

created with PyMOL 2.5.2

@<TRIPOS>MOLECULE

CoilPDB

1358 1357 50

SMALL

USER_CHARGES

@<TRIPOS>ATOM

1	C1	103.715	21.451	41.880	C.3	1	HED1	0.000
2	N1	103.088	19.050	45.783	N.3	1	HED1	0.000
3	O1	102.159	18.913	42.643	O.3	1	HED1	0.000
4	C2	104.431	20.068	41.444	C.3	1	HED1	0.000
5	O2	102.980	16.875	41.999	O.3	1	HED1	0.000
6	C3	103.558	18.933	40.781	C.3	1	HED1	0.000
7	C5	102.886	18.101	41.877	C.3	1	HED1	0.000
8	C6	101.383	18.400	43.770	C.3	1	HED1	0.000
9	C7	102.346	18.016	45.004	C.3	1	HED1	0.000
10	C8	103.685	20.113	44.907	C.3	1	HED1	0.000
11	C9	104.188	18.390	46.529	C.3	1	HED1	0.000
12	C10	104.619	18.085	39.977	C.3	1	HED1	0.000
13	H01	103.275	22.093	41.107	H	1	HED1	0.000
14	H02	102.809	21.303	42.482	H	1	HED1	0.000
15	H03	104.366	22.033	42.544	H	1	HED1	0.000
16	H04	102.439	19.492	46.450	H	1	HED1	0.000
17	H05	104.971	19.685	42.319	H	1	HED1	0.000
18	H06	105.202	20.393	40.733	H	1	HED1	0.000
19	H10	100.851	17.488	43.470	H	1	HED1	0.000
20	H11	100.620	19.120	44.092	H	1	HED1	0.000
21	H12	102.966	17.192	44.647	H	1	HED1	0.000
22	H13	101.628	17.586	45.703	H	1	HED1	0.000
23	H14	102.830	20.676	44.530	H	1	HED1	0.000
24	H15	104.318	20.778	45.497	H	1	HED1	0.000

25	H16	104.221	19.704 44.049	H	1	HED1	0.000
26	H17	104.539	19.057 47.318	H	1	HED1	0.000
27	H18	103.780	17.560 47.108	H	1	HED1	0.000
28	H19	105.049	18.195 45.888	H	1	HED1	0.000
29	H20	105.441	17.752 40.622	H	1	HED1	0.000
30	H21	104.187	17.199 39.496	H	1	HED1	0.000
31	H22	105.133	18.687 39.218	H	1	HED1	0.000
32	N1	105.484	20.328 35.592	N.3	2	PLY2	0.000
33	O1	103.046	18.778 36.957	O.3	2	PLY2	0.000
34	C2	102.491	19.564 39.812	C.3	2	PLY2	0.000
35	O2	102.457	16.729 37.619	O.3	2	PLY2	0.000
36	C3	101.534	18.662 38.886	C.3	2	PLY2	0.000
37	C5	102.399	17.905 37.801	C.3	2	PLY2	0.000
38	C6	103.848	18.271 35.919	C.3	2	PLY2	0.000
39	C7	104.328	19.500 35.045	C.3	2	PLY2	0.000
40	C8	105.011	21.156 36.774	C.3	2	PLY2	0.000
41	C9	105.978	21.231 34.557	C.3	2	PLY2	0.000
42	C10	100.680	19.642 38.063	C.3	2	PLY2	0.000
43	H04	106.218	19.691 35.935	H	2	PLY2	0.000
44	H05	103.075	20.269 39.207	H	2	PLY2	0.000
45	H06	101.829	20.192 40.420	H	2	PLY2	0.000
46	H10	103.355	17.568 35.237	H	2	PLY2	0.000
47	H11	104.771	17.778 36.250	H	2	PLY2	0.000
48	H12	103.485	20.180 34.910	H	2	PLY2	0.000
49	H13	104.668	19.103 34.087	H	2	PLY2	0.000
50	H14	104.103	21.717 36.553	H	2	PLY2	0.000
51	H15	104.842	20.572 37.680	H	2	PLY2	0.000
52	H16	105.892	21.749 37.022	H	2	PLY2	0.000
53	H17	106.501	22.068 35.021	H	2	PLY2	0.000
54	H18	106.677	20.695 33.913	H	2	PLY2	0.000
55	H19	105.110	21.643 34.039	H	2	PLY2	0.000

