	19.103	-0.518	0.00
ATOM	85	NE2	GLN	549	31.872	25.847	21.143	-0.311	0.00

ATOM	86	HE21	GLN	549	32.372	25.025	20.830	0.155	0.00
ATOM	87	HE22	GLN	549	31.624	25.933	22.139	0.324	0.00
ATOM	88	CB	ASN	156	30.277	22.588	28.275	-0.510	0.00
ATOM	89	h	ASN	156	30.395	22.537	29.363	0.111	0.00
ATOM	90	HB2	ASN	156	31.160	23.080	27.856	0.098	0.00
ATOM	91	CG	ASN	156	28.984	23.329	27.959	0.451	0.00
ATOM	92	OD1	ASN	156	27.885	22.770	28.021	-0.474	0.00
ATOM	93	ND2	ASN	156	29.114	24.651	27.684	-0.242	0.00
ATOM	94	HD21	ASN	156	28.267	25.151	27.448	0.224	0.00
ATOM	95	HD22	ASN	156	29.947	25.074	27.284	0.218	0.00
ATOM	96	HB3	ASN	156	30.207	21.566	27.895	0.108	0.00

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ATOM	1	h	VAL	162	22.444	18.822	25.026	0.095	0.00
ATOM	2	C	VAL	162	22.681	19.797	25.489	0.303	0.00
ATOM	3	O	VAL	162	23.671	20.437	25.164	-0.502	0.00
ATOM	4	N	GLY	163	21.765	20.175	26.409	-0.199	0.00
ATOM	5	H	GLY	163	21.001	19.569	26.668	0.173	0.00
ATOM	6	h	GLY	163	21.903	21.030	26.934	0.194	0.00
ATOM	7	h	HIP	164	22.606	23.128	23.395	0.110	0.00
ATOM	8	CB	HIP	164	23.623	23.237	22.997	-0.543	0.00
ATOM	9	HB2	HIP	164	23.942	22.254	22.631	0.120	0.00
ATOM	10	HB3	HIP	164	23.579	23.922	22.146	0.120	0.00
ATOM	11	CG	HIP	164	24.565	23.770	24.027	0.130	0.00
ATOM	12	ND1	HIP	164	24.929	23.051	25.158	-0.282	0.00
ATOM	13	HD1	HIP	164	24.594	22.110	25.370	0.372	0.00
ATOM	14	CE1	HIP	164	25.770	23.790	25.906	0.102	0.00
ATOM	15	HE1	HIP	164	26.265	23.464	26.819	0.224	0.00
ATOM	16	NE2	HIP	164	25.954	24.956	25.296	-0.268	0.00
ATOM	17	HE2	HIP	164	26.596	25.808	25.670	0.594	0.00
ATOM	18	CD2	HIP	164	25.221	24.966	24.130	-0.238	0.00
ATOM	19	HD2	HIP	164	25.230	25.826	23.479	0.172	0.00

ATOM	20	h	HIE	281	22.547	25.163	30.194	0.080	0.00
ATOM	21	CB	HIE	281	22.848	26.185	29.924	-0.562	0.00
ATOM	22	HB2	HIE	281	22.294	26.480	29.027	0.089	0.00
ATOM	23	HB3	HIE	281	22.529	26.837	30.748	0.093	0.00
ATOM	24	CG	HIE	281	24.332	26.285	29.668	-0.141	0.00
ATOM	25	ND1	HIE	281	25.331	25.972	30.589	-0.348	0.00
ATOM	26	CE1	HIE	281	26.462	26.199	29.952	0.175	0.00
ATOM	27	HE1	HIE	281	27.453	26.050	30.362	0.106	0.00
ATOM	28	NE2	HIE	281	26.262	26.645	28.684	-0.264	0.00
ATOM	29	HE2	HIE	281	26.941	26.811	27.927	0.317	0.00
ATOM	30	CD2	HIE	281	24.901	26.696	28.487	0.227	0.00
ATOM	31	HD2	HIE	281	24.473	27.005	27.543	0.180	0.00
ATOM	32	h	SER	282	21.938	26.749	25.637	0.100	0.00
ATOM	33	CB	SER	282	22.623	27.103	24.858	-0.102	0.00
ATOM	34	HB2	SER	282	22.743	26.289	24.123	0.089	0.00
ATOM	35	HB3	SER	282	22.136	27.950	24.346	0.103	0.00
ATOM	36	OG	SER	282	23.829	27.464	25.481	-0.453	0.00
ATOM	37	HG	SER	282	24.462	27.818	24.809	0.383	0.00
ATOM	38	h	GLY	432	23.492	30.588	23.084	0.096	0.00
ATOM	39	C	GLY	432	23.807	31.648	23.004	0.234	0.00
ATOM	40	O	GLY	432	23.020	32.582	23.042	-0.447	0.00
ATOM	41	N	CYX	433	25.159	31.767	22.886	-0.230	0.00
ATOM	42	H	CYX	433	25.695	30.934	22.651	0.259	0.00
ATOM	43	CA	CYX	433	25.755	33.081	22.692	-0.063	0.00
ATOM	44	HA	CYX	433	25.115	33.796	23.208	0.155	0.00
ATOM	45	CB	CYX	433	27.174	33.141	23.272	0.066	0.00
ATOM	46	HB2	CYX	433	27.802	32.339	22.874	0.114	0.00
ATOM	47	HB3	CYX	433	27.636	34.094	22.997	0.100	0.00
ATOM	48	SG	CYX	433	27.217	33.108	25.112	-0.255	0.00
ATOM	49	C	CYX	433	25.739	33.551	21.220	0.357	0.00
ATOM	50	O	CYX	433	25.274	34.645	20.933	-0.503	0.00
ATOM	51	N	VAL	434	26.313	32.720	20.307	-0.435	0.00

ATOM	52	H	VAL	434	26.547	31.749	20.507	0.299	0.00
ATOM	53	h	VAL	434	26.236	33.003	19.340	0.189	0.00
ATOM	54	h	GLU	435	26.982	29.445	18.569	0.102	0.00
ATOM	55	CG	GLU	435	26.884	28.523	19.144	-0.403	0.00
ATOM	56	HG2	GLU	435	26.105	27.885	18.716	0.100	0.00
ATOM	57	HG3	GLU	435	27.830	27.972	19.092	0.132	0.00
ATOM	58	CD	GLU	435	26.577	28.838	20.594	0.611	0.00
ATOM	59	OE1	GLU	435	26.136	27.808	21.279	-0.433	0.00
ATOM	60	OE2	GLU	435	26.753	29.956	21.083	-0.580	0.00
ATOM	61	h	ASP	447	29.139	25.251	22.705	0.107	0.00
ATOM	62	CB	ASP	447	28.913	25.620	23.710	-0.201	0.01
ATOM	63	HB2	ASP	447	28.197	26.442	23.631	0.117	0.00
ATOM	64	HB3	ASP	447	28.438	24.818	24.283	0.109	0.00
ATOM	65	CG	ASP	447	30.193	26.078	24.429	0.447	0.00
ATOM	66	OD1	ASP	447	31.296	25.978	23.863	-0.579	0.00
ATOM	67	OD2	ASP	447	30.018	26.534	25.623	-0.823	0.00
ATOM	68	O1	GOL	788	25.777	28.307	23.735	-0.490	0.22
ATOM	69	H01	GOL	788	25.979	28.077	22.285	0.397	0.00
ATOM	70	C1	GOL	788	26.886	28.661	24.333	-0.155	0.43
ATOM	71	H11	GOL	788	27.746	28.930	23.712	0.157	-0.03
ATOM	72	H12	GOL	788	26.550	31.941	25.243	0.068	0.00
ATOM	73	C2	GOL	788	27.071	28.611	25.738	-0.198	0.19
ATOM	74	O2	GOL	788	27.429	26.828	26.242	-0.454	0.19
ATOM	75	H02	GOL	788	28.384	26.718	25.957	0.378	-0.01
ATOM	76	H2	GOL	788	26.164	28.645	26.337	0.171	-0.01
ATOM	77	C3	GOL	788	28.267	29.326	26.346	-0.338	-0.02
ATOM	78	H31	GOL	788	28.020	30.394	26.432	0.129	0.01
ATOM	79	H32	GOL	788	28.413	28.952	27.372	0.103	0.01
ATOM	80	O3	GOL	788	29.445	29.254	25.579	-0.398	0.00
ATOM	81	H03	GOL	788	29.794	28.334	25.631	0.316	0.00
ATOM	82	h	GLN	549	31.658	27.782	20.871	0.087	0.00
ATOM	83	CD	GLN	549	31.852	26.854	20.297	0.213	0.00

ATOM	84	OE1	GLN	549	32.132	26.869	19.103	-0.524	0.00
ATOM	85	NE2	GLN	549	31.728	25.755	21.073	-0.310	0.00
ATOM	86	HE21	GLN	549	31.931	24.860	20.648	0.155	0.00
ATOM	87	HE22	GLN	549	31.552	25.810	22.090	0.337	0.00
ATOM	88	CB	ASN	156	30.277	22.588	28.275	-0.521	0.00
ATOM	89	h	ASN	156	30.363	22.522	29.366	0.108	0.00
ATOM	90	HB2	ASN	156	31.168	23.091	27.887	0.096	0.00
ATOM	91	CG	ASN	156	28.985	23.317	27.929	0.455	0.00
ATOM	92	OD1	ASN	156	27.890	22.751	28.021	-0.480	0.00
ATOM	93	ND2	ASN	156	29.117	24.618	27.586	-0.243	0.00
ATOM	94	HD21	ASN	156	28.286	25.135	27.320	0.228	0.00
ATOM	95	HD22	ASN	156	29.971	25.031	27.224	0.216	0.00
ATOM	96	HB3	ASN	156	30.229	21.569	27.882	0.105	0.00

TITLE In2

ATOM	1	h	VAL	162	22.368	18.682	25.139	0.088	0.00
ATOM	2	C	VAL	162	22.655	19.680	25.517	0.292	0.00
ATOM	3	O	VAL	162	23.669	20.246	25.136	-0.490	0.00
ATOM	4	N	GLY	163	21.765	20.175	26.409	-0.201	0.00
ATOM	5	H	GLY	163	20.977	19.629	26.723	0.168	0.00
ATOM	6	h	GLY	163	21.948	21.064	26.858	0.195	0.00
ATOM	7	h	HIP	164	22.595	23.138	23.372	0.099	0.00
ATOM	8	CB	HIP	164	23.623	23.237	22.997	-0.547	0.00
ATOM	9	HB2	HIP	164	23.914	22.260	22.589	0.114	0.00
ATOM	10	HB3	HIP	164	23.606	23.955	22.172	0.110	0.00
ATOM	11	CG	HIP	164	24.565	23.704	24.053	0.182	0.00
ATOM	12	ND1	HIP	164	24.884	22.957	25.174	-0.266	0.00
ATOM	13	HD1	HIP	164	24.550	22.012	25.354	0.329	0.00
ATOM	14	CE1	HIP	164	25.746	23.686	25.934	0.072	0.00
ATOM	15	HE1	HIP	164	26.194	23.335	26.857	0.194	0.00
ATOM	16	NE2	HIP	164	25.993	24.856	25.369	-0.430	0.00
ATOM	17	HE2	HIP	164	27.035	26.177	25.989	0.526	0.00

ATOM	18	CD2	HIP	164	25.267	24.873	24.198	-0.210	0.00
ATOM	19	HD2	HIP	164	25.297	25.721	23.528	0.134	0.00
ATOM	20	h	HIE	281	22.591	25.128	30.074	0.082	0.00
ATOM	21	CB	HIE	281	22.848	26.185	29.924	-0.532	0.00
ATOM	22	HB2	HIE	281	22.290	26.554	29.057	0.091	0.00
ATOM	23	HB3	HIE	281	22.495	26.727	30.812	0.090	0.00
ATOM	24	CG	HIE	281	24.330	26.368	29.700	0.077	0.00
ATOM	25	ND1	HIE	281	25.331	25.972	30.589	-0.351	0.00
ATOM	26	CE1	HIE	281	26.459	26.291	29.991	0.139	0.00
ATOM	27	HE1	HIE	281	27.451	26.103	30.384	0.106	0.00
ATOM	28	NE2	HIE	281	26.262	26.889	28.787	-0.169	0.00
ATOM	29	HE2	HIE	281	26.955	27.038	28.045	0.287	0.00
ATOM	30	CD2	HIE	281	24.902	26.927	28.582	-0.029	0.00
ATOM	31	HD2	HIE	281	24.470	27.335	27.677	0.157	0.00
ATOM	32	h	SER	282	21.617	27.240	25.269	0.103	0.00
ATOM	33	CB	SER	282	22.623	27.103	24.858	-0.158	0.00
ATOM	34	HB2	SER	282	23.035	26.163	25.249	0.127	0.00
ATOM	35	HB3	SER	282	22.530	27.008	23.764	0.087	0.00
ATOM	36	OG	SER	282	23.385	28.236	25.242	-0.463	0.00
ATOM	37	HG	SER	282	24.265	28.180	24.822	0.381	0.00
ATOM	38	h	GLY	432	23.532	30.608	23.240	0.122	0.00
ATOM	39	C	GLY	432	23.822	31.663	23.080	0.234	0.00
ATOM	40	O	GLY	432	23.020	32.582	23.042	-0.443	0.00
ATOM	41	N	CYX	433	25.179	31.820	22.980	-0.246	0.00
ATOM	42	H	CYX	433	25.734	30.999	22.753	0.246	0.00
ATOM	43	CA	CYX	433	25.733	33.146	22.746	-0.123	-0.01
ATOM	44	HA	CYX	433	25.046	33.854	23.209	0.160	0.00
ATOM	45	CB	CYX	433	27.124	33.284	23.380	0.099	0.01
ATOM	46	HB2	CYX	433	27.789	32.472	23.069	0.110	0.00
ATOM	47	HB3	CYX	433	27.576	34.228	23.062	0.102	0.00
ATOM	48	SG	CYX	433	27.069	33.377	25.221	-0.244	0.00
ATOM	49	C	CYX	433	25.753	33.570	21.261	0.365	0.00

ATOM	50	O	CYX	433	25.274	34.645	20.933-0.498	0.00
ATOM	51	N	VAL	434	26.375	32.731	20.386-0.430	0.00
ATOM	52	H	VAL	434	26.605	31.765	20.605 0.298	0.00
ATOM	53	h	VAL	434	26.315	32.991	19.411 0.191	0.00
ATOM	54	h	GLU	435	27.000	29.450	18.581 0.106	0.00
ATOM	55	CG	GLU	435	26.884	28.523	19.144-0.402	0.00
ATOM	56	HG2	GLU	435	26.080	27.914	18.721 0.106	0.00
ATOM	57	HG3	GLU	435	27.812	27.944	19.073 0.137	0.00
ATOM	58	CD	GLU	435	26.606	28.828	20.597 0.623	0.00
ATOM	59	OE1	GLU	435	26.175	27.779	21.280-0.363	0.00
ATOM	60	OE2	GLU	435	26.783	29.930	21.110-0.562	0.00
ATOM	61	h	ASP	447	29.144	25.094	22.780 0.101	0.00
ATOM	62	CB	ASP	447	28.913	25.620	23.710-0.147	0.00
ATOM	63	HB2	ASP	447	28.165	26.391	23.496 0.112	0.00
ATOM	64	HB3	ASP	447	28.455	24.921	24.415 0.123	0.00
ATOM	65	CG	ASP	447	30.177	26.248	24.317 0.330	0.00
ATOM	66	OD1	ASP	447	31.276	26.121	23.750-0.556	0.00
ATOM	67	OD2	ASP	447	30.004	26.885	25.427-0.799	0.00
ATOM	68	O1	GOL	788	25.918	28.476	23.826-0.271	0.29
ATOM	69	H01	GOL	788	26.040	28.051	22.246 0.325	0.00
ATOM	70	C1	GOL	788	27.025	28.890	24.285-0.746	0.00
ATOM	71	H11	GOL	788	27.890	28.958	23.616 0.175-0.01	
ATOM	72	H12	GOL	788	26.230	32.330	25.380 0.069	0.00
ATOM	73	C2	GOL	788	27.227	29.281	25.625 0.436	0.65
ATOM	74	O2	GOL	788	27.625	26.836	26.450-0.677	0.04
ATOM	75	H02	GOL	788	28.530	26.831	25.994 0.449	0.00
ATOM	76	H2	GOL	788	26.371	29.283	26.295 0.145-0.03	
ATOM	77	C3	GOL	788	28.550	29.766	26.135-0.107-0.03	
ATOM	78	H31	GOL	788	28.460	30.849	26.327 0.144	0.04
ATOM	79	H32	GOL	788	28.723	29.298	27.120 0.113	0.03
ATOM	80	O3	GOL	788	29.625	29.583	25.254-0.429	0.00
ATOM	81	H03	GOL	788	29.909	28.634	25.310 0.325	0.00