56	H20	101.154	20.467	37.517	H	2	PLY2	0.000
57	H21	100.058	19.217	37.267	H	2	PLY2	0.000
58	H22	99.980	20.107	38.769	H	2	PLY2	0.000
59	N1	96.544	19.844	43.063	N.3	3	PLY3	0.000
60	O1	97.846	18.773	40.525	O.3	3	PLY3	0.000
61	C2	100.556	17.789	39.804	C.3	3	PLY3	0.000
62	O2	97.667	18.776	38.200	O.3	3	PLY3	0.000
63	C3	99.207	17.125	39.301	C.3	3	PLY3	0.000
64	C5	98.141	18.258	39.241	C.3	3	PLY3	0.000
65	C6	96.970	19.878	40.582	C.3	3	PLY3	0.000
66	C7	97.259	20.574	41.883	C.3	3	PLY3	0.000
67	C8	95.049	20.152	43.101	C.3	3	PLY3	0.000
68	C9	97.077	20.325	44.419	C.3	3	PLY3	0.000
69	C10	98.674	16.066	40.348	C.3	3	PLY3	0.000
70	H04	96.724	18.832	42.998	H	3	PLY3	0.000
71	H05	100.342	18.404	40.687	H	3	PLY3	0.000
72	H06	101.134	16.924	40.153	H	3	PLY3	0.000
73	H10	95.925	19.547	40.537	H	3	PLY3	0.000
74	H11	97.007	20.556	39.721	H	3	PLY3	0.000
75	H12	96.957	21.622	41.885	H	3	PLY3	0.000
76	H13	98.344	20.509	41.974	H	3	PLY3	0.000
77	H14	94.612	19.682	43.983	H	3	PLY3	0.000
78	H15	94.857	21.226	43.130	H	3	PLY3	0.000
79	H16	94.640	19.632	42.234	H	3	PLY3	0.000
80	H17	98.134	20.055	44.421	H	3	PLY3	0.000
81	H18	96.814	21.356	44.660	H	3	PLY3	0.000
82	H19	96.608	19.658	45.143	H	3	PLY3	0.000
83	H20	97.584	15.954	40.408	H	3	PLY3	0.000
84	H21	99.322	15.183	40.278	H	3	PLY3	0.000
85	H22	98.960	16.456	41.332	H	3	PLY3	0.000
86	N1	102.369	11.835	37.487	N.3	4	PLY4	0.000

87	O1	99.907	13.458	38.097	O.3	4	PLY4	0.000
88	C2	99.489	16.368	37.899	C.3	4	PLY4	0.000
89	O2	97.637	13.262	38.529	O.3	4	PLY4	0.000
90	C3	98.521	15.257	37.254	C.3	4	PLY4	0.000
91	C5	98.583	13.930	38.097	C.3	4	PLY4	0.000
92	C6	100.292		12.268	38.864	C.3	4	PLY4 0.000
93	C7	101.805		12.222	38.831	C.3	4	PLY4 0.000
94	C8	103.806		11.445	37.599	C.3	4	PLY4 0.000
95	C9	102.353		13.080	36.605	C.3	4	PLY4 0.000
96	C10	99.154	14.954	35.846	C.3	4	PLY4	0.000
97	H04	101.819		11.086	37.042	H	4	PLY4 0.000
98	H05	100.412		15.812	38.107	H	4	PLY4 0.000
99	H06	99.775	17.094	37.128	H	4	PLY4	0.000
100	H10	99.853	11.294	38.615	H	4	PLY4	0.000
101	H11	100.167		12.309	39.953	H	4	PLY4 0.000
102	H12	102.166		11.438	39.498	H	4	PLY4 0.000
103	H13	102.166		13.164	39.248	H	4	PLY4 0.000
104	H14	104.160		11.086	36.632	H	4	PLY4 0.000
105	H15	104.389		12.328	37.863	H	4	PLY4 0.000
106	H16	103.952		10.636	38.317	H	4	PLY4 0.000
107	H17	101.296		13.255	36.397	H	4	PLY4 0.000
108	H18	102.759		13.971	37.087	H	4	PLY4 0.000
109	H19	102.890		12.925	35.669	H	4	PLY4 0.000
110	H20	100.184		14.576	35.865	H	4	PLY4 0.000
111	H21	98.562	14.227	35.276	H	4	PLY4	0.000
112	H22	99.174	15.890	35.275	H	4	PLY4	0.000
113	N1	95.871	11.260	39.099	N.3	5	PLY5	0.000
114	O1	94.528	13.433	38.074	O.3	5	PLY5	0.000
115	C2	97.020	15.986	37.069	C.3	5	PLY5	0.000
116	O2	95.329	15.338	39.177	O.3	5	PLY5	0.000
117	C3	95.651	15.124	36.754	C.3	5	PLY5	0.000