ATOM	82	h	GLN	549	31.729	27.713	20.922	0.090	0.00
ATOM	83	CD	GLN	549	31.862	26.807	20.298	0.210	0.00
ATOM	84	OE1	GLN	549	32.132	26.869	19.103	-0.525	0.00
ATOM	85	NE2	GLN	549	31.679	25.681	21.018	-0.304	0.00
ATOM	86	HE21	GLN	549	31.824	24.795	20.553	0.157	0.00
ATOM	87	HE22	GLN	549	31.514	25.722	22.037	0.329	0.00
ATOM	88	CB	ASN	156	30.277	22.588	28.275	-0.556	0.00
ATOM	89	h	ASN	156	30.206	22.125	29.264	0.107	0.00
ATOM	90	HB2	ASN	156	31.211	23.155	28.210	0.086	0.00
ATOM	91	CG	ASN	156	29.032	23.432	28.041	0.499	0.00
ATOM	92	OD1	ASN	156	27.910	22.949	28.197	-0.471	0.00
ATOM	93	ND2	ASN	156	29.254	24.720	27.683	-0.267	0.00
ATOM	94	HD21	ASN	156	28.473	25.314	27.404	0.272	0.00
ATOM	95	HD22	ASN	156	30.159	25.043	27.370	0.185	0.00
ATOM	96	HB3	ASN	156	30.302	21.779	27.536	0.104	0.00

TITLE TS3

ATOM	1	h	VAL	162	22.047	18.557	25.180	0.089	0.00
ATOM	2	C	VAL	162	22.480	19.535	25.455	0.291	0.00
ATOM	3	O	VAL	162	23.494	19.963	24.921	-0.484	0.00
ATOM	4	N	GLY	163	21.765	20.175	26.409	-0.204	0.00
ATOM	5	H	GLY	163	20.969	19.738	26.850	0.170	0.00
ATOM	6	h	GLY	163	22.093	21.061	26.775	0.198	0.00
ATOM	7	h	HIP	164	22.590	23.091	23.341	0.098	0.00
ATOM	8	CB	HIP	164	23.623	23.237	22.997	-0.565	0.00
ATOM	9	HB2	HIP	164	23.906	22.338	22.434	0.114	0.00
ATOM	10	HB3	HIP	164	23.624	24.081	22.301	0.110	0.00
ATOM	11	CG	HIP	164	24.559	23.508	24.122	0.257	0.00
ATOM	12	ND1	HIP	164	24.820	22.593	25.125	-0.264	0.00
ATOM	13	HD1	HIP	164	24.445	21.645	25.164	0.340	0.00
ATOM	14	CE1	HIP	164	25.711	23.156	25.984	0.132	0.00
ATOM	15	HE1	HIP	164	26.139	22.644	26.839	0.181	0.00

ATOM	16	NE2	HIP	164	26.034	24.379	25.596	-0.293	0.00
ATOM	17	HE2	HIP	164	26.798	26.119	26.010	0.298	0.00
ATOM	18	CD2	HIP	164	25.321	24.603	24.436	-0.330	0.00
ATOM	19	HD2	HIP	164	25.404	25.535	23.894	0.141	0.00
ATOM	20	h	HIE	281	22.579	25.133	30.087	0.082	0.00
ATOM	21	CB	HIE	281	22.848	26.185	29.924	-0.535	0.00
ATOM	22	HB2	HIE	281	22.290	26.550	29.056	0.091	0.00
ATOM	23	HB3	HIE	281	22.504	26.741	30.806	0.090	0.00
ATOM	24	CG	HIE	281	24.330	26.349	29.692	-0.006	0.00
ATOM	25	ND1	HIE	281	25.331	25.972	30.589	-0.363	0.00
ATOM	26	CE1	HIE	281	26.460	26.250	29.967	0.126	0.00
ATOM	27	HE1	HIE	281	27.451	26.069	30.363	0.103	0.00
ATOM	28	NE2	HIE	281	26.260	26.804	28.742	-0.168	0.00
ATOM	29	HE2	HIE	281	26.921	26.952	27.970	0.294	0.00
ATOM	30	CD2	HIE	281	24.899	26.859	28.550	0.038	0.00
ATOM	31	HD2	HIE	281	24.470	27.258	27.641	0.165	0.00
ATOM	32	h	SER	282	21.646	27.166	25.348	0.104	0.00
ATOM	33	CB	SER	282	22.623	27.103	24.858	-0.157	0.00
ATOM	34	HB2	SER	282	23.103	26.161	25.157	0.130	0.00
ATOM	35	HB3	SER	282	22.453	27.076	23.769	0.088	0.00
ATOM	36	OG	SER	282	23.358	28.248	25.264	-0.432	0.00
ATOM	37	HG	SER	282	24.228	28.245	24.825	0.332	0.00
ATOM	38	h	GLY	432	23.425	30.596	23.357	0.114	0.00
ATOM	39	C	GLY	432	23.767	31.618	23.103	0.255	0.00
ATOM	40	O	GLY	432	23.020	32.582	23.042	-0.449	0.00
ATOM	41	N	CYX	433	25.110	31.684	22.902	-0.259	0.00
ATOM	42	H	CYX	433	25.628	30.821	22.782	0.253	0.00
ATOM	43	CA	CYX	433	25.749	32.952	22.598	0.292	0.01
ATOM	44	HA	CYX	433	25.300	33.716	23.236	0.137	0.00
ATOM	45	CB	CYX	433	27.258	32.864	22.870	-0.322	-0.02
ATOM	46	HB2	CYX	433	27.718	32.061	22.286	0.123	0.01
ATOM	47	HB3	CYX	433	27.731	33.802	22.557	0.120	0.01

ATOM	48	SG	CYX	433	27.735	32.688	24.636-0.162	0.41
ATOM	49	C	CYX	433	25.507	33.464	21.152 0.252	0.00
ATOM	50	O	CYX	433	25.274	34.645	20.933-0.502	0.00
ATOM	51	N	VAL	434	25.609	32.529	20.168-0.418	0.00
ATOM	52	H	VAL	434	25.957	31.592	20.348 0.256	0.00
ATOM	53	h	VAL	434	25.556	32.863	19.217 0.189	0.00
ATOM	54	h	GLU	435	27.056	29.445	18.587 0.109	0.00
ATOM	55	CG	GLU	435	26.884	28.523	19.144-0.435	0.00
ATOM	56	HG2	GLU	435	26.016	27.992	18.740 0.108	0.00
ATOM	57	HG3	GLU	435	27.751	27.862	19.034 0.135	0.00
ATOM	58	CD	GLU	435	26.668	28.834	20.603 0.643	0.00
ATOM	59	OE1	GLU	435	26.391	27.765	21.338-0.358	0.00
ATOM	60	OE2	GLU	435	26.741	29.966	21.069-0.562	0.00
ATOM	61	h	ASP	447	29.189	25.383	22.679 0.112	0.00
ATOM	62	CB	ASP	447	28.913	25.620	23.710-0.190	0.00
ATOM	63	HB2	ASP	447	28.023	26.255	23.706 0.084	0.00
ATOM	64	HB3	ASP	447	28.635	24.695	24.227 0.123	0.00
ATOM	65	CG	ASP	447	30.071	26.309	24.450 0.374	0.00
ATOM	66	OD1	ASP	447	31.176	26.437	23.898-0.558	0.00
ATOM	67	OD2	ASP	447	29.802	26.716	25.648-0.789	0.00
ATOM	68	O1	GOL	788	26.044	28.720	23.829-0.336	0.14
ATOM	69	H01	GOL	788	26.248	28.062	22.289 0.348	0.00
ATOM	70	C1	GOL	788	27.123	28.997	24.391-0.834	0.01
ATOM	71	H11	GOL	788	28.068	28.626	23.975 0.174-0.01	
ATOM	72	H12	GOL	788	27.462	31.186	24.893 0.281-0.08	
ATOM	73	C2	GOL	788	27.248	29.890	25.530 0.636	0.52
ATOM	74	O2	GOL	788	27.253	26.969	26.197-0.530	0.01
ATOM	75	H02	GOL	788	28.224	26.803	25.989 0.391	0.00
ATOM	76	H2	GOL	788	26.310	30.127	26.035 0.137-0.02	
ATOM	77	C3	GOL	788	28.488	29.793	26.406-0.261-0.04	
ATOM	78	H31	GOL	788	28.627	30.755	26.922 0.127	0.02
ATOM	79	H32	GOL	788	28.263	29.049	27.186 0.118	0.03

ATOM	80	O3	GOL	788	29.659	29.489	25.696	-0.402	0.00
ATOM	81	HO3	GOL	788	29.836	28.517	25.744	0.310	0.00
ATOM	82	h	GLN	549	31.596	27.933	20.766	0.085	0.00
ATOM	83	CD	GLN	549	31.834	26.960	20.289	0.210	0.00
ATOM	84	OE1	GLN	549	32.132	26.869	19.103	-0.523	0.00
ATOM	85	NE2	GLN	549	31.740	25.941	21.169	-0.310	0.00
ATOM	86	HE21	GLN	549	31.979	25.015	20.839	0.158	0.00
ATOM	87	HE22	GLN	549	31.532	26.091	22.170	0.340	0.00
ATOM	88	CB	ASN	156	30.277	22.588	28.275	-0.444	0.00
ATOM	89	h	ASN	156	30.234	22.352	29.343	0.106	0.00
ATOM	90	HB2	ASN	156	31.024	23.370	28.110	0.092	0.00
ATOM	91	CG	ASN	156	28.883	22.965	27.800	0.431	0.00
ATOM	92	OD1	ASN	156	27.938	22.190	27.970	-0.496	0.00
ATOM	93	ND2	ASN	156	28.757	24.173	27.203	-0.309	0.00
ATOM	94	HD21	ASN	156	27.858	24.421	26.800	0.256	0.00
ATOM	95	HD22	ASN	156	29.530	24.789	26.977	0.210	0.00
ATOM	96	HB3	ASN	156	30.592	21.679	27.752	0.105	0.00

TITLE Pro

ATOM	1	h	VAL	162	21.985	18.517	25.221	0.088	0.00
ATOM	2	C	VAL	162	22.445	19.493	25.459	0.290	0.00
ATOM	3	O	VAL	162	23.455	19.883	24.890	-0.484	0.00
ATOM	4	N	GLY	163	21.765	20.175	26.409	-0.205	0.00
ATOM	5	H	GLY	163	20.971	19.768	26.880	0.171	0.00
ATOM	6	h	GLY	163	22.120	21.063	26.742	0.200	0.00
ATOM	7	h	HIP	164	22.594	23.064	23.340	0.097	0.00
ATOM	8	CB	HIP	164	23.623	23.237	22.997	-0.567	0.00
ATOM	9	HB2	HIP	164	23.906	22.375	22.378	0.112	0.00
ATOM	10	HB3	HIP	164	23.612	24.120	22.352	0.110	0.00
ATOM	11	CG	HIP	164	24.566	23.448	24.125	0.246	0.00
ATOM	12	ND1	HIP	164	24.828	22.491	25.089	-0.270	0.00
ATOM	13	HD1	HIP	164	24.439	21.548	25.101	0.342	0.00

ATOM	14	CE1	HIP	164	25.734	23.012	25.958	0.177	0.00
ATOM	15	HE1	HIP	164	26.166	22.471	26.792	0.181	0.00
ATOM	16	NE2	HIP	164	26.063	24.246	25.612	-0.292	0.00
ATOM	17	HE2	HIP	164	26.809	25.967	25.955	0.293	0.00
ATOM	18	CD2	HIP	164	25.341	24.523	24.471	-0.354	0.00
ATOM	19	HD2	HIP	164	25.425	25.476	23.966	0.146	0.00
ATOM	20	h	HIE	281	22.565	25.142	30.122	0.083	0.00
ATOM	21	CB	HIE	281	22.848	26.185	29.924	-0.557	0.00
ATOM	22	HB2	HIE	281	22.292	26.529	29.046	0.091	0.00
ATOM	23	HB3	HIE	281	22.515	26.774	30.789	0.090	0.00
ATOM	24	CG	HIE	281	24.330	26.322	29.682	-0.153	0.00
ATOM	25	ND1	HIE	281	25.331	25.972	30.589	-0.355	0.00
ATOM	26	CE1	HIE	281	26.460	26.210	29.951	0.148	0.00
ATOM	27	HE1	HIE	281	27.451	26.036	30.349	0.104	0.00
ATOM	28	NE2	HIE	281	26.259	26.713	28.704	-0.182	0.00
ATOM	29	HE2	HIE	281	26.916	26.832	27.925	0.301	0.00
ATOM	30	CD2	HIE	281	24.898	26.777	28.517	0.164	0.00
ATOM	31	HD2	HIE	281	24.468	27.145	27.596	0.171	0.00
ATOM	32	h	SER	282	21.654	27.137	25.366	0.102	0.00
ATOM	33	CB	SER	282	22.623	27.103	24.858	-0.156	0.00
ATOM	34	HB2	SER	282	23.130	26.171	25.144	0.127	0.00
ATOM	35	HB3	SER	282	22.432	27.073	23.772	0.085	0.00
ATOM	36	OG	SER	282	23.340	28.261	25.251	-0.450	0.00
ATOM	37	HG	SER	282	24.198	28.270	24.785	0.365	0.00
ATOM	38	h	GLY	432	23.470	30.626	23.465	0.123	0.00
ATOM	39	C	GLY	432	23.793	31.645	23.176	0.226	0.00
ATOM	40	O	GLY	432	23.020	32.582	23.042	-0.442	0.00
ATOM	41	N	CYX	433	25.147	31.742	23.024	-0.198	0.00
ATOM	42	H	CYX	433	25.670	30.886	22.873	0.250	0.00
ATOM	43	CA	CYX	433	25.726	33.011	22.625	0.191	0.04
ATOM	44	HA	CYX	433	25.282	33.792	23.246	0.137	0.00
ATOM	45	CB	CYX	433	27.256	33.030	22.790	-0.122	-0.08

ATOM	46	HB2	CYX	433	27.712	32.153	22.309	0.111	0.03
ATOM	47	HB3	CYX	433	27.657	33.906	22.267	0.122	0.02
ATOM	48	SG	CYX	433	27.885	33.084	24.493	-0.171	0.97
ATOM	49	C	CYX	433	25.402	33.455	21.181	0.228	0.00
ATOM	50	O	CYX	433	25.274	34.645	20.933	-0.514	0.00
ATOM	51	N	VAL	434	25.334	32.476	20.241	-0.403	0.00
ATOM	52	H	VAL	434	25.647	31.528	20.430	0.247	0.00
ATOM	53	h	VAL	434	25.244	32.778	19.281	0.187	0.00
ATOM	54	h	GLU	435	26.958	29.466	18.601	0.110	0.00
ATOM	55	CG	GLU	435	26.884	28.523	19.144	-0.398	0.00
ATOM	56	HG2	GLU	435	26.091	27.900	18.718	0.108	0.00
ATOM	57	HG3	GLU	435	27.824	27.968	19.047	0.136	0.00
ATOM	58	CD	GLU	435	26.603	28.791	20.606	0.664	0.00
ATOM	59	OE1	GLU	435	26.438	27.689	21.326	-0.391	0.00
ATOM	60	OE2	GLU	435	26.537	29.919	21.085	-0.591	0.00
ATOM	61	h	ASP	447	29.263	25.227	22.752	0.110	0.00
ATOM	62	CB	ASP	447	28.913	25.620	23.710	-0.216	0.00
ATOM	63	HB2	ASP	447	28.078	26.301	23.517	0.098	0.00
ATOM	64	HB3	ASP	447	28.521	24.796	24.315	0.113	0.00
ATOM	65	CG	ASP	447	30.048	26.351	24.450	0.444	0.00
ATOM	66	OD1	ASP	447	31.151	26.507	23.898	-0.581	0.00
ATOM	67	OD2	ASP	447	29.760	26.772	25.637	-0.779	0.00
ATOM	68	O1	GOL	788	25.913	28.424	23.906	-0.359	0.00
ATOM	69	H01	GOL	788	26.248	27.940	22.280	0.385	0.00
ATOM	70	C1	GOL	788	26.897	28.728	24.600	-0.696	0.02
ATOM	71	H11	GOL	788	27.902	28.467	24.246	0.166	0.00
ATOM	72	H12	GOL	788	26.751	30.655	25.331	0.130	0.01
ATOM	73	C2	GOL	788	26.849	29.649	25.775	0.615	-0.01
ATOM	74	O2	GOL	788	27.226	26.834	26.150	-0.430	0.00
ATOM	75	H02	GOL	788	28.214	26.726	25.954	0.353	0.00
ATOM	76	H2	GOL	788	25.935	29.477	26.355	0.130	0.00
ATOM	77	C3	GOL	788	28.119	29.624	26.655	-0.387	0.00

ATOM	78	H31	GOL	788	28.135	30.546	27.251	0.118	0.00
ATOM	79	H32	GOL	788	28.061	28.785	27.354	0.113	0.00
ATOM	80	O3	GOL	788	29.308	29.581	25.887	-0.400	0.00
ATOM	81	H03	GOL	788	29.621	28.649	25.842	0.300	0.00
ATOM	82	h	GLN	549	31.450	27.928	20.714	0.081	0.00
ATOM	83	CD	GLN	549	31.799	26.969	20.279	0.212	0.00
ATOM	84	OE1	GLN	549	32.132	26.869	19.103	-0.523	0.00
ATOM	85	NE2	GLN	549	31.791	25.978	21.195	-0.312	0.00
ATOM	86	HE21	GLN	549	32.133	25.071	20.906	0.158	0.00
ATOM	87	HE22	GLN	549	31.549	26.143	22.187	0.345	0.00
ATOM	88	CB	ASN	156	30.277	22.588	28.275	-0.438	0.00
ATOM	89	h	ASN	156	30.238	22.278	29.324	0.107	0.00
ATOM	90	HB2	ASN	156	30.987	23.414	28.170	0.092	0.00
ATOM	91	CG	ASN	156	28.873	22.929	27.812	0.415	0.00
ATOM	92	OD1	ASN	156	27.953	22.120	27.963	-0.496	0.00
ATOM	93	ND2	ASN	156	28.710	24.146	27.243	-0.318	0.00
ATOM	94	HD21	ASN	156	27.809	24.364	26.827	0.272	0.00
ATOM	95	HD22	ASN	156	29.472	24.775	27.017	0.203	0.00
ATOM	96	HB3	ASN	156	30.642	21.733	27.695	0.105	0.00

TITLE Suba

ATOM	1	h	VAL	162	22.339	18.644	25.171	0.089	0.00
ATOM	2	C	VAL	162	22.637	19.649	25.519	0.295	0.00
ATOM	3	O	VAL	162	23.652	20.196	25.112	-0.488	0.00
ATOM	4	N	GLY	163	21.765	20.175	26.409	-0.204	0.00
ATOM	5	H	GLY	163	20.965	19.653	26.733	0.170	0.00
ATOM	6	h	GLY	163	21.952	21.080	26.823	0.195	0.00
ATOM	7	h	HIP	164	22.581	23.246	23.344	0.100	0.00
ATOM	8	CB	HIP	164	23.623	23.237	22.997	-0.545	0.00
ATOM	9	HB2	HIP	164	23.839	22.222	22.639	0.113	0.00
ATOM	10	HB3	HIP	164	23.694	23.919	22.145	0.120	0.00
ATOM	11	CG	HIP	164	24.574	23.661	24.066	0.161	0.00

ATOM	12	ND1	HIP	164	24.814	22.901	25.197	-0.240	0.00
ATOM	13	HD1	HIP	164	24.451	21.962	25.355	0.336	0.00
ATOM	14	CE1	HIP	164	25.696	23.577	25.977	0.102	0.00
ATOM	15	HE1	HIP	164	26.091	23.173	26.901	0.173	0.00
ATOM	16	NE2	HIP	164	26.039	24.730	25.419	-0.355	0.00
ATOM	17	HE2	HIP	164	26.808	26.549	25.740	0.413	0.00
ATOM	18	CD2	HIP	164	25.342	24.786	24.225	-0.237	0.00
ATOM	19	HD2	HIP	164	25.442	25.632	23.561	0.168	0.00
ATOM	20	h	HIE	281	22.534	25.176	30.222	0.083	0.00
ATOM	21	CB	HIE	281	22.848	26.185	29.924	-0.561	0.00
ATOM	22	HB2	HIE	281	22.292	26.467	29.025	0.093	0.00
ATOM	23	HB3	HIE	281	22.552	26.864	30.735	0.094	0.00
ATOM	24	CG	HIE	281	24.334	26.251	29.653	-0.315	0.00
ATOM	25	ND1	HIE	281	25.331	25.972	30.589	-0.333	0.00
ATOM	26	CE1	HIE	281	26.465	26.140	29.945	0.190	0.00
ATOM	27	HE1	HIE	281	27.453	26.000	30.364	0.103	0.00
ATOM	28	NE2	HIE	281	26.270	26.513	28.652	-0.238	0.00
ATOM	29	HE2	HIE	281	26.963	26.696	27.930	0.284	0.00
ATOM	30	CD2	HIE	281	24.909	26.587	28.451	0.357	0.00
ATOM	31	HD2	HIE	281	24.485	26.870	27.494	0.177	0.00
ATOM	32	h	SER	282	21.824	27.083	25.608	0.092	0.00
ATOM	33	CB	SER	282	22.623	27.103	24.858	-0.129	0.00
ATOM	34	HB2	SER	282	22.861	26.064	24.583	0.117	0.00
ATOM	35	HB3	SER	282	22.229	27.615	23.964	0.099	0.00
ATOM	36	OG	SER	282	23.723	27.781	25.427	-0.363	0.00
ATOM	37	HG	SER	282	24.443	27.837	24.759	0.275	0.00
ATOM	38	h	GLY	432	23.366	30.565	23.066	0.089	0.00
ATOM	39	C	GLY	432	23.747	31.601	22.972	0.247	0.00
ATOM	40	O	GLY	432	23.020	32.582	23.042	-0.462	0.00
ATOM	41	N	CYX	433	25.097	31.634	22.802	-0.223	0.00
ATOM	42	H	CYX	433	25.546	30.793	22.420	0.283	0.00
ATOM	43	CA	CYX	433	25.744	32.906	22.533	0.133	0.03



ATOM	44	HA	CYX	433	25.314	33.656	23.199	0.134	0.00
ATOM	45	CB	CYX	433	27.266	32.812	22.739	-0.084	-0.07
ATOM	46	HB2	CYX	433	27.658	31.926	22.217	0.118	0.03
ATOM	47	HB3	CYX	433	27.754	33.683	22.285	0.110	0.02
ATOM	48	SG	CYX	433	27.836	32.694	24.459	-0.203	0.97
ATOM	49	C	CYX	433	25.486	33.451	21.108	0.269	0.00
ATOM	50	O	CYX	433	25.274	34.645	20.933	-0.520	0.01
ATOM	51	N	VAL	434	25.573	32.534	20.110	-0.436	0.00
ATOM	52	H	VAL	434	25.840	31.557	20.270	0.288	0.00
ATOM	53	h	VAL	434	25.469	32.875	19.165	0.185	0.00
ATOM	54	h	GLU	435	25.985	28.785	18.572	0.087	0.00
ATOM	55	CG	GLU	435	26.884	28.523	19.144	-0.452	0.00
ATOM	56	HG2	GLU	435	27.157	27.487	18.931	0.105	0.00
ATOM	57	HG3	GLU	435	27.686	29.192	18.813	0.102	0.00
ATOM	58	CD	GLU	435	26.612	28.731	20.639	0.764	0.00
ATOM	59	OE1	GLU	435	26.605	27.706	21.378	-0.624	0.00
ATOM	60	OE2	GLU	435	26.404	29.921	21.023	-0.775	0.00
ATOM	61	h	ASP	447	29.205	25.083	22.806	0.130	0.00
ATOM	62	CB	ASP	447	28.913	25.620	23.710	-0.208	0.00
ATOM	63	HB2	ASP	447	28.265	26.454	23.418	0.177	0.00
ATOM	64	HB3	ASP	447	28.323	24.963	24.354	0.123	0.00
ATOM	65	CG	ASP	447	30.155	26.105	24.420	0.390	0.00
ATOM	66	OD1	ASP	447	31.289	26.003	23.992	-0.475	0.00
ATOM	67	OD2	ASP	447	29.951	26.665	25.634	-0.589	0.00
ATOM	68	O1	GOL	788	26.025	27.957	23.889	-0.382	0.00
ATOM	69	H01	GOL	788	26.197	27.940	22.883	0.377	0.00
ATOM	70	C1	GOL	788	26.916	28.884	24.487	-0.158	-0.01
ATOM	71	H11	GOL	788	27.906	28.831	24.016	0.153	0.00
ATOM	72	H12	GOL	788	26.556	29.917	24.387	0.165	0.01
ATOM	73	C2	GOL	788	27.035	28.564	25.969	0.033	0.02
ATOM	74	O2	GOL	788	27.444	27.179	26.167	-0.503	0.00
ATOM	75	H02	GOL	788	28.965	26.796	25.794	0.444	0.00

ATOM	76	H2	GOL	788	26.054	28.683	26.446	0.190	0.00
ATOM	77	C3	GOL	788	28.035	29.462	26.699	-0.484	0.00
ATOM	78	H31	GOL	788	27.612	30.470	26.739	0.144	0.00
ATOM	79	H32	GOL	788	28.139	29.103	27.735	0.100	0.00
ATOM	80	O3	GOL	788	29.295	29.598	26.060	-0.311	0.00
ATOM	81	HO3	GOL	788	29.755	28.742	26.068	0.226	0.00
ATOM	82	h	GLN	549	31.070	27.554	20.709	0.090	0.00
ATOM	83	CD	GLN	549	31.735	26.793	20.256	0.240	0.00
ATOM	84	OE1	GLN	549	32.132	26.869	19.103	-0.499	0.00
ATOM	85	NE2	GLN	549	32.019	25.788	21.123	-0.292	0.00
ATOM	86	HE21	GLN	549	32.671	25.077	20.820	0.164	0.00
ATOM	87	HE22	GLN	549	31.757	25.832	22.107	0.273	0.00
ATOM	88	CB	ASN	156	30.277	22.588	28.275	-0.458	0.00
ATOM	89	h	ASN	156	30.202	22.052	29.224	0.114	0.00
ATOM	90	HB2	ASN	156	30.992	23.410	28.376	0.088	0.00
ATOM	91	CG	ASN	156	28.888	23.047	27.858	0.420	0.00
ATOM	92	OD1	ASN	156	27.902	22.332	28.019	-0.454	0.00
ATOM	93	ND2	ASN	156	28.824	24.281	27.289	-0.313	0.00
ATOM	94	HD21	ASN	156	27.954	24.576	26.860	0.254	0.00
ATOM	95	HD22	ASN	156	29.648	24.824	27.069	0.192	0.00
ATOM	96	HB3	ASN	156	30.660	21.886	27.525	0.111	0.00

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ATOM	1	h	VAL	162	22.535	18.809	25.088	0.091	0.00
ATOM	2	C	VAL	162	22.726	19.802	25.532	0.293	0.00
ATOM	3	O	VAL	162	23.708	20.465	25.231	-0.496	0.00
ATOM	4	N	GLY	163	21.765	20.175	26.409	-0.198	0.00
ATOM	5	H	GLY	163	21.002	19.559	26.647	0.170	0.00
ATOM	6	h	GLY	163	21.854	21.051	26.908	0.192	0.00
ATOM	7	h	HIP	164	22.583	23.248	23.350	0.103	0.00
ATOM	8	CB	HIP	164	23.623	23.237	22.997	-0.543	0.00
ATOM	9	HB2	HIP	164	23.877	22.197	22.760	0.115	0.00

ATOM	10	HB3	HIP	164	23.665	23.818	22.072	0.117	0.00
ATOM	11	CG	HIP	164	24.560	23.816	24.007	0.118	0.00
ATOM	12	ND1	HIP	164	24.842	23.182	25.203	-0.223	0.00
ATOM	13	HD1	HIP	164	24.506	22.255	25.458	0.341	0.00
ATOM	14	CE1	HIP	164	25.685	23.974	25.913	0.070	0.00
ATOM	15	HE1	HIP	164	26.088	23.681	26.875	0.178	0.00
ATOM	16	NE2	HIP	164	25.961	25.087	25.249	-0.422	0.00
ATOM	17	HE2	HIP	164	26.810	26.651	25.725	0.521	0.00
ATOM	18	CD2	HIP	164	25.267	24.993	24.056	-0.214	0.00
ATOM	19	HD2	HIP	164	25.331	25.773	23.309	0.166	0.00
ATOM	20	h	HIE	281	22.548	25.159	30.177	0.082	0.00
ATOM	21	CB	HIE	281	22.848	26.185	29.924	-0.551	0.00
ATOM	22	HB2	HIE	281	22.291	26.497	29.035	0.093	0.00
ATOM	23	HB3	HIE	281	22.538	26.824	30.761	0.096	0.00
ATOM	24	CG	HIE	281	24.332	26.287	29.664	-0.199	0.00
ATOM	25	ND1	HIE	281	25.331	25.972	30.589	-0.335	0.00
ATOM	26	CE1	HIE	281	26.463	26.205	29.961	0.187	0.00
ATOM	27	HE1	HIE	281	27.453	26.061	30.373	0.109	0.00
ATOM	28	NE2	HIE	281	26.263	26.647	28.686	-0.269	0.00
ATOM	29	HE2	HIE	281	26.948	26.904	27.979	0.286	0.00
ATOM	30	CD2	HIE	281	24.900	26.703	28.485	0.335	0.00
ATOM	31	HD2	HIE	281	24.475	27.021	27.541	0.169	0.00
ATOM	32	h	SER	282	21.907	26.873	25.655	0.094	0.00
ATOM	33	CB	SER	282	22.623	27.103	24.858	-0.120	0.00
ATOM	34	HB2	SER	282	22.876	26.166	24.343	0.117	0.00
ATOM	35	HB3	SER	282	22.125	27.775	24.141	0.102	0.00
ATOM	36	OG	SER	282	23.746	27.708	25.471	-0.374	0.00
ATOM	37	HG	SER	282	24.401	27.960	24.792	0.289	0.00
ATOM	38	h	GLY	432	23.269	30.579	22.694	0.067	0.00
ATOM	39	C	GLY	432	23.694	31.603	22.755	0.280	0.00
ATOM	40	O	GLY	432	23.020	32.582	23.042	-0.460	0.00
ATOM	41	N	CYX	433	25.017	31.623	22.491	-0.263	0.00

ATOM	42	H	CYX	433	25.502	30.793	22.145	0.259	0.00
ATOM	43	CA	CYX	433	25.761	32.870	22.507	0.282	0.00
ATOM	44	HA	CYX	433	25.221	33.561	23.154	0.144	0.00
ATOM	45	CB	CYX	433	27.180	32.633	23.045	-0.374	-0.01
ATOM	46	HB2	CYX	433	27.710	31.898	22.434	0.119	0.01
ATOM	47	HB3	CYX	433	27.748	33.568	23.008	0.103	0.01
ATOM	48	SG	CYX	433	27.209	32.081	24.798	-0.189	0.34
ATOM	49	C	CYX	433	25.759	33.533	21.110	0.251	0.00
ATOM	50	O	CYX	433	25.274	34.645	20.933	-0.516	0.00
ATOM	51	N	VAL	434	26.344	32.800	20.118	-0.441	0.00
ATOM	52	H	VAL	434	26.549	31.805	20.238	0.288	0.00
ATOM	53	h	VAL	434	26.234	33.158	19.179	0.185	0.00
ATOM	54	h	GLU	435	25.999	28.899	18.617	0.092	0.00
ATOM	55	CG	GLU	435	26.884	28.523	19.144	-0.468	0.00
ATOM	56	HG2	GLU	435	26.979	27.449	18.967	0.102	0.00
ATOM	57	HG3	GLU	435	27.754	29.045	18.733	0.106	0.00
ATOM	58	CD	GLU	435	26.748	28.840	20.637	0.761	0.00
ATOM	59	OE1	GLU	435	26.607	27.867	21.445	-0.626	0.00
ATOM	60	OE2	GLU	435	26.763	30.054	20.968	-0.738	0.00
ATOM	61	h	ASP	447	29.181	24.999	22.853	0.127	0.00
ATOM	62	CB	ASP	447	28.913	25.620	23.710	-0.216	0.00
ATOM	63	HB2	ASP	447	28.387	26.505	23.332	0.185	0.00
ATOM	64	HB3	ASP	447	28.219	25.083	24.359	0.144	0.00
ATOM	65	CG	ASP	447	30.170	26.013	24.449	0.398	0.00
ATOM	66	OD1	ASP	447	31.302	25.858	24.034	-0.464	0.00
ATOM	67	OD2	ASP	447	29.970	26.562	25.669	-0.620	0.00
ATOM	68	O1	GOL	788	26.100	28.479	23.857	-0.277	0.15
ATOM	69	H01	GOL	788	26.310	28.315	22.841	0.361	0.00
ATOM	70	C1	GOL	788	27.163	29.036	24.493	-0.345	0.56
ATOM	71	H11	GOL	788	28.108	28.992	23.945	0.166	-0.01
ATOM	72	H12	GOL	788	27.088	30.562	24.576	0.279	-0.06
ATOM	73	C2	GOL	788	27.240	28.684	25.959	-0.064	-0.01