118	C5	95.100	14.690	38.099	C.3	5	PLY5	0.000
119	C6	93.982	12.915	39.251	C.3	5	PLY5	0.000
120	C7	94.945	12.031	40.043	C.3	5	PLY5	0.000
121	C8	95.139	10.306	38.228	C.3	5	PLY5	0.000
122	C9	97.017	10.668	39.856	C.3	5	PLY5	0.000
123	C10	95.891	14.000	35.736	C.3	5	PLY5	0.000
124	H04	96.212	11.944	38.409	H	5	PLY5	0.000
125	H05	97.082	16.720	36.255	H	5	PLY5	0.000
126	H06	96.710	16.566	37.947	H	5	PLY5	0.000
127	H10	93.125	12.283	38.987	H	5	PLY5	0.000
128	H11	93.526	13.732	39.823	H	5	PLY5	0.000
129	H12	94.491	11.319	40.734	H	5	PLY5	0.000
130	H13	95.542	12.779	40.566	H	5	PLY5	0.000
131	H14	95.911	9.848	37.607	H	5	PLY5	0.000
132	H15	94.583	9.576	38.819	H	5	PLY5	0.000
133	H16	94.349	10.838	37.696	H	5	PLY5	0.000
134	H17	96.693	10.057	40.700	H	5	PLY5	0.000
135	H18	97.587	10.029	39.179	H	5	PLY5	0.000
136	H19	97.676	11.492	40.134	H	5	PLY5	0.000
137	H20	96.286	14.590	34.900	H	5	PLY5	0.000
138	H21	96.622	13.256	36.075	H	5	PLY5	0.000
139	H22	94.985	13.476	35.408	H	5	PLY5	0.000
140	N1	88.243	15.198	39.999	N.3	6	PLY6	0.000
141	O1	91.214	15.692	37.440	O.3	6	PLY6	0.000
142	C2	94.736	16.266	36.072	C.3	6	PLY6	0.000
143	O2	92.997	16.664	38.394	O.3	6	PLY6	0.000
144	C3	93.150	16.035	35.964	C.3	6	PLY6	0.000
145	C5	92.499	16.164	37.416	C.3	6	PLY6	0.000
146	C6	90.529	15.726	38.761	C.3	6	PLY6	0.000
147	C7	89.064	15.163	38.682	C.3	6	PLY6	0.000
148	C8	86.979	14.426	39.802	C.3	6	PLY6	0.000

149	C9	87.948	16.622	40.347	C.3	6	PLY6	0.000
150	C10	92.790	14.655	35.340	C.3	6	PLY6	0.000
151	H04	88.799	14.812	40.776	H	6	PLY6	0.000
152	H05	95.073	16.359	35.032	H	6	PLY6	0.000
153	H06	94.913	17.200	36.619	H	6	PLY6	0.000
154	H10	90.524	16.777	39.075	H	6	PLY6	0.000
155	H11	91.064	15.207	39.566	H	6	PLY6	0.000
156	H12	89.060	14.189	38.189	H	6	PLY6	0.000
157	H13	88.527	15.810	37.987	H	6	PLY6	0.000
158	H14	87.132	13.531	39.198	H	6	PLY6	0.000
159	H15	86.347	14.350	40.688	H	6	PLY6	0.000
160	H16	86.467	15.031	39.052	H	6	PLY6	0.000
161	H17	87.312	16.662	41.232	H	6	PLY6	0.000
162	H18	88.871	17.148	40.593	H	6	PLY6	0.000
163	H19	87.521	17.051	39.439	H	6	PLY6	0.000
164	H20	91.737	14.461	35.097	H	6	PLY6	0.000
165	H21	93.301	14.484	34.385	H	6	PLY6	0.000
166	H22	92.964	13.807	36.014	H	6	PLY6	0.000
167	N1	94.236	23.325	33.370	N.3	7	PLY7	0.000
168	O1	94.060	20.345	33.811	O.3	7	PLY7	0.000
169	C2	92.405	17.023	34.904	C.3	7	PLY7	0.000
170	O2	94.429	18.150	33.160	O.3	7	PLY7	0.000
171	C3	92.635	18.619	34.781	C.3	7	PLY7	0.000
172	C5	93.796	18.997	33.784	C.3	7	PLY7	0.000
173	C6	95.169	20.870	33.113	C.3	7	PLY7	0.000
174	C7	95.427	22.333	33.666	C.3	7	PLY7	0.000
175	C8	93.776	23.472	31.906	C.3	7	PLY7	0.000
176	C9	94.599	24.712	33.873	C.3	7	PLY7	0.000
177	C10	92.826	19.121	36.260	C.3	7	PLY7	0.000
178	H04	93.420	22.953	33.878	H	7	PLY7	0.000
179	H05	91.334	16.894	35.105	H	7	PLY7	0.000