ATOM	74	O2	GOL	788	27.493	27.246	26.159	-0.526	0.02
ATOM	75	HO2	GOL	788	28.987	26.743	25.810	0.458	0.00
ATOM	76	H2	GOL	788	26.273	28.903	26.430	0.188	0.00
ATOM	77	C3	GOL	788	28.343	29.430	26.720	-0.357	0.00
ATOM	78	H31	GOL	788	28.048	30.476	26.824	0.149	0.00
ATOM	79	H32	GOL	788	28.408	29.002	27.734	0.099	0.00
ATOM	80	O3	GOL	788	29.603	29.446	26.073	-0.332	0.00
ATOM	81	HO3	GOL	788	29.981	28.550	26.082	0.232	0.00
ATOM	82	h	GLN	549	31.174	27.609	20.750	0.090	0.00
ATOM	83	CD	GLN	549	31.765	26.806	20.267	0.236	0.00
ATOM	84	OE1	GLN	549	32.132	26.869	19.103	-0.498	0.00
ATOM	85	NE2	GLN	549	32.002	25.772	21.113	-0.278	0.00
ATOM	86	HE21	GLN	549	32.581	25.013	20.779	0.163	0.00
ATOM	87	HE22	GLN	549	31.754	25.804	22.101	0.262	0.00
ATOM	88	CB	ASN	156	30.277	22.588	28.275	-0.472	0.00
ATOM	89	h	ASN	156	30.478	22.558	29.352	0.112	0.00
ATOM	90	HB2	ASN	156	31.095	23.129	27.789	0.090	0.00
ATOM	91	CG	ASN	156	28.915	23.228	28.045	0.404	0.00
ATOM	92	OD1	ASN	156	27.870	22.600	28.179	-0.443	0.00
ATOM	93	ND2	ASN	156	28.940	24.558	27.745	-0.258	0.00
ATOM	94	HD21	ASN	156	28.056	25.002	27.539	0.239	0.00
ATOM	95	HD22	ASN	156	29.769	25.025	27.403	0.195	0.00
ATOM	96	HB3	ASN	156	30.250	21.559	27.910	0.113	0.00

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ATOM	1	h	VAL	162	22.451	18.709	25.150	0.090	0.00
ATOM	2	C	VAL	162	22.693	19.714	25.539	0.296	0.00
ATOM	3	O	VAL	162	23.698	20.315	25.188	-0.493	0.00
ATOM	4	N	GLY	163	21.765	20.175	26.409	-0.200	0.00
ATOM	5	H	GLY	163	20.979	19.608	26.689	0.169	0.00
ATOM	6	h	GLY	163	21.900	21.072	26.859	0.193	0.00
ATOM	7	h	HIP	164	22.587	23.207	23.362	0.101	0.00

ATOM	8	CB	HIP	164	23.623	23.237	22.997	-0.542	0.00
ATOM	9	HB2	HIP	164	23.881	22.224	22.664	0.114	0.00
ATOM	10	HB3	HIP	164	23.648	23.897	22.126	0.118	0.00
ATOM	11	CG	HIP	164	24.569	23.736	24.039	0.117	0.00
ATOM	12	ND1	HIP	164	24.861	23.023	25.189	-0.252	0.00
ATOM	13	HD1	HIP	164	24.518	22.085	25.392	0.344	0.00
ATOM	14	CE1	HIP	164	25.720	23.761	25.936	0.110	0.00
ATOM	15	HE1	HIP	164	26.137	23.409	26.872	0.177	0.00
ATOM	16	NE2	HIP	164	25.996	24.912	25.339	-0.396	0.00
ATOM	17	HE2	HIP	164	26.858	26.437	25.818	0.509	0.00
ATOM	18	CD2	HIP	164	25.286	24.901	24.153	-0.237	0.00
ATOM	19	HD2	HIP	164	25.345	25.727	23.460	0.159	0.00
ATOM	20	h	HIE	281	22.551	25.159	30.180	0.082	0.00
ATOM	21	CB	HIE	281	22.848	26.185	29.924	-0.553	0.00
ATOM	22	HB2	HIE	281	22.292	26.493	29.033	0.092	0.00
ATOM	23	HB3	HIE	281	22.535	26.825	30.759	0.095	0.00
ATOM	24	CG	HIE	281	24.332	26.289	29.666	-0.180	0.01
ATOM	25	ND1	HIE	281	25.331	25.972	30.589	-0.332	0.00
ATOM	26	CE1	HIE	281	26.463	26.205	29.964	0.176	0.00
ATOM	27	HE1	HIE	281	27.453	26.058	30.377	0.108	0.00
ATOM	28	NE2	HIE	281	26.265	26.654	28.694	-0.291	0.00
ATOM	29	HE2	HIE	281	26.953	26.878	27.976	0.293	0.00
ATOM	30	CD2	HIE	281	24.904	26.708	28.490	0.333	0.00
ATOM	31	HD2	HIE	281	24.478	27.027	27.546	0.165	0.00
ATOM	32	h	SER	282	21.829	27.066	25.612	0.095	0.00
ATOM	33	CB	SER	282	22.623	27.103	24.858	-0.130	0.00
ATOM	34	HB2	SER	282	22.891	26.071	24.590	0.122	0.00
ATOM	35	HB3	SER	282	22.213	27.600	23.964	0.101	0.00
ATOM	36	OG	SER	282	23.704	27.819	25.422	-0.374	0.00
ATOM	37	HG	SER	282	24.407	27.919	24.748	0.303	0.00
ATOM	38	h	GLY	432	23.391	30.572	23.166	0.085	0.00
ATOM	39	C	GLY	432	23.760	31.607	23.023	0.223	0.00

ATOM	40	O	GLY	432	23.020	32.582	23.042-0.461	0.00
ATOM	41	N	CYX	433	25.109	31.649	22.859-0.227	0.01
ATOM	42	H	CYX	433	25.568	30.798	22.524 0.271-0.01	
ATOM	43	CA	CYX	433	25.737	32.919	22.536 0.267	0.00
ATOM	44	HA	CYX	433	25.343	33.677	23.214 0.133	0.00
ATOM	45	CB	CYX	433	27.266	32.845	22.665-0.203	0.00
ATOM	46	HB2	CYX	433	27.666	32.060	22.017 0.126	0.00
ATOM	47	HB3	CYX	433	27.684	33.801	22.337 0.112	0.00
ATOM	48	SG	CYX	433	27.911	32.599	24.369-0.213	0.01
ATOM	49	C	CYX	433	25.415	33.443	21.120 0.247	0.01
ATOM	50	O	CYX	433	25.274	34.645	20.933-0.524-0.01	
ATOM	51	N	VAL	434	25.366	32.509	20.134-0.435	0.00
ATOM	52	H	VAL	434	25.663	31.541	20.282 0.284	0.00
ATOM	53	h	VAL	434	25.266	32.856	19.190 0.181	0.00
ATOM	54	h	GLU	435	25.956	28.669	18.578 0.090	0.00
ATOM	55	CG	GLU	435	26.884	28.523	19.144-0.462	0.00
ATOM	56	HG2	GLU	435	27.255	27.512	18.964 0.107	0.00
ATOM	57	HG3	GLU	435	27.608	29.257	18.778 0.105	0.00
ATOM	58	CD	GLU	435	26.608	28.762	20.629 0.763	0.00
ATOM	59	OE1	GLU	435	26.631	27.747	21.398-0.605	0.00
ATOM	60	OE2	GLU	435	26.359	29.939	20.995-0.755	0.00
ATOM	61	h	ASP	447	29.191	25.003	22.853 0.127	0.00
ATOM	62	CB	ASP	447	28.913	25.620	23.710-0.221	0.00
ATOM	63	HB2	ASP	447	28.361	26.489	23.336 0.185	0.00
ATOM	64	HB3	ASP	447	28.242	25.063	24.368 0.136	0.00
ATOM	65	CG	ASP	447	30.168	26.053	24.434 0.405	0.00
ATOM	66	OD1	ASP	447	31.298	25.927	24.001-0.476	0.00
ATOM	67	OD2	ASP	447	29.975	26.607	25.650-0.607	0.00
ATOM	68	O1	GOL	788	25.999	28.185	23.776-0.300	0.15
ATOM	69	H01	GOL	788	26.232	28.077	22.743 0.393	0.00
ATOM	70	C1	GOL	788	27.037	28.743	24.435-0.189	0.83
ATOM	71	H11	GOL	788	27.935	28.970	23.866 0.178-0.05	

ATOM	72	H12	GOL	788	27.504	31.316	24.496	0.108	0.00
ATOM	73	C2	GOL	788	27.100	28.515	25.893	-0.055	0.01
ATOM	74	O2	GOL	788	27.492	27.102	26.225	-0.453	0.03
ATOM	75	H02	GOL	788	28.984	26.735	25.821	0.436	0.01
ATOM	76	H2	GOL	788	26.107	28.650	26.339	0.192	0.00
ATOM	77	C3	GOL	788	28.100	29.414	26.626	-0.552	0.00
ATOM	78	H31	GOL	788	27.687	30.426	26.664	0.138	0.00
ATOM	79	H32	GOL	788	28.191	29.059	27.666	0.101	0.00
ATOM	80	O3	GOL	788	29.365	29.531	26.000	-0.324	0.00
ATOM	81	H03	GOL	788	29.812	28.668	26.015	0.233	0.00
ATOM	82	h	GLN	549	31.089	27.557	20.720	0.090	0.00
ATOM	83	CD	GLN	549	31.741	26.790	20.258	0.240	0.00
ATOM	84	OE1	GLN	549	32.132	26.869	19.103	-0.503	0.00
ATOM	85	NE2	GLN	549	32.020	25.779	21.118	-0.286	0.00
ATOM	86	HE21	GLN	549	32.659	25.060	20.806	0.163	0.00
ATOM	87	HE22	GLN	549	31.758	25.813	22.103	0.272	0.00
ATOM	88	CB	ASN	156	30.277	22.588	28.275	-0.460	0.00
ATOM	89	h	ASN	156	30.449	22.531	29.356	0.112	0.00
ATOM	90	HB2	ASN	156	31.091	23.166	27.826	0.089	0.00
ATOM	91	CG	ASN	156	28.902	23.190	28.026	0.396	0.00
ATOM	92	OD1	ASN	156	27.874	22.536	28.173	-0.446	0.00
ATOM	93	ND2	ASN	156	28.895	24.509	27.687	-0.264	0.00
ATOM	94	HD21	ASN	156	28.004	24.936	27.472	0.245	0.00
ATOM	95	HD22	ASN	156	29.721	24.998	27.367	0.193	0.00
ATOM	96	HB3	ASN	156	30.293	21.569	27.882	0.112	0.00

TITLE TS2a

ATOM	1	h	VAL	162	22.140	18.559	25.203	0.088	0.00
ATOM	2	C	VAL	162	22.534	19.553	25.486	0.292	0.00
ATOM	3	O	VAL	162	23.552	20.007	24.985	-0.486	0.00
ATOM	4	N	GLY	163	21.765	20.175	26.409	-0.204	0.00
ATOM	5	H	GLY	163	20.964	19.719	26.819	0.169	0.00



ATOM	6	h	GLY	163	22.049	21.075	26.775	0.198	0.00
ATOM	7	h	HIP	164	22.600	23.088	23.370	0.097	0.00
ATOM	8	CB	HIP	164	23.623	23.237	22.997	-0.543	0.00
ATOM	9	HB2	HIP	164	23.907	22.326	22.455	0.111	0.00
ATOM	10	HB3	HIP	164	23.597	24.061	22.278	0.115	0.00
ATOM	11	CG	HIP	164	24.582	23.553	24.094	0.214	0.00
ATOM	12	ND1	HIP	164	24.874	22.661	25.110	-0.277	0.00
ATOM	13	HD1	HIP	164	24.500	21.715	25.184	0.335	0.00
ATOM	14	CE1	HIP	164	25.777	23.250	25.937	0.162	0.00
ATOM	15	HE1	HIP	164	26.209	22.752	26.799	0.175	0.00
ATOM	16	NE2	HIP	164	26.083	24.469	25.521	-0.300	0.00
ATOM	17	HE2	HIP	164	26.989	26.359	25.908	0.233	-0.01
ATOM	18	CD2	HIP	164	25.340	24.664	24.370	-0.319	-0.01
ATOM	19	HD2	HIP	164	25.396	25.594	23.820	0.144	0.00
ATOM	20	h	HIE	281	22.558	25.152	30.157	0.082	0.00
ATOM	21	CB	HIE	281	22.848	26.185	29.924	-0.550	0.00
ATOM	22	HB2	HIE	281	22.291	26.506	29.038	0.092	0.00
ATOM	23	HB3	HIE	281	22.527	26.805	30.771	0.091	0.00
ATOM	24	CG	HIE	281	24.333	26.304	29.671	-0.126	0.00
ATOM	25	ND1	HIE	281	25.331	25.972	30.589	-0.347	0.00
ATOM	26	CE1	HIE	281	26.463	26.205	29.958	0.168	0.00
ATOM	27	HE1	HIE	281	27.452	26.044	30.368	0.101	0.00
ATOM	28	NE2	HIE	281	26.270	26.678	28.699	-0.232	0.00
ATOM	29	HE2	HIE	281	26.965	26.846	27.961	0.288	0.00
ATOM	30	CD2	HIE	281	24.909	26.737	28.500	0.228	0.00
ATOM	31	HD2	HIE	281	24.481	27.079	27.566	0.166	0.00
ATOM	32	h	SER	282	21.730	27.194	25.488	0.096	0.00
ATOM	33	CB	SER	282	22.623	27.103	24.858	-0.155	0.00
ATOM	34	HB2	SER	282	22.987	26.067	24.927	0.119	0.00
ATOM	35	HB3	SER	282	22.315	27.289	23.815	0.088	0.00
ATOM	36	OG	SER	282	23.566	28.049	25.321	-0.447	0.00
ATOM	37	HG	SER	282	24.354	28.023	24.730	0.382	0.00

ATOM	38	h	GLY	432	23.491	30.599	23.281	0.118	0.00
ATOM	39	C	GLY	432	23.803	31.645	23.095	0.213	0.00
ATOM	40	O	GLY	432	23.020	32.582	23.042	-0.449	0.00
ATOM	41	N	CYX	433	25.157	31.768	22.973	-0.242	0.01
ATOM	42	H	CYX	433	25.696	30.929	22.766	0.266	-0.01
ATOM	43	CA	CYX	433	25.725	33.078	22.691	-0.052	0.00
ATOM	44	HA	CYX	433	25.105	33.808	23.211	0.153	0.00
ATOM	45	CB	CYX	433	27.169	33.174	23.199	0.062	0.00
ATOM	46	HB2	CYX	433	27.778	32.346	22.823	0.108	0.00
ATOM	47	HB3	CYX	433	27.614	34.109	22.847	0.102	0.00
ATOM	48	SG	CYX	433	27.283	33.250	25.037	-0.243	0.00
ATOM	49	C	CYX	433	25.638	33.510	21.210	0.361	0.00
ATOM	50	O	CYX	433	25.274	34.645	20.933	-0.509	0.00
ATOM	51	N	VAL	434	26.032	32.602	20.281	-0.446	0.00
ATOM	52	H	VAL	434	26.280	31.638	20.499	0.305	0.00
ATOM	53	h	VAL	434	25.951	32.881	19.313	0.189	0.00
ATOM	54	h	GLU	435	27.119	29.456	18.629	0.103	0.00
ATOM	55	CG	GLU	435	26.884	28.523	19.144	-0.410	0.00
ATOM	56	HG2	GLU	435	26.019	28.042	18.675	0.104	0.00
ATOM	57	HG3	GLU	435	27.729	27.833	19.053	0.123	0.00
ATOM	58	CD	GLU	435	26.597	28.783	20.610	0.653	0.00
ATOM	59	OE1	GLU	435	26.269	27.706	21.279	-0.460	0.00
ATOM	60	OE2	GLU	435	26.679	29.907	21.114	-0.604	0.00
ATOM	61	h	ASP	447	29.181	25.154	22.760	0.120	0.00
ATOM	62	CB	ASP	447	28.913	25.620	23.710	-0.191	0.00
ATOM	63	HB2	ASP	447	28.273	26.485	23.511	0.157	0.00
ATOM	64	HB3	ASP	447	28.330	24.919	24.314	0.138	0.00
ATOM	65	CG	ASP	447	30.171	26.047	24.438	0.409	0.01
ATOM	66	OD1	ASP	447	31.295	25.946	23.968	-0.489	0.00
ATOM	67	OD2	ASP	447	29.990	26.546	25.665	-0.680	0.00
ATOM	68	O1	GOL	788	25.855	28.155	23.718	-0.415	0.23
ATOM	69	HO1	GOL	788	26.070	27.942	22.294	0.412	0.00

ATOM	70	C1	GOL	788	26.931	28.628	24.294	-0.221	0.49
ATOM	71	H11	GOL	788	27.770	28.934	23.663	0.155	-0.04
ATOM	72	H12	GOL	788	26.460	32.203	25.261	0.060	0.00
ATOM	73	C2	GOL	788	27.107	28.646	25.706	-0.182	0.17
ATOM	74	O2	GOL	788	27.617	27.006	26.298	-0.311	0.16
ATOM	75	HO2	GOL	788	28.963	26.680	25.886	0.481	0.00
ATOM	76	H2	GOL	788	26.183	28.678	26.283	0.189	-0.01
ATOM	77	C3	GOL	788	28.229	29.486	26.289	-0.366	-0.03
ATOM	78	H31	GOL	788	27.915	30.536	26.290	0.136	0.01
ATOM	79	H32	GOL	788	28.384	29.191	27.338	0.102	0.01
ATOM	80	O3	GOL	788	29.436	29.448	25.548	-0.363	0.00
ATOM	81	HO3	GOL	788	29.841	28.571	25.671	0.258	0.00
ATOM	82	h	GLN	549	31.604	27.763	20.865	0.086	0.00
ATOM	83	CD	GLN	549	31.870	26.848	20.298	0.221	0.00
ATOM	84	OE1	GLN	549	32.132	26.869	19.103	-0.505	0.00
ATOM	85	NE2	GLN	549	31.854	25.748	21.087	-0.284	0.00
ATOM	86	HE21	GLN	549	32.117	24.864	20.672	0.162	0.00
ATOM	87	HE22	GLN	549	31.675	25.795	22.092	0.287	0.00
ATOM	88	CB	ASN	156	30.277	22.588	28.275	-0.412	0.00
ATOM	89	h	ASN	156	30.266	22.194	29.296	0.109	0.00
ATOM	90	HB2	ASN	156	30.991	23.415	28.216	0.088	0.00
ATOM	91	CG	ASN	156	28.860	22.974	27.884	0.376	0.00
ATOM	92	OD1	ASN	156	27.928	22.183	28.025	-0.476	0.00
ATOM	93	ND2	ASN	156	28.713	24.225	27.381	-0.312	0.00
ATOM	94	HD21	ASN	156	27.817	24.511	27.000	0.270	0.00
ATOM	95	HD22	ASN	156	29.503	24.819	27.170	0.190	0.00
ATOM	96	HB3	ASN	156	30.617	21.781	27.617	0.107	0.00

TITLE TSsb

ATOM	1	h	VAL	162	22.621	18.860	25.089	0.094	0.00
ATOM	2	C	VAL	162	22.762	19.853	25.554	0.295	0.00
ATOM	3	O	VAL	162	23.726	20.556	25.288	-0.498	0.00

ATOM	4	N	GLY	163	21.765	20.175	26.409	-0.196	0.00
ATOM	5	H	GLY	163	21.018	19.528	26.614	0.172	0.00
ATOM	6	h	GLY	163	21.805	21.047	26.922	0.193	0.00
ATOM	7	h	HIP	164	22.590	23.250	23.367	0.107	0.00
ATOM	8	CB	HIP	164	23.623	23.237	22.997	-0.532	0.00
ATOM	9	HB2	HIP	164	23.883	22.196	22.776	0.117	0.00
ATOM	10	HB3	HIP	164	23.652	23.805	22.064	0.123	0.00
ATOM	11	CG	HIP	164	24.570	23.841	23.988	0.084	0.00
ATOM	12	ND1	HIP	164	24.882	23.229	25.194	-0.258	0.00
ATOM	13	HD1	HIP	164	24.545	22.308	25.473	0.364	0.00
ATOM	14	CE1	HIP	164	25.714	24.030	25.891	0.114	0.00
ATOM	15	HE1	HIP	164	26.163	23.773	26.843	0.217	0.00
ATOM	16	NE2	HIP	164	25.950	25.133	25.188	-0.434	0.00
ATOM	17	HE2	HIP	164	26.625	26.090	25.578	0.696	0.00
ATOM	18	CD2	HIP	164	25.253	25.030	24.000	-0.165	0.00
ATOM	19	HD2	HIP	164	25.306	25.811	23.259	0.188	0.00
ATOM	20	h	HIE	281	22.520	25.185	30.242	0.081	0.00
ATOM	21	CB	HIE	281	22.848	26.185	29.924	-0.578	0.00
ATOM	22	HB2	HIE	281	22.295	26.456	29.019	0.092	0.00
ATOM	23	HB3	HIE	281	22.556	26.882	30.721	0.095	0.00
ATOM	24	CG	HIE	281	24.329	26.233	29.653	-0.350	0.00
ATOM	25	ND1	HIE	281	25.331	25.972	30.589	-0.340	0.00
ATOM	26	CE1	HIE	281	26.459	26.128	29.926	0.198	0.00
ATOM	27	HE1	HIE	281	27.452	25.997	30.338	0.103	0.00
ATOM	28	NE2	HIE	281	26.252	26.472	28.626	-0.297	0.00
ATOM	29	HE2	HIE	281	26.924	26.658	27.875	0.341	0.00
ATOM	30	CD2	HIE	281	24.890	26.542	28.440	0.391	0.00
ATOM	31	HD2	HIE	281	24.456	26.820	27.487	0.179	0.00
ATOM	32	h	SER	282	21.832	27.005	25.612	0.095	0.00
ATOM	33	CB	SER	282	22.623	27.103	24.858	-0.111	0.00
ATOM	34	HB2	SER	282	22.804	26.106	24.426	0.107	0.00
ATOM	35	HB3	SER	282	22.238	27.755	24.056	0.104	0.00

ATOM	36	OG	SER	282	23.756	27.641	25.494	-0.372	0.00
ATOM	37	HG	SER	282	24.455	27.813	24.820	0.288	0.00
ATOM	38	h	GLY	432	23.369	30.565	23.060	0.083	0.00
ATOM	39	C	GLY	432	23.750	31.602	22.971	0.239	0.00
ATOM	40	O	GLY	432	23.020	32.582	23.042	-0.464	0.00
ATOM	41	N	CYX	433	25.098	31.635	22.803	-0.211	0.00
ATOM	42	H	CYX	433	25.552	30.790	22.437	0.277	0.00
ATOM	43	CA	CYX	433	25.749	32.906	22.537	0.133	0.03
ATOM	44	HA	CYX	433	25.323	33.656	23.205	0.134	0.00
ATOM	45	CB	CYX	433	27.269	32.798	22.749	-0.073	-0.07
ATOM	46	HB2	CYX	433	27.661	31.926	22.206	0.118	0.03
ATOM	47	HB3	CYX	433	27.765	33.679	22.323	0.109	0.03
ATOM	48	SG	CYX	433	27.829	32.639	24.471	-0.205	0.97
ATOM	49	C	CYX	433	25.494	33.452	21.111	0.269	0.00
ATOM	50	O	CYX	433	25.274	34.645	20.933	-0.525	0.01
ATOM	51	N	VAL	434	25.589	32.537	20.112	-0.432	0.00
ATOM	52	H	VAL	434	25.857	31.560	20.272	0.290	0.00
ATOM	53	h	VAL	434	25.485	32.879	19.167	0.182	0.00
ATOM	54	h	GLU	435	26.036	28.877	18.545	0.085	0.00
ATOM	55	CG	GLU	435	26.884	28.523	19.144	-0.455	0.00
ATOM	56	HG2	GLU	435	27.070	27.470	18.921	0.102	0.00
ATOM	57	HG3	GLU	435	27.757	29.119	18.855	0.104	0.00
ATOM	58	CD	GLU	435	26.582	28.734	20.634	0.770	0.00
ATOM	59	OE1	GLU	435	26.528	27.711	21.373	-0.630	0.00
ATOM	60	OE2	GLU	435	26.407	29.929	21.015	-0.770	0.00
ATOM	61	h	ASP	447	29.247	25.106	22.806	0.125	0.00
ATOM	62	CB	ASP	447	28.913	25.620	23.710	-0.226	0.00
ATOM	63	HB2	ASP	447	28.182	26.384	23.427	0.166	0.00
ATOM	64	HB3	ASP	447	28.410	24.908	24.368	0.117	0.00
ATOM	65	CG	ASP	447	30.110	26.229	24.413	0.416	0.00
ATOM	66	OD1	ASP	447	31.252	26.189	23.977	-0.509	0.00
ATOM	67	OD2	ASP	447	29.848	26.805	25.586	-0.654	0.00

ATOM	68	O1	GOL	788	25.951	28.020	23.894	-0.376	0.00
ATOM	69	H01	GOL	788	26.146	28.021	22.899	0.362	0.00
ATOM	70	C1	GOL	788	26.921	28.800	24.578	-0.068	-0.01
ATOM	71	H11	GOL	788	27.900	28.712	24.092	0.131	0.00
ATOM	72	H12	GOL	788	26.647	29.866	24.569	0.144	0.01
ATOM	73	C2	GOL	788	27.018	28.337	26.030	0.022	0.01
ATOM	74	O2	GOL	788	27.421	26.954	26.127	-0.752	0.00
ATOM	75	H02	GOL	788	28.800	26.833	25.770	0.509	0.00
ATOM	76	H2	GOL	788	26.020	28.427	26.482	0.173	0.00
ATOM	77	C3	GOL	788	27.954	29.247	26.843	-0.536	0.00
ATOM	78	H31	GOL	788	27.455	30.211	26.985	0.136	0.00
ATOM	79	H32	GOL	788	28.097	28.800	27.841	0.094	0.00
ATOM	80	O3	GOL	788	29.196	29.552	26.227	-0.313	0.00
ATOM	81	H03	GOL	788	29.685	28.724	26.076	0.233	0.00
ATOM	82	h	GLN	549	31.022	27.593	20.660	0.091	0.00
ATOM	83	CD	GLN	549	31.712	26.829	20.251	0.238	0.00
ATOM	84	OE1	GLN	549	32.132	26.869	19.103	-0.505	0.00
ATOM	85	NE2	GLN	549	31.998	25.866	21.162	-0.300	0.00
ATOM	86	HE21	GLN	549	32.678	25.165	20.901	0.161	0.00
ATOM	87	HE22	GLN	549	31.723	25.951	22.143	0.288	0.00
ATOM	88	CB	ASN	156	30.277	22.588	28.275	-0.521	0.00
ATOM	89	h	ASN	156	30.169	22.207	29.295	0.113	0.00
ATOM	90	HB2	ASN	156	31.207	23.160	28.206	0.085	0.00
ATOM	91	CG	ASN	156	29.035	23.396	27.923	0.463	0.00
ATOM	92	OD1	ASN	156	27.916	22.886	27.934	-0.453	0.00
ATOM	93	ND2	ASN	156	29.249	24.704	27.627	-0.243	0.00
ATOM	94	HD21	ASN	156	28.475	25.271	27.303	0.255	0.00
ATOM	95	HD22	ASN	156	30.168	25.079	27.440	0.186	0.00
ATOM	96	HB3	ASN	156	30.337	21.723	27.607	0.110	0.00

TITLE TSIn

ATOM	1	h	VAL	162	22.573	18.864	25.055	0.095	0.00
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ATOM	2	C	VAL	162	22.738	19.848	25.530	0.298	0.00
ATOM	3	O	VAL	162	23.709	20.539	25.253	-0.500	0.00
ATOM	4	N	GLY	163	21.765	20.175	26.409	-0.196	0.00
ATOM	5	H	GLY	163	21.013	19.536	26.623	0.172	0.00
ATOM	6	h	GLY	163	21.831	21.038	26.934	0.192	0.00
ATOM	7	h	HIP	164	22.591	23.235	23.370	0.109	0.00
ATOM	8	CB	HIP	164	23.623	23.237	22.997	-0.552	0.00
ATOM	9	HB2	HIP	164	23.890	22.202	22.756	0.118	0.00
ATOM	10	HB3	HIP	164	23.645	23.823	22.075	0.123	0.00
ATOM	11	CG	HIP	164	24.569	23.828	23.997	0.091	0.00
ATOM	12	ND1	HIP	164	24.881	23.194	25.192	-0.260	0.00
ATOM	13	HD1	HIP	164	24.538	22.270	25.457	0.369	0.00
ATOM	14	CE1	HIP	164	25.721	23.975	25.900	0.127	0.00
ATOM	15	HE1	HIP	164	26.175	23.701	26.846	0.219	0.00
ATOM	16	NE2	HIP	164	25.962	25.086	25.213	-0.361	0.00
ATOM	17	HE2	HIP	164	26.638	26.009	25.607	0.645	0.00
ATOM	18	CD2	HIP	164	25.260	25.011	24.025	-0.201	0.00
ATOM	19	HD2	HIP	164	25.315	25.803	23.295	0.180	0.00
ATOM	20	h	HIE	281	22.523	25.184	30.241	0.081	0.00
ATOM	21	CB	HIE	281	22.848	26.185	29.924	-0.576	0.00
ATOM	22	HB2	HIE	281	22.295	26.455	29.019	0.090	0.00
ATOM	23	HB3	HIE	281	22.553	26.880	30.721	0.095	0.00
ATOM	24	CG	HIE	281	24.329	26.238	29.655	-0.266	0.00
ATOM	25	ND1	HIE	281	25.331	25.972	30.589	-0.344	0.00
ATOM	26	CE1	HIE	281	26.460	26.140	29.931	0.188	0.00
ATOM	27	HE1	HIE	281	27.452	26.009	30.343	0.104	0.00
ATOM	28	NE2	HIE	281	26.254	26.496	28.634	-0.309	0.00
ATOM	29	HE2	HIE	281	26.926	26.678	27.879	0.345	0.00
ATOM	30	CD2	HIE	281	24.892	26.560	28.445	0.359	0.00
ATOM	31	HD2	HIE	281	24.460	26.836	27.492	0.181	0.00
ATOM	32	h	SER	282	21.919	26.818	25.648	0.096	0.00
ATOM	33	CB	SER	282	22.623	27.103	24.858	-0.099	0.00

ATOM	34	HB2	SER	282	22.770	26.228	24.205	0.099	0.00
ATOM	35	HB3	SER	282	22.150	27.899	24.260	0.108	0.00
ATOM	36	OG	SER	282	23.811	27.528	25.481	-0.382	0.00
ATOM	37	HG	SER	282	24.456	27.805	24.796	0.310	0.00
ATOM	38	h	GLY	432	23.384	30.568	23.100	0.076	0.00
ATOM	39	C	GLY	432	23.758	31.607	22.994	0.223	0.00
ATOM	40	O	GLY	432	23.020	32.582	23.042	-0.465	0.00
ATOM	41	N	CYX	433	25.106	31.646	22.837	-0.217	0.00
ATOM	42	H	CYX	433	25.568	30.797	22.499	0.270	0.00
ATOM	43	CA	CYX	433	25.748	32.917	22.542	0.250	0.00
ATOM	44	HA	CYX	433	25.339	33.670	23.217	0.132	0.00
ATOM	45	CB	CYX	433	27.272	32.827	22.714	-0.195	0.00
ATOM	46	HB2	CYX	433	27.682	32.040	22.075	0.124	0.00
ATOM	47	HB3	CYX	433	27.710	33.779	22.400	0.109	0.00
ATOM	48	SG	CYX	433	27.870	32.574	24.435	-0.218	0.01
ATOM	49	C	CYX	433	25.456	33.448	21.120	0.261	0.01
ATOM	50	O	CYX	433	25.274	34.645	20.933	-0.523	-0.01
ATOM	51	N	VAL	434	25.472	32.520	20.127	-0.440	0.00
ATOM	52	H	VAL	434	25.766	31.552	20.280	0.288	0.00
ATOM	53	h	VAL	434	25.376	32.867	19.183	0.181	0.00
ATOM	54	h	GLU	435	26.038	28.873	18.541	0.088	0.00
ATOM	55	CG	GLU	435	26.884	28.523	19.144	-0.467	0.00
ATOM	56	HG2	GLU	435	27.072	27.468	18.930	0.104	0.00
ATOM	57	HG3	GLU	435	27.757	29.117	18.854	0.108	0.00
ATOM	58	CD	GLU	435	26.580	28.749	20.628	0.763	0.00
ATOM	59	OE1	GLU	435	26.540	27.729	21.384	-0.617	0.00
ATOM	60	OE2	GLU	435	26.389	29.937	21.003	-0.755	0.00
ATOM	61	h	ASP	447	29.246	25.102	22.808	0.124	0.00
ATOM	62	CB	ASP	447	28.913	25.620	23.710	-0.222	0.00
ATOM	63	HB2	ASP	447	28.213	26.408	23.419	0.165	0.00
ATOM	64	HB3	ASP	447	28.382	24.919	24.357	0.115	0.00
ATOM	65	CG	ASP	447	30.116	26.199	24.430	0.429	0.00