180	H06	92.653	16.621	33.914	H	7	PLY7	0.000
181	H10	94.972	20.925	32.036	H	7	PLY7	0.000
182	H11	96.070	20.286	33.339	H	7	PLY7	0.000
183	H12	96.357	22.677	33.209	H	7	PLY7	0.000
184	H13	95.596	22.286	34.742	H	7	PLY7	0.000
185	H14	93.306	22.568	31.516	H	7	PLY7	0.000
186	H15	92.990	24.229	31.915	H	7	PLY7	0.000
187	H16	94.648	23.859	31.376	H	7	PLY7	0.000
188	H17	93.744	25.389	33.850	H	7	PLY7	0.000
189	H18	94.753	24.537	34.939	H	7	PLY7	0.000
190	H19	95.521	25.119	33.455	H	7	PLY7	0.000
191	H20	93.787	18.784	36.669	H	7	PLY7	0.000
192	H21	92.931	20.210	36.188	H	7	PLY7	0.000
193	H22	92.084	18.798	37.000	H	7	PLY7	0.000
194	N1	91.666	15.290	29.207	N.3	8	PLY8	0.000
195	O1	91.077	16.595	32.088	O.3	8	PLY8	0.000
196	C2	91.175	19.171	34.386	C.3	8	PLY8	0.000
197	O2	89.392	16.657	33.673	O.3	8	PLY8	0.000
198	C3	90.452	18.808	33.009	C.3	8	PLY8	0.000
199	C5	90.165	17.269	32.933	C.3	8	PLY8	0.000
200	C6	90.826	15.229	31.746	C.3	8	PLY8	0.000
201	C7	91.756	14.716	30.642	C.3	8	PLY8	0.000
202	C8	92.988	15.001	28.460	C.3	8	PLY8	0.000
203	C9	91.379	16.781	29.196	C.3	8	PLY8	0.000
204	C10	91.247	19.346	31.852	C.3	8	PLY8	0.000
205	H04	90.928	14.794	28.686	H	8	PLY8	0.000
206	H05	91.251	20.263	34.306	H	8	PLY8	0.000
207	H06	90.498	19.034	35.238	H	8	PLY8	0.000
208	H10	89.847	15.149	31.257	H	8	PLY8	0.000
209	H11	90.912	14.503	32.564	H	8	PLY8	0.000
210	H12	91.638	13.636	30.536	H	8	PLY8	0.000

211	H13	92.756	14.941	31.013	H	8	PLY8	0.000
212	H14	92.949	15.520	27.501	H	8	PLY8	0.000
213	H15	93.777	15.455	29.062	H	8	PLY8	0.000
214	H16	93.211	13.955	28.242	H	8	PLY8	0.000
215	H17	91.361	17.124	28.161	H	8	PLY8	0.000
216	H18	90.338	17.019	29.417	H	8	PLY8	0.000
217	H19	92.108	17.324	29.800	H	8	PLY8	0.000
218	H20	90.812	18.999	30.906	H	8	PLY8	0.000
219	H21	91.452	20.423	31.881	H	8	PLY8	0.000
220	H22	92.194	18.793	31.823	H	8	PLY8	0.000
221	N1	86.527	21.118	27.132	N.3	9	PLY9	0.000
222	O1	87.509	19.713	29.517	O.3	9	PLY9	0.000
223	C2	89.035	19.577	33.055	C.3	9	PLY9	0.000
224	O2	88.503	17.994	30.643	O.3	9	PLY9	0.000
225	C3	88.230	20.077	31.756	C.3	9	PLY9	0.000
226	C5	88.054	19.113	30.588	C.3	9	PLY9	0.000
227	C6	87.087	18.872	28.378	C.3	9	PLY9	0.000
228	C7	86.965	19.627	27.021	C.3	9	PLY9	0.000
229	C8	86.030	21.772	25.820	C.3	9	PLY9	0.000
230	C9	87.684	21.908	27.557	C.3	9	PLY9	0.000
231	C10	88.845	21.431	31.242	C.3	9	PLY9	0.000
232	H04	85.864	21.267	27.906	H	9	PLY9	0.000
233	H05	89.149	20.553	33.541	H	9	PLY9	0.000
234	H06	88.244	19.088	33.638	H	9	PLY9	0.000
235	H10	86.180	18.282	28.558	H	9	PLY9	0.000
236	H11	87.834	18.083	28.224	H	9	PLY9	0.000
237	H12	86.180	19.151	26.433	H	9	PLY9	0.000
238	H13	87.834	19.497	26.375	H	9	PLY9	0.000
239	H14	86.842	22.176	25.213	H	9	PLY9	0.000
240	H15	85.295	21.151	25.306	H	9	PLY9	0.000
241	H16	85.373	22.580	26.145	H	9	PLY9	0.000

242	H17	87.862	21.571	28.580	H	9	PLY9	0.000
243	H18	88.549	21.639	26.950	H	9	PLY9	0.000
244	H19	87.583	22.995	27.563	H	9	PLY9	0.000
245	H20	89.095	22.051	32.111	H	9	PLY9	0.000
246	H21	89.757	21.245	30.662	H	9	PLY9	0.000
247	H22	88.204	22.097	30.651	H	9	PLY9	0.000
248	N1	84.956	15.074	30.073	N.3	10	PLY10	0.000
249	O1	86.231	17.127	31.784	O.3	10	PLY10	0.000
250	C2	86.795	20.454	32.318	C.3	10	PLY10	0.000
251	O2	86.508	17.411	34.029	O.3	10	PLY10	0.000
252	C3	85.710	19.366	32.705	C.3	10	PLY10	0.000
253	C5	86.307	17.901	32.922	C.3	10	PLY10	0.000
254	C6	86.650	15.677	31.919	C.3	10	PLY10	0.000
255	C7	86.369	14.882	30.598	C.3	10	PLY10	0.000
256	C8	83.896	14.824	31.149	C.3	10	PLY10	0.000
257	C9	84.776	14.118	28.860	C.3	10	PLY10	0.000
258	C10	84.666	19.298	31.468	C.3	10	PLY10	0.000
259	H04	84.892	16.051	29.754	H	10	PLY10	0.000
260	H05	86.293	21.160	31.645	H	10	PLY10	0.000
261	H06	86.909	21.074	33.216	H	10	PLY10	0.000
262	H10	86.066	15.281	32.759	H	10	PLY10	0.000
263	H11	87.707	15.672	32.215	H	10	PLY10	0.000
264	H12	86.346	13.820	30.848	H	10	PLY10	0.000
265	H13	87.188	15.086	29.906	H	10	PLY10	0.000
266	H14	82.865	14.789	30.794	H	10	PLY10	0.000
267	H15	83.910	13.798	31.519	H	10	PLY10	0.000
268	H16	83.894	15.427	32.058	H	10	PLY10	0.000
269	H17	83.844	14.304	28.326	H	10	PLY10	0.000
270	H18	85.528	14.238	28.078	H	10	PLY10	0.000
271	H19	84.778	13.079	29.193	H	10	PLY10	0.000
272	H20	84.147	20.254	31.328	H	10	PLY10	0.000

273	H21	85.224	19.139	30.537	H	10	PLY10	0.000
274	H22	83.850	18.565	31.493	H	10	PLY10	0.000
275	N1	79.741	23.269	31.336	N.3	11	PLY11	0.000
276	O1	81.934	21.374	32.606	O.3	11	PLY11	0.000
277	C2	84.929	19.797	34.026	C.3	11	PLY11	0.000
278	O2	82.162	19.231	33.329	O.3	11	PLY11	0.000
279	C3	83.817	20.887	34.092	C.3	11	PLY11	0.000
280	C5	82.518	20.396	33.350	C.3	11	PLY11	0.000
281	C6	80.957	21.005	31.623	C.3	11	PLY11	0.000
282	C7	80.561	22.165	30.733	C.3	11	PLY11	0.000
283	C8	79.221	24.268	30.324	C.3	11	PLY11	0.000
284	C9	80.435	24.137	32.438	C.3	11	PLY11	0.000
285	C10	84.315	22.234	33.437	C.3	11	PLY11	0.000
286	H04	78.958	22.773	31.784	H	11	PLY11	0.000
287	H05	85.627	20.188	34.777	H	11	PLY11	0.000
288	H06	84.568	18.913	34.567	H	11	PLY11	0.000
289	H10	80.002	20.665	32.043	H	11	PLY11	0.000
290	H11	81.450	20.320	30.921	H	11	PLY11	0.000
291	H12	80.045	21.772	29.856	H	11	PLY11	0.000
292	H13	81.482	22.660	30.422	H	11	PLY11	0.000
293	H14	78.540	23.742	29.654	H	11	PLY11	0.000
294	H15	78.725	25.059	30.888	H	11	PLY11	0.000
295	H16	80.072	24.695	29.791	H	11	PLY11	0.000
296	H17	81.188	24.758	31.951	H	11	PLY11	0.000
297	H18	79.713	24.624	33.095	H	11	PLY11	0.000
298	H19	80.905	23.403	33.095	H	11	PLY11	0.000
299	H20	85.336	22.444	33.779	H	11	PLY11	0.000
300	H21	84.403	22.083	32.354	H	11	PLY11	0.000
301	H22	83.716	23.135	33.619	H	11	PLY11	0.000
302	N1	85.751	25.592	38.254	N.3	12	PLY12	0.000
303	O1	84.079	23.957	36.151	O.3	12	PLY12	0.000