ATOM	66	OD1	ASP	447	31.255	26.164	23.984	-0.508	0.00
ATOM	67	OD2	ASP	447	29.859	26.744	25.616	-0.673	0.00
ATOM	68	O1	GOL	788	25.950	28.142	23.805	-0.341	0.12
ATOM	69	H01	GOL	788	26.177	28.080	22.784	0.390	0.01
ATOM	70	C1	GOL	788	26.985	28.667	24.514	-0.138	0.88
ATOM	71	H11	GOL	788	27.888	28.913	23.961	0.170	-0.06
ATOM	72	H12	GOL	788	27.483	31.284	24.554	0.113	0.01
ATOM	73	C2	GOL	788	27.048	28.307	25.957	0.033	-0.02
ATOM	74	O2	GOL	788	27.448	26.901	26.157	-0.636	0.04
ATOM	75	H02	GOL	788	28.798	26.775	25.806	0.506	0.00
ATOM	76	H2	GOL	788	26.044	28.403	26.393	0.173	0.00
ATOM	77	C3	GOL	788	27.980	29.233	26.754	-0.628	0.00
ATOM	78	H31	GOL	788	27.487	30.205	26.863	0.130	0.00
ATOM	79	H32	GOL	788	28.103	28.814	27.767	0.097	0.00
ATOM	80	O3	GOL	788	29.232	29.504	26.148	-0.334	0.00
ATOM	81	H03	GOL	788	29.716	28.666	26.039	0.242	0.00
ATOM	82	h	GLN	549	31.085	27.642	20.679	0.090	0.00
ATOM	83	CD	GLN	549	31.727	26.844	20.257	0.237	0.00
ATOM	84	OE1	GLN	549	32.132	26.869	19.103	-0.507	0.00
ATOM	85	NE2	GLN	549	31.975	25.864	21.160	-0.298	0.00
ATOM	86	HE21	GLN	549	32.611	25.127	20.885	0.161	0.00
ATOM	87	HE22	GLN	549	31.711	25.951	22.144	0.290	0.00
ATOM	88	CB	ASN	156	30.277	22.588	28.275	-0.514	0.00
ATOM	89	h	ASN	156	30.194	22.223	29.304	0.113	0.00
ATOM	90	HB2	ASN	156	31.200	23.168	28.178	0.086	0.00
ATOM	91	CG	ASN	156	29.022	23.380	27.936	0.458	0.00
ATOM	92	OD1	ASN	156	27.911	22.851	27.937	-0.460	0.00
ATOM	93	ND2	ASN	156	29.215	24.697	27.670	-0.245	0.00
ATOM	94	HD21	ASN	156	28.431	25.257	27.354	0.255	0.00
ATOM	95	HD22	ASN	156	30.126	25.085	27.469	0.188	0.00
ATOM	96	HB3	ASN	156	30.331	21.713	27.621	0.110	0.00

TITLE Sub

REMARK Unproductive steps (Note! Asn156 has been removed from the model)

ATOM	1	h	VAL	162	23.269	18.920	25.801	0.100	0.00
ATOM	2	C	VAL	162	23.028	19.983	25.972	0.323	0.00
ATOM	3	O	VAL	162	23.849	20.867	25.765	-0.537	0.00
ATOM	4	N	GLY	163	21.765	20.175	26.409	-0.197	0.00
ATOM	5	H	GLY	163	21.153	19.396	26.603	0.175	0.00
ATOM	6	h	GLY	163	21.447	21.108	26.638	0.189	0.00
ATOM	7	h	HIP	164	22.566	23.371	23.259	0.111	0.00
ATOM	8	CB	HIP	164	23.623	23.237	22.997	-0.549	0.00
ATOM	9	HB2	HIP	164	23.833	22.161	22.986	0.118	0.00
ATOM	10	HB3	HIP	164	23.769	23.626	21.986	0.127	0.00
ATOM	11	CG	HIP	164	24.513	23.957	23.952	0.177	0.00
ATOM	12	ND1	HIP	164	24.657	23.550	25.272	-0.213	0.00
ATOM	13	HD1	HIP	164	24.278	22.679	25.650	0.377	0.00
ATOM	14	CE1	HIP	164	25.447	24.421	25.918	0.074	0.00
ATOM	15	HE1	HIP	164	25.718	24.384	26.961	0.187	0.00
ATOM	16	NE2	HIP	164	25.811	25.365	25.061	-0.270	0.00
ATOM	17	HE2	HIP	164	26.392	26.213	25.338	0.591	0.00
ATOM	18	CD2	HIP	164	25.252	25.104	23.830	-0.213	0.00
ATOM	19	HD2	HIP	164	25.422	25.755	22.985	0.209	0.00
ATOM	20	h	HIE	281	22.538	25.166	30.194	0.082	0.00
ATOM	21	CB	HIE	281	22.848	26.185	29.924	-0.540	0.00
ATOM	22	HB2	HIE	281	22.293	26.489	29.031	0.093	0.00
ATOM	23	HB3	HIE	281	22.544	26.839	30.752	0.098	0.00
ATOM	24	CG	HIE	281	24.333	26.271	29.661	-0.305	0.00
ATOM	25	ND1	HIE	281	25.331	25.972	30.589	-0.368	0.00
ATOM	26	CE1	HIE	281	26.464	26.178	29.945	0.210	0.00
ATOM	27	HE1	HIE	281	27.454	26.046	30.363	0.105	0.00
ATOM	28	NE2	HIE	281	26.267	26.587	28.661	-0.299	0.00
ATOM	29	HE2	HIE	281	26.946	26.830	27.929	0.323	0.00
ATOM	30	CD2	HIE	281	24.903	26.656	28.471	0.351	0.00

ATOM	31	HD2	HIE	281	24.473	26.987	27.533	0.185	0.00
ATOM	32	h	SER	282	21.914	26.761	25.622	0.096	0.00
ATOM	33	CB	SER	282	22.623	27.103	24.858	-0.126	0.00
ATOM	34	HB2	SER	282	22.817	26.262	24.173	0.097	0.00
ATOM	35	HB3	SER	282	22.129	27.899	24.278	0.112	0.00
ATOM	36	OG	SER	282	23.780	27.554	25.520	-0.410	0.00
ATOM	37	HG	SER	282	24.442	27.869	24.858	0.313	0.00
ATOM	38	h	GLY	432	23.378	30.567	23.022	0.078	0.00
ATOM	39	C	GLY	432	23.755	31.607	22.955	0.250	0.00
ATOM	40	O	GLY	432	23.020	32.582	23.042	-0.456	0.00
ATOM	41	N	CYX	433	25.104	31.647	22.795	-0.222	0.00
ATOM	42	H	CYX	433	25.560	30.808	22.414	0.280	0.00
ATOM	43	CA	CYX	433	25.748	32.923	22.545	0.110	0.03
ATOM	44	HA	CYX	433	25.286	33.669	23.193	0.136	0.00
ATOM	45	CB	CYX	433	27.265	32.852	22.806	-0.084	-0.07
ATOM	46	HB2	CYX	433	27.686	31.953	22.335	0.123	0.03
ATOM	47	HB3	CYX	433	27.759	33.711	22.337	0.109	0.02
ATOM	48	SG	CYX	433	27.765	32.809	24.551	-0.205	0.97
ATOM	49	C	CYX	433	25.524	33.459	21.112	0.299	0.00
ATOM	50	O	CYX	433	25.274	34.645	20.933	-0.525	0.00
ATOM	51	N	VAL	434	25.679	32.551	20.115	-0.442	0.00
ATOM	52	H	VAL	434	25.950	31.575	20.281	0.299	0.00
ATOM	53	h	VAL	434	25.588	32.891	19.168	0.183	0.00
ATOM	54	h	GLU	435	26.153	29.029	18.502	0.084	0.00
ATOM	55	CG	GLU	435	26.884	28.523	19.144	-0.460	0.00
ATOM	56	HG2	GLU	435	26.924	27.461	18.889	0.100	0.00
ATOM	57	HG3	GLU	435	27.860	28.980	18.950	0.110	0.00
ATOM	58	CD	GLU	435	26.508	28.732	20.621	0.769	0.00
ATOM	59	OE1	GLU	435	26.310	27.711	21.340	-0.648	0.00
ATOM	60	OE2	GLU	435	26.431	29.933	21.019	-0.752	0.00
ATOM	61	h	ASP	447	29.291	25.043	22.862	0.110	0.00
ATOM	62	CB	ASP	447	28.913	25.620	23.710	-0.262	0.00

ATOM	63	HB2	ASP	447	28.171	26.334	23.333	0.140	0.00
ATOM	64	HB3	ASP	447	28.412	24.945	24.411	0.094	0.00
ATOM	65	CG	ASP	447	30.059	26.365	24.415	0.520	0.00
ATOM	66	OD1	ASP	447	31.182	26.422	23.888	-0.590	0.00
ATOM	67	OD2	ASP	447	29.761	26.903	25.548	-0.747	0.00
ATOM	68	O1	GOL	788	25.923	28.136	23.913	-0.438	0.00
ATOM	69	H01	GOL	788	26.040	28.089	22.908	0.369	0.00
ATOM	70	C1	GOL	788	26.954	28.949	24.471	-0.301	-0.02
ATOM	71	H11	GOL	788	27.906	28.763	23.962	0.159	0.00
ATOM	72	H12	GOL	788	26.715	30.015	24.359	0.149	0.02
ATOM	73	C2	GOL	788	27.101	28.645	25.957	0.211	0.01
ATOM	74	O2	GOL	788	27.361	27.239	26.175	-0.577	0.00
ATOM	75	H02	GOL	788	28.355	27.032	25.897	0.455	0.00
ATOM	76	H2	GOL	788	26.143	28.844	26.455	0.144	0.00
ATOM	77	C3	GOL	788	28.171	29.524	26.626	-0.461	0.00
ATOM	78	H31	GOL	788	27.779	30.546	26.689	0.124	0.00
ATOM	79	H32	GOL	788	28.305	29.160	27.661	0.081	0.00
ATOM	80	O3	GOL	788	29.395	29.609	25.932	-0.353	0.00
ATOM	81	H03	GOL	788	29.764	28.701	25.833	0.277	0.00
ATOM	82	h	GLN	549	31.038	27.702	20.616	0.088	0.00
ATOM	83	CD	GLN	549	31.688	26.885	20.246	0.229	0.00
ATOM	84	OE1	GLN	549	32.132	26.869	19.103	-0.524	0.00
ATOM	85	NE2	GLN	549	31.892	25.941	21.191	-0.323	0.00
ATOM	86	HE21	GLN	549	32.540	25.197	20.966	0.156	0.00
ATOM	87	HE22	GLN	549	31.604	26.080	22.172	0.337	0.00

TITLE TS1'

REMARK Unproductive steps (Note! Asn156 has been removed from the model)

ATOM	1	h	VAL	162	23.510	19.098	26.378	0.102	0.00
ATOM	2	C	VAL	162	23.109	20.121	26.282	0.330	0.00
ATOM	3	O	VAL	162	23.840	21.080	26.071	-0.546	0.00
ATOM	4	N	GLY	163	21.765	20.175	26.409	-0.199	0.00

ATOM	5	H	GLY	163	21.226	19.352	26.636	0.176	0.00
ATOM	6	h	GLY	163	21.293	21.070	26.387	0.189	0.00
ATOM	7	h	HIP	164	22.558	23.380	23.220	0.110	0.00
ATOM	8	CB	HIP	164	23.623	23.237	22.997	-0.524	0.00
ATOM	9	HB2	HIP	164	23.839	22.164	23.053	0.116	0.00
ATOM	10	HB3	HIP	164	23.798	23.569	21.971	0.128	0.00
ATOM	11	CG	HIP	164	24.480	24.021	23.939	0.163	0.00
ATOM	12	ND1	HIP	164	24.570	23.714	25.291	-0.228	0.00
ATOM	13	HD1	HIP	164	24.188	22.866	25.719	0.387	0.00
ATOM	14	CE1	HIP	164	25.313	24.642	25.911	0.048	0.00
ATOM	15	HE1	HIP	164	25.522	24.693	26.969	0.198	0.00
ATOM	16	NE2	HIP	164	25.705	25.528	25.004	-0.212	0.00
ATOM	17	HE2	HIP	164	26.199	26.422	25.230	0.521	0.00
ATOM	18	CD2	HIP	164	25.207	25.170	23.769	-0.188	0.00
ATOM	19	HD2	HIP	164	25.395	25.770	22.891	0.215	0.00
ATOM	20	h	HIE	281	22.565	25.138	30.099	0.083	0.00
ATOM	21	CB	HIE	281	22.848	26.185	29.924	-0.518	0.00
ATOM	22	HB2	HIE	281	22.291	26.551	29.056	0.094	0.00
ATOM	23	HB3	HIE	281	22.518	26.753	30.803	0.099	0.00
ATOM	24	CG	HIE	281	24.330	26.338	29.688	-0.113	0.00
ATOM	25	ND1	HIE	281	25.331	25.972	30.589	-0.366	0.00
ATOM	26	CE1	HIE	281	26.460	26.299	29.985	0.211	0.00
ATOM	27	HE1	HIE	281	27.451	26.160	30.396	0.105	0.00
ATOM	28	NE2	HIE	281	26.254	26.844	28.753	-0.254	0.00
ATOM	29	HE2	HIE	281	26.917	27.200	28.058	0.299	0.00
ATOM	30	CD2	HIE	281	24.892	26.877	28.554	0.203	-0.01
ATOM	31	HD2	HIE	281	24.458	27.280	27.647	0.183	0.00
ATOM	32	h	SER	282	21.977	26.672	25.632	0.095	0.00
ATOM	33	CB	SER	282	22.623	27.103	24.858	-0.126	0.00
ATOM	34	HB2	SER	282	22.877	26.306	24.142	0.098	0.00
ATOM	35	HB3	SER	282	22.033	27.861	24.318	0.114	0.00
ATOM	36	OG	SER	282	23.750	27.652	25.497	-0.413	0.00

ATOM	37	HG	SER	282	24.389	27.963	24.811	0.293	0.00
ATOM	38	h	GLY	432	23.374	30.587	22.754	0.074	0.00
ATOM	39	C	GLY	432	23.753	31.628	22.829	0.270	0.00
ATOM	40	O	GLY	432	23.020	32.582	23.042	-0.451	0.00
ATOM	41	N	CYX	433	25.097	31.685	22.679	-0.261	0.00
ATOM	42	H	CYX	433	25.562	30.875	22.253	0.318	0.00
ATOM	43	CA	CYX	433	25.784	32.969	22.627	0.164	0.00
ATOM	44	HA	CYX	433	25.204	33.673	23.224	0.143	0.00
ATOM	45	CB	CYX	433	27.215	32.844	23.191	-0.264	-0.01
ATOM	46	HB2	CYX	433	27.723	31.973	22.765	0.106	0.01
ATOM	47	HB3	CYX	433	27.794	33.726	22.900	0.106	0.01
ATOM	48	SG	CYX	433	27.303	32.780	25.041	-0.294	0.34
ATOM	49	C	CYX	433	25.759	33.546	21.185	0.286	0.00
ATOM	50	O	CYX	433	25.274	34.645	20.933	-0.511	0.00
ATOM	51	N	VAL	434	26.331	32.745	20.236	-0.418	0.00
ATOM	52	H	VAL	434	26.497	31.747	20.398	0.280	0.00
ATOM	53	h	VAL	434	26.206	33.046	19.279	0.183	0.00
ATOM	54	h	GLU	435	26.348	29.218	18.488	0.088	0.00
ATOM	55	CG	GLU	435	26.884	28.523	19.144	-0.389	0.00
ATOM	56	HG2	GLU	435	26.710	27.496	18.814	0.095	0.00
ATOM	57	HG3	GLU	435	27.952	28.752	19.053	0.112	0.00
ATOM	58	CD	GLU	435	26.444	28.730	20.593	0.714	0.00
ATOM	59	OE1	GLU	435	26.054	27.713	21.242	-0.672	0.00
ATOM	60	OE2	GLU	435	26.518	29.908	21.044	-0.730	0.00
ATOM	61	h	ASP	447	29.383	24.940	22.995	0.106	0.00
ATOM	62	CB	ASP	447	28.913	25.620	23.710	-0.237	0.00
ATOM	63	HB2	ASP	447	28.124	26.177	23.190	0.138	0.00
ATOM	64	HB3	ASP	447	28.447	25.040	24.514	0.093	0.00
ATOM	65	CG	ASP	447	29.937	26.610	24.286	0.461	0.00
ATOM	66	OD1	ASP	447	31.067	26.706	23.784	-0.562	0.00
ATOM	67	OD2	ASP	447	29.523	27.312	25.284	-0.745	0.00
ATOM	68	O1	GOL	788	25.839	28.096	23.781	-0.506	0.00

ATOM	69	H01	GOL	788	25.855	28.038	22.761	0.438	0.00
ATOM	70	C1	GOL	788	26.860	29.003	24.179	-0.566	0.04
ATOM	71	H11	GOL	788	27.827	28.705	23.754	0.165	0.00
ATOM	72	H12	GOL	788	26.633	30.013	23.836	0.213	0.00
ATOM	73	C2	GOL	788	26.940	29.016	25.700	0.402	-0.01
ATOM	74	O2	GOL	788	27.170	27.669	26.196	-0.503	0.02
ATOM	75	H02	GOL	788	28.093	27.396	25.852	0.411	0.00
ATOM	76	H2	GOL	788	25.961	29.312	26.090	0.155	0.00
ATOM	77	C3	GOL	788	27.950	30.037	26.216	-0.576	0.49
ATOM	78	H31	GOL	788	27.626	31.297	25.434	0.231	-0.05
ATOM	79	H32	GOL	788	27.693	30.494	27.178	0.109	0.00
ATOM	80	O3	GOL	788	29.280	29.792	26.145	-0.359	0.16
ATOM	81	H03	GOL	788	29.506	28.955	25.647	0.347	0.00
ATOM	82	h	GLN	549	31.000	27.698	20.590	0.090	0.00
ATOM	83	CD	GLN	549	31.670	26.889	20.237	0.230	0.00
ATOM	84	OE1	GLN	549	32.132	26.869	19.103	-0.522	0.00
ATOM	85	NE2	GLN	549	31.873	25.958	21.197	-0.321	0.00
ATOM	86	HE21	GLN	549	32.551	25.233	20.999	0.158	0.00
ATOM	87	HE22	GLN	549	31.580	26.135	22.169	0.329	0.00

TITLE In1'

REMARK Unproductive steps (Note! Asn156 has been removed from the model)

ATOM	1	h	VAL	162	23.260	18.922	25.775	0.101	0.00
ATOM	2	C	VAL	162	23.024	19.984	25.960	0.322	0.00
ATOM	3	O	VAL	162	23.846	20.868	25.757	-0.536	0.00
ATOM	4	N	GLY	163	21.765	20.175	26.409	-0.198	0.00
ATOM	5	H	GLY	163	21.151	19.396	26.599	0.176	0.00
ATOM	6	h	GLY	163	21.452	21.106	26.652	0.189	0.00
ATOM	7	h	HIP	164	22.562	23.377	23.242	0.110	0.00
ATOM	8	CB	HIP	164	23.623	23.237	22.997	-0.547	0.00
ATOM	9	HB2	HIP	164	23.827	22.160	22.991	0.118	0.00
ATOM	10	HB3	HIP	164	23.786	23.623	21.988	0.127	0.00

ATOM	11	CG	HIP	164	24.501	23.956	23.963	0.164	0.00
ATOM	12	ND1	HIP	164	24.624	23.558	25.288	-0.209	0.00
ATOM	13	HD1	HIP	164	24.247	22.684	25.663	0.373	0.00
ATOM	14	CE1	HIP	164	25.400	24.436	25.941	0.077	0.00
ATOM	15	HE1	HIP	164	25.653	24.410	26.990	0.190	0.00
ATOM	16	NE2	HIP	164	25.775	25.375	25.083	-0.297	0.00
ATOM	17	HE2	HIP	164	26.342	26.231	25.361	0.604	0.00
ATOM	18	CD2	HIP	164	25.237	25.103	23.846	-0.205	0.00
ATOM	19	HD2	HIP	164	25.416	25.750	22.999	0.207	0.00
ATOM	20	h	HIE	281	22.546	25.157	30.167	0.082	0.00
ATOM	21	CB	HIE	281	22.848	26.185	29.924	-0.535	0.00
ATOM	22	HB2	HIE	281	22.292	26.507	29.038	0.092	0.00
ATOM	23	HB3	HIE	281	22.537	26.815	30.767	0.098	0.00
ATOM	24	CG	HIE	281	24.333	26.291	29.668	-0.264	0.01
ATOM	25	ND1	HIE	281	25.331	25.972	30.589	-0.365	0.00
ATOM	26	CE1	HIE	281	26.465	26.218	29.961	0.211	0.00
ATOM	27	HE1	HIE	281	27.454	26.086	30.380	0.105	0.00
ATOM	28	NE2	HIE	281	26.268	26.670	28.693	-0.293	0.00
ATOM	29	HE2	HIE	281	26.947	26.940	27.971	0.316	0.00
ATOM	30	CD2	HIE	281	24.906	26.725	28.495	0.335	-0.02
ATOM	31	HD2	HIE	281	24.477	27.076	27.564	0.175	0.00
ATOM	32	h	SER	282	21.905	26.837	25.643	0.098	0.00
ATOM	33	CB	SER	282	22.623	27.103	24.858	-0.129	0.00
ATOM	34	HB2	SER	282	22.821	26.201	24.257	0.100	0.00
ATOM	35	HB3	SER	282	22.140	27.844	24.201	0.113	0.00
ATOM	36	OG	SER	282	23.775	27.609	25.490	-0.407	0.00
ATOM	37	HG	SER	282	24.443	27.873	24.812	0.305	0.00
ATOM	38	h	GLY	432	23.412	30.574	23.062	0.080	0.00
ATOM	39	C	GLY	432	23.774	31.619	22.991	0.236	0.00
ATOM	40	O	GLY	432	23.020	32.582	23.042	-0.453	0.00
ATOM	41	N	CYX	433	25.130	31.680	22.869	-0.259	0.00
ATOM	42	H	CYX	433	25.588	30.849	22.474	0.292	0.00



ATOM	43	CA	CYX	433	25.736	32.974	22.588	0.170	0.00
ATOM	44	HA	CYX	433	25.236	33.717	23.209	0.141	0.00
ATOM	45	CB	CYX	433	27.246	32.990	22.875	-0.159	0.00
ATOM	46	HB2	CYX	433	27.740	32.123	22.426	0.123	0.00
ATOM	47	HB3	CYX	433	27.671	33.888	22.418	0.111	0.00
ATOM	48	SG	CYX	433	27.727	33.130	24.648	-0.244	0.00
ATOM	49	C	CYX	433	25.508	33.461	21.140	0.313	0.01
ATOM	50	O	CYX	433	25.274	34.645	20.933	-0.525	-0.01
ATOM	51	N	VAL	434	25.639	32.527	20.164	-0.451	0.00
ATOM	52	H	VAL	434	25.912	31.554	20.340	0.307	0.00
ATOM	53	h	VAL	434	25.547	32.853	19.212	0.184	0.00
ATOM	54	h	GLU	435	26.169	29.052	18.504	0.084	0.00
ATOM	55	CG	GLU	435	26.884	28.523	19.144	-0.435	0.00
ATOM	56	HG2	GLU	435	26.912	27.466	18.871	0.100	0.00
ATOM	57	HG3	GLU	435	27.870	28.967	18.968	0.110	0.00
ATOM	58	CD	GLU	435	26.499	28.710	20.622	0.741	0.00
ATOM	59	OE1	GLU	435	26.333	27.672	21.328	-0.646	0.00
ATOM	60	OE2	GLU	435	26.387	29.900	21.037	-0.759	0.00
ATOM	61	h	ASP	447	29.320	25.004	22.904	0.109	0.00
ATOM	62	CB	ASP	447	28.913	25.620	23.710	-0.260	0.00
ATOM	63	HB2	ASP	447	28.158	26.288	23.279	0.144	0.00
ATOM	64	HB3	ASP	447	28.422	24.976	24.446	0.094	0.00
ATOM	65	CG	ASP	447	30.023	26.447	24.376	0.488	0.00
ATOM	66	OD1	ASP	447	31.137	26.550	23.842	-0.582	0.00
ATOM	67	OD2	ASP	447	29.698	27.011	25.491	-0.770	0.00
ATOM	68	O1	GOL	788	25.968	28.076	23.881	-0.450	0.00
ATOM	69	H01	GOL	788	26.075	28.033	22.870	0.388	0.00
ATOM	70	C1	GOL	788	26.982	28.913	24.426	-0.405	0.06
ATOM	71	H11	GOL	788	27.952	28.700	23.960	0.150	0.00
ATOM	72	H12	GOL	788	26.746	29.969	24.248	0.186	0.00
ATOM	73	C2	GOL	788	27.080	28.689	25.941	0.572	-0.11
ATOM	74	O2	GOL	788	27.296	27.266	26.199	-0.577	0.01

ATOM	75	H02	GOL	788	28.270	27.054	25.914	0.432	0.00
ATOM	76	H2	GOL	788	26.105	28.920	26.383	0.141	0.00
ATOM	77	C3	GOL	788	28.101	29.546	26.622	-0.721	0.94
ATOM	78	H31	GOL	788	27.490	31.853	25.012	0.087	0.00
ATOM	79	H32	GOL	788	27.790	30.458	27.121	0.125	-0.05
ATOM	80	O3	GOL	788	29.412	29.549	26.275	-0.329	0.15
ATOM	81	H03	GOL	788	29.691	28.659	25.923	0.345	0.00
ATOM	82	h	GLN	549	30.997	27.681	20.597	0.088	0.00
ATOM	83	CD	GLN	549	31.671	26.879	20.238	0.229	0.00
ATOM	84	OE1	GLN	549	32.132	26.869	19.103	-0.522	0.00
ATOM	85	NE2	GLN	549	31.882	25.942	21.190	-0.323	0.00
ATOM	86	HE21	GLN	549	32.559	25.219	20.982	0.158	0.00
ATOM	87	HE22	GLN	549	31.591	26.099	22.167	0.336	0.00

TITLE Suba

REMARK Unproductive steps (Note! Asn156 has been removed from the model)

ATOM	1	h	VAL	162	23.067	18.630	26.110	0.092	0.00
ATOM	2	C	VAL	162	22.993	19.732	26.102	0.301	0.00
ATOM	3	O	VAL	162	23.949	20.440	25.824	-0.503	0.00
ATOM	4	N	GLY	163	21.753	20.176	26.416	-0.205	0.00
ATOM	5	H	GLY	163	21.019	19.537	26.683	0.170	0.00
ATOM	6	h	GLY	163	21.577	21.170	26.480	0.193	0.00
ATOM	7	h	HIP	164	22.571	23.258	23.327	0.097	0.00
ATOM	8	CB	HIP	164	23.620	23.230	23.001	-0.574	0.00
ATOM	9	HB2	HIP	164	23.863	22.186	22.763	0.109	0.00
ATOM	10	HB3	HIP	164	23.694	23.810	22.077	0.121	0.00
ATOM	11	CG	HIP	164	24.540	23.801	24.028	0.082	0.00
ATOM	12	ND1	HIP	164	24.741	23.221	25.271	-0.243	0.00
ATOM	13	HD1	HIP	164	24.390	22.311	25.566	0.356	0.00
ATOM	14	CE1	HIP	164	25.582	24.028	25.969	0.117	0.00
ATOM	15	HE1	HIP	164	25.898	23.817	26.981	0.139	0.00
ATOM	16	NE2	HIP	164	25.928	25.087	25.260	-0.423	0.00

ATOM	17	HE2	HIP	164	26.797	26.607	25.720	0.618	0.00
ATOM	18	CD2	HIP	164	25.287	24.952	24.046	-0.113	0.00
ATOM	19	HD2	HIP	164	25.405	25.694	23.269	0.166	0.00
ATOM	20	h	HIE	281	22.529	25.179	30.222	0.081	0.00
ATOM	21	CB	HIE	281	22.846	26.187	29.924	-0.547	0.00
ATOM	22	HB2	HIE	281	22.292	26.471	29.024	0.094	0.00
ATOM	23	HB3	HIE	281	22.550	26.866	30.734	0.095	0.00
ATOM	24	CG	HIE	281	24.331	26.252	29.655	-0.356	0.00
ATOM	25	ND1	HIE	281	25.328	25.970	30.591	-0.372	0.00
ATOM	26	CE1	HIE	281	26.462	26.146	29.945	0.212	0.00
ATOM	27	HE1	HIE	281	27.451	26.016	30.367	0.100	0.00
ATOM	28	NE2	HIE	281	26.267	26.521	28.651	-0.258	0.00
ATOM	29	HE2	HIE	281	26.954	26.731	27.925	0.297	0.00
ATOM	30	CD2	HIE	281	24.905	26.595	28.454	0.393	0.00
ATOM	31	HD2	HIE	281	24.481	26.890	27.501	0.177	0.00
ATOM	32	h	SER	282	21.814	27.052	25.591	0.093	0.00
ATOM	33	CB	SER	282	22.627	27.100	24.857	-0.136	0.00
ATOM	34	HB2	SER	282	22.874	26.072	24.551	0.117	0.00
ATOM	35	HB3	SER	282	22.245	27.637	23.973	0.102	0.00
ATOM	36	OG	SER	282	23.710	27.767	25.466	-0.385	0.00
ATOM	37	HG	SER	282	24.435	27.870	24.808	0.306	0.00
ATOM	38	h	GLY	432	23.388	30.559	23.067	0.088	0.00
ATOM	39	C	GLY	432	23.766	31.596	22.970	0.247	-0.01
ATOM	40	O	GLY	432	23.037	32.576	23.035	-0.459	0.01
ATOM	41	N	CYX	433	25.116	31.630	22.804	-0.226	0.00
ATOM	42	H	CYX	433	25.569	30.787	22.430	0.283	0.00
ATOM	43	CA	CYX	433	25.760	32.903	22.533	0.133	0.03
ATOM	44	HA	CYX	433	25.319	33.654	23.189	0.135	0.00
ATOM	45	CB	CYX	433	27.281	32.821	22.759	-0.092	-0.08
ATOM	46	HB2	CYX	433	27.684	31.922	22.270	0.120	0.03
ATOM	47	HB3	CYX	433	27.771	33.680	22.286	0.111	0.02
ATOM	48	SG	CYX	433	27.828	32.763	24.491	-0.207	0.97

ATOM	49	C	CYX	433	25.514	33.439	21.103	0.282	0.00
ATOM	50	O	CYX	433	25.297	34.632	20.925	-0.521	0.00
ATOM	51	N	VAL	434	25.614	32.521	20.108	-0.441	0.00
ATOM	52	H	VAL	434	25.884	31.545	20.272	0.299	0.00
ATOM	53	h	VAL	434	25.516	32.861	19.162	0.183	0.00
ATOM	54	h	GLU	435	26.013	28.803	18.566	0.087	0.00
ATOM	55	CG	GLU	435	26.895	28.504	19.145	-0.486	0.00
ATOM	56	HG2	GLU	435	27.130	27.459	18.932	0.104	0.00
ATOM	57	HG3	GLU	435	27.726	29.142	18.822	0.103	0.00
ATOM	58	CD	GLU	435	26.621	28.722	20.640	0.781	0.00
ATOM	59	OE1	GLU	435	26.591	27.705	21.388	-0.622	0.00
ATOM	60	OE2	GLU	435	26.434	29.918	21.016	-0.782	0.00
ATOM	61	h	ASP	447	29.227	24.944	22.903	0.121	0.00
ATOM	62	CB	ASP	447	28.915	25.602	23.716	-0.269	0.00
ATOM	63	HB2	ASP	447	28.294	26.401	23.290	0.183	0.00
ATOM	64	HB3	ASP	447	28.291	25.052	24.424	0.133	0.00
ATOM	65	CG	ASP	447	30.144	26.178	24.387	0.472	0.00
ATOM	66	OD1	ASP	447	31.273	26.103	23.935	-0.516	0.00
ATOM	67	OD2	ASP	447	29.937	26.803	25.557	-0.540	0.00
ATOM	68	O1	GOL	788	25.982	28.095	23.899	-0.391	0.00
ATOM	69	HO1	GOL	788	26.175	28.027	22.905	0.366	0.00
ATOM	70	C1	GOL	788	26.940	28.951	24.498	-0.352	-0.02
ATOM	71	H11	GOL	788	27.921	28.831	24.023	0.155	0.00
ATOM	72	H12	GOL	788	26.653	30.008	24.405	0.151	0.01
ATOM	73	C2	GOL	788	27.050	28.621	25.979	0.249	0.01
ATOM	74	O2	GOL	788	27.434	27.235	26.178	-0.622	0.00
ATOM	75	HO2	GOL	788	28.957	26.849	25.775	0.435	0.00
ATOM	76	H2	GOL	788	26.067	28.760	26.450	0.172	0.00
ATOM	77	C3	GOL	788	28.055	29.513	26.711	-0.506	0.00
ATOM	78	H31	GOL	788	27.627	30.518	26.780	0.140	0.00
ATOM	79	H32	GOL	788	28.178	29.131	27.738	0.093	0.00
ATOM	80	O3	GOL	788	29.304	29.675	26.059	-0.312	0.00

ATOM	81	H03	GOL	788	29.747	28.811	25.992	0.230	0.00
ATOM	82	h	GLN	549	30.933	27.513	20.677	0.094	0.00
ATOM	83	CD	GLN	549	31.677	26.817	20.242	0.239	0.00
ATOM	84	OE1	GLN	549	32.096	26.934	19.099	-0.508	0.00
ATOM	85	NE2	GLN	549	32.026	25.839	21.113	-0.295	0.00
ATOM	86	HE21	GLN	549	32.762	25.204	20.832	0.162	0.00
ATOM	87	HE22	GLN	549	31.752	25.875	22.096	0.283	0.00

TITLE TS1a'

REMARK Unproductive steps (Note! Asn156 has been removed from the model)

ATOM	1	h	VAL	162	23.200	18.715	26.309	0.092	0.00
ATOM	2	C	VAL	162	23.050	19.807	26.225	0.305	0.00
ATOM	3	O	VAL	162	23.974	20.567	25.980	-0.509	0.00
ATOM	4	N	GLY	163	21.761	20.174	26.411	-0.204	0.00
ATOM	5	H	GLY	163	21.053	19.500	26.664	0.170	0.00
ATOM	6	h	GLY	163	21.513	21.155	26.402	0.191	0.00
ATOM	7	h	HIP	164	22.571	23.303	23.282	0.096	0.00
ATOM	8	CB	HIP	164	23.630	23.230	23.000	-0.553	0.00
ATOM	9	HB2	HIP	164	23.858	22.168	22.841	0.107	0.00
ATOM	10	HB3	HIP	164	23.754	23.747	22.045	0.120	0.00
ATOM	11	CG	HIP	164	24.525	23.852	24.028	0.136	0.00
ATOM	12	ND1	HIP	164	24.672	23.351	25.312	-0.224	0.00
ATOM	13	HD1	HIP	164	24.321	22.454	25.645	0.348	0.00
ATOM	14	CE1	HIP	164	25.491	24.198	25.993	0.100	0.00
ATOM	15	HE1	HIP	164	25.761	24.045	27.028	0.140	0.00
ATOM	16	NE2	HIP	164	25.874	25.213	25.240	-0.354	0.00
ATOM	17	HE2	HIP	164	26.658	26.985	25.724	0.476	0.00
ATOM	18	CD2	HIP	164	25.281	24.999	24.010	-0.199	0.00
ATOM	19	HD2	HIP	164	25.426	25.689	23.192	0.165	0.00
ATOM	20	h	HIE	281	22.551	25.146	30.117	0.081	0.00
ATOM	21	CB	HIE	281	22.841	26.187	29.922	-0.519	0.00
ATOM	22	HB2	HIE	281	22.287	26.540	29.047	0.094	0.00

ATOM	23	HB3	HIE	281	22.519	26.776	30.791	0.095	0.00
ATOM	24	CG	HIE	281	24.325	26.320	29.679	-0.131	0.00
ATOM	25	ND1	HIE	281	25.323	25.972	30.593	-0.370	0.00
ATOM	26	CE1	HIE	281	26.455	26.262	29.983	0.207	0.00
ATOM	27	HE1	HIE	281	27.445	26.126	30.401	0.100	0.00
ATOM	28	NE2	HIE	281	26.257	26.768	28.733	-0.225	0.00
ATOM	29	HE2	HIE	281	26.935	27.084	28.042	0.261	0.00
ATOM	30	CD2	HIE	281	24.896	26.810	28.528	0.247	-0.01
ATOM	31	HD2	HIE	281	24.469	27.168	27.598	0.162	0.00
ATOM	32	h	SER	282	21.787	27.168	25.553	0.096	0.00
ATOM	33	CB	SER	282	22.630	27.099	24.854	-0.156	0.00
ATOM	34	HB2	SER	282	22.895	26.038	24.737	0.123	0.00
ATOM	35	HB3	SER	282	22.284	27.475	23.877	0.104	0.00
ATOM	36	OG	SER	282	23.685	27.872	25.384	-0.387	0.00
ATOM	37	HG	SER	282	24.413	27.897	24.722	0.289	0.00
ATOM	38	h	GLY	432	23.370	30.574	22.768	0.085	0.00
ATOM	39	C	GLY	432	23.757	31.611	22.827	0.274	0.00
ATOM	40	O	GLY	432	23.037	32.576	23.033	-0.448	0.00
ATOM	41	N	CYX	433	25.103	31.662	22.670	-0.298	0.00
ATOM	42	H	CYX	433	25.568	30.852	22.246	0.322	0.00
ATOM	43	CA	CYX	433	25.787	32.947	22.619	0.184	0.00
ATOM	44	HA	CYX	433	25.205	33.650	23.215	0.145	0.00
ATOM	45	CB	CYX	433	27.216	32.819	23.188	-0.281	0.00
ATOM	46	HB2	CYX	433	27.720	31.942	22.772	0.107	0.01
ATOM	47	HB3	CYX	433	27.803	33.695	22.896	0.109	0.01
ATOM	48	SG	CYX	433	27.310	32.786	25.040	-0.265	0.35
ATOM	49	C	CYX	433	25.768	33.528	21.176	0.283	0.00
ATOM	50	O	CYX	433	25.298	34.634	20.927	-0.508	0.00
ATOM	51	N	VAL	434	26.328	32.718	20.228	-0.423	0.00
ATOM	52	H	VAL	434	26.491	31.720	20.393	0.284	0.00
ATOM	53	h	VAL	434	26.207	33.018	19.270	0.184	0.00
ATOM	54	h	GLU	435	26.085	28.919	18.549	0.092	0.00

ATOM	55	CG	GLU	435	26.906	28.508	19.149	-0.440	0.00
ATOM	56	HG2	GLU	435	27.036	27.453	18.900	0.104	0.00
ATOM	57	HG3	GLU	435	27.810	29.066	18.882	0.105	0.00
ATOM	58	CD	GLU	435	26.592	28.695	20.628	0.750	0.00
ATOM	59	OE1	GLU	435	26.357	27.645	21.296	-0.644	0.00
ATOM	60	OE2	GLU	435	26.579	29.879	21.071	-0.763	0.00
ATOM	61	h	ASP	447	29.337	24.839	23.071	0.119	0.00
ATOM	62	CB	ASP	447	28.921	25.608	23.723	-0.240	0.00
ATOM	63	HB2	ASP	447	28.237	26.236	23.136	0.179	0.00
ATOM	64	HB3	ASP	447	28.323	25.152	24.517	0.132	0.00
ATOM	65	CG	ASP	447	30.042	26.457	24.278	0.432	0.00
ATOM	66	OD1	ASP	447	31.186	26.447	23.860	-0.487	0.00
ATOM	67	OD2	ASP	447	29.723	27.287	25.287	-0.563	0.00
ATOM	68	O1	GOL	788	25.936	28.013	23.774	-0.438	0.00
ATOM	69	HO1	GOL	788	26.031	27.916	22.757	0.427	0.00
ATOM	70	C1	GOL	788	26.827	29.018	24.196	-0.411	0.02
ATOM	71	H11	GOL	788	27.835	28.854	23.780	0.143	0.00
ATOM	72	H12	GOL	788	26.499	30.012	23.884	0.219	0.00
ATOM	73	C2	GOL	788	26.875	28.991	25.715	0.222	0.01
ATOM	74	O2	GOL	788	27.258	27.651	26.164	-0.470	0.01
ATOM	75	HO2	GOL	788	28.764	27.228	25.579	0.429	0.00
ATOM	76	H2	GOL	788	25.867	29.197	26.093	0.189	0.00
ATOM	77	C3	GOL	788	27.798	30.048	26.292	-0.615	0.52
ATOM	78	H31	GOL	788	27.501	31.303	25.481	0.233	-0.06
ATOM	79	H32	GOL	788	27.493	30.471	27.251	0.123	0.00
ATOM	80	O3	GOL	788	29.149	29.857	26.294	-0.327	0.14
ATOM	81	HO3	GOL	788	29.435	29.202	25.629	0.294	0.00
ATOM	82	h	GLN	549	30.932	27.538	20.679	0.093	0.00
ATOM	83	CD	GLN	549	31.665	26.830	20.245	0.238	0.00
ATOM	84	OE1	GLN	549	32.065	26.922	19.094	-0.503	0.00
ATOM	85	NE2	GLN	549	32.022	25.868	21.132	-0.291	0.00
ATOM	86	HE21	GLN	549	32.756	25.229	20.859	0.165	0.00

ATOM 87 HE22 GLN 549 31.764 25.947 22.116 0.273 0.00

TITLE In1a'

REMARK Unproductive steps (Note! Asn156 has been removed from the model)

ATOM	1	h	VAL	162	23.067	18.629	26.096	0.092	0.00
ATOM	2	C	VAL	162	22.994	19.732	26.096	0.303	0.00
ATOM	3	O	VAL	162	23.951	20.440	25.821	-0.506	0.00
ATOM	4	N	GLY	163	21.756	20.175	26.414	-0.203	0.00
ATOM	5	H	GLY	163	21.020	19.536	26.677	0.170	0.00
ATOM	6	h	GLY	163	21.581	21.169	26.486	0.192	0.00
ATOM	7	h	HIP	164	22.571	23.273	23.312	0.097	0.00
ATOM	8	CB	HIP	164	23.624	23.230	23.001	-0.558	0.00
ATOM	9	HB2	HIP	164	23.856	22.181	22.773	0.109	0.00
ATOM	10	HB3	HIP	164	23.718	23.803	22.074	0.120	0.00
ATOM	11	CG	HIP	164	24.537	23.796	24.036	0.141	0.00
ATOM	12	ND1	HIP	164	24.721	23.224	25.284	-0.251	0.00
ATOM	13	HD1	HIP	164	24.371	22.312	25.578	0.355	0.00
ATOM	14	CE1	HIP	164	25.557	24.032	25.986	0.108	0.00
ATOM	15	HE1	HIP	164	25.861	23.828	27.003	0.140	0.00
ATOM	16	NE2	HIP	164	25.915	25.085	25.274	-0.427	0.00
ATOM	17	HE2	HIP	164	26.761	26.600	25.734	0.627	0.01
ATOM	18	CD2	HIP	164	25.289	24.943	24.054	-0.155	0.00
ATOM	19	HD2	HIP	164	25.417	25.679	23.273	0.162	0.00
ATOM	20	h	HIE	281	22.534	25.171	30.200	0.081	0.00
ATOM	21	CB	HIE	281	22.844	26.187	29.923	-0.538	0.00
ATOM	22	HB2	HIE	281	22.290	26.483	29.027	0.093	0.00
ATOM	23	HB3	HIE	281	22.540	26.848	30.746	0.096	0.00
ATOM	24	CG	HIE	281	24.330	26.270	29.661	-0.340	0.00
ATOM	25	ND1	HIE	281	25.326	25.971	30.592	-0.368	0.00
ATOM	26	CE1	HIE	281	26.461	26.178	29.958	0.216	0.00
ATOM	27	HE1	HIE	281	27.449	26.048	30.382	0.100	0.00
ATOM	28	NE2	HIE	281	26.269	26.588	28.676	-0.264	0.00



ATOM	29	HE2	HIE	281	26.958	26.820	27.958	0.292	0.00
ATOM	30	CD2	HIE	281	24.908	26.652	28.473	0.393	-0.01
ATOM	31	HD2	HIE	281	24.485	26.966	27.526	0.170	0.00
ATOM	32	h	SER	282	21.787	27.184	25.554	0.097	0.00
ATOM	33	CB	SER	282	22.628	27.100	24.856	-0.147	0.00
ATOM	34	HB2	SER	282	22.883	26.035	24.749	0.118	0.00
ATOM	35	HB3	SER	282	22.286	27.469	23.875	0.103	0.00
ATOM	36	OG	SER	282	23.691	27.868	25.380	-0.387	0.00
ATOM	37	HG	SER	282	24.434	27.872	24.736	0.306	0.00
ATOM	38	h	GLY	432	23.424	30.568	23.129	0.094	0.00
ATOM	39	C	GLY	432	23.786	31.608	23.012	0.237	0.00
ATOM	40	O	GLY	432	23.037	32.576	23.034	-0.452	0.00
ATOM	41	N	CYX	433	25.143	31.663	22.880	-0.277	0.00
ATOM	42	H	CYX	433	25.595	30.827	22.490	0.296	0.00
ATOM	43	CA	CYX	433	25.753	32.949	22.570	0.165	0.00
ATOM	44	HA	CYX	433	25.288	33.703	23.206	0.142	0.00
ATOM	45	CB	CYX	433	27.272	32.936	22.801	-0.125	0.00
ATOM	46	HB2	CYX	433	27.726	32.057	22.332	0.121	0.00
ATOM	47	HB3	CYX	433	27.700	33.826	22.330	0.110	0.00
ATOM	48	SG	CYX	433	27.824	33.064	24.554	-0.247	0.00
ATOM	49	C	CYX	433	25.490	33.439	21.130	0.297	0.00
ATOM	50	O	CYX	433	25.298	34.632	20.926	-0.527	0.00
ATOM	51	N	VAL	434	25.546	32.496	20.155	-0.446	0.00
ATOM	52	H	VAL	434	25.818	31.522	20.327	0.303	0.00
ATOM	53	h	VAL	434	25.442	32.821	19.204	0.183	0.00
ATOM	54	h	GLU	435	26.014	28.794	18.569	0.087	0.00
ATOM	55	CG	GLU	435	26.900	28.505	19.147	-0.466	0.00
ATOM	56	HG2	GLU	435	27.156	27.467	18.926	0.105	0.00
ATOM	57	HG3	GLU	435	27.720	29.161	18.832	0.104	0.00
ATOM	58	CD	GLU	435	26.621	28.705	20.645	0.775	0.00
ATOM	59	OE1	GLU	435	26.648	27.678	21.384	-0.625	0.00
ATOM	60	OE2	GLU	435	26.378	29.884	21.034	-0.795	0.00

ATOM	61	h	ASP	447	29.274	24.899	22.966	0.121	0.00
ATOM	62	CB	ASP	447	28.917	25.604	23.719	-0.279	0.00
ATOM	63	HB2	ASP	447	28.262	26.333	23.225	0.186	0.00
ATOM	64	HB3	ASP	447	28.315	25.082	24.466	0.129	0.00
ATOM	65	CG	ASP	447	30.105	26.306	24.343	0.469	0.00
ATOM	66	OD1	ASP	447	31.234	26.292	23.885	-0.511	0.00
ATOM	67	OD2	ASP	447	29.858	26.992	25.472	-0.569	0.00
ATOM	68	O1	GOL	788	26.042	28.010	23.879	-0.396	0.00
ATOM	69	H01	GOL	788	26.234	27.965	22.877	0.378	0.00
ATOM	70	C1	GOL	788	26.941	28.914	24.484	-0.414	0.08
ATOM	71	H11	GOL	788	27.945	28.824	24.045	0.146	0.00
ATOM	72	H12	GOL	788	26.613	29.954	24.350	0.182	0.00
ATOM	73	C2	GOL	788	27.009	28.629	25.987	0.587	-0.17
ATOM	74	O2	GOL	788	27.391	27.231	26.199	-0.627	0.01
ATOM	75	H02	GOL	788	28.885	26.935	25.739	0.434	0.00
ATOM	76	H2	GOL	788	26.007	28.764	26.411	0.175	0.00
ATOM	77	C3	GOL	788	27.945	29.517	26.737	-0.788	0.99
ATOM	78	H31	GOL	788	27.404	31.851	24.966	0.084	0.00
ATOM	79	H32	GOL	788	27.560	30.372	27.281	0.133	-0.05
ATOM	80	O3	GOL	788	29.250	29.682	26.376	-0.293	0.13
ATOM	81	H03	GOL	788	29.608	28.872	25.960	0.285	0.00
ATOM	82	h	GLN	549	30.824	27.423	20.630	0.096	0.00
ATOM	83	CD	GLN	549	31.640	26.792	20.227	0.238	0.00
ATOM	84	OE1	GLN	549	32.082	26.932	19.097	-0.505	0.00
ATOM	85	NE2	GLN	549	32.045	25.857	21.123	-0.299	0.00
ATOM	86	HE21	GLN	549	32.856	25.303	20.879	0.164	0.00
ATOM	87	HE22	GLN	549	31.761	25.913	22.102	0.283	0.00