304	C2	83.479	21.050	35.576	C.3	12	PLY12	0.000
305	O2	81.971	24.358	35.372	O.3	12	PLY12	0.000
306	C3	82.428	22.066	36.204	C.3	12	PLY12	0.000
307	C5	82.782	23.613	35.899	C.3	12	PLY12	0.000
308	C6	84.589	25.278	35.914	C.3	12	PLY12	0.000
309	C7	85.863	25.585	36.737	C.3	12	PLY12	0.000
310	C8	86.964	26.356	38.984	C.3	12	PLY12	0.000
311	C9	85.881	24.161	38.751	C.3	12	PLY12	0.000
312	C10	82.548	21.887	37.730	C.3	12	PLY12	0.000
313	H04	84.886	26.074	38.538	H	12	PLY12	0.000
314	H05	84.395	21.216	36.156	H	12	PLY12	0.000
315	H06	83.188	20.047	35.913	H	12	PLY12	0.000
316	H10	83.845	26.058	36.115	H	12	PLY12	0.000
317	H11	84.865	25.414	34.861	H	12	PLY12	0.000
318	H12	86.171	26.598	36.470	H	12	PLY12	0.000
319	H13	86.589	24.801	36.515	H	12	PLY12	0.000
320	H14	87.125	27.318	38.497	H	12	PLY12	0.000
321	H15	86.644	26.511	40.016	H	12	PLY12	0.000
322	H16	87.806	25.671	38.869	H	12	PLY12	0.000
323	H17	86.777	23.660	38.381	H	12	PLY12	0.000
324	H18	85.844	24.242	39.838	H	12	PLY12	0.000
325	H19	84.978	23.644	38.424	H	12	PLY12	0.000
326	H20	81.780	22.419	38.306	H	12	PLY12	0.000
327	H21	82.455	20.854	38.087	H	12	PLY12	0.000
328	H22	83.483	22.315	38.112	H	12	PLY12	0.000
329	N1	79.801	16.897	36.308	N.3	13	PLY13	0.000
330	O1	79.965	19.664	37.380	O.3	13	PLY13	0.000
331	C2	80.996	21.747	35.692	C.3	13	PLY13	0.000
332	O2	79.438	21.200	38.993	O.3	13	PLY13	0.000
333	C3	79.756	21.935	36.590	C.3	13	PLY13	0.000
334	C5	79.688	20.965	37.817	C.3	13	PLY13	0.000

335	C6	79.883	18.546	38.286	C.3	13	PLY13	0.000
336	C7	80.508	17.266	37.632	C.3	13	PLY13	0.000
337	C8	80.417	17.711	35.170	C.3	13	PLY13	0.000
338	C9	78.301	17.105	36.247	C.3	13	PLY13	0.000
339	C10	78.576	21.526	35.735	C.3	13	PLY13	0.000
340	H04	79.958	15.882	36.234	H	13	PLY13	0.000
341	H05	80.922	20.683	35.436	H	13	PLY13	0.000
342	H06	80.897	22.223	34.708	H	13	PLY13	0.000
343	H10	78.814	18.456	38.517	H	13	PLY13	0.000
344	H11	80.497	18.795	39.160	H	13	PLY13	0.000
345	H12	80.540	16.418	38.317	H	13	PLY13	0.000
346	H13	81.573	17.385	37.427	H	13	PLY13	0.000
347	H14	79.912	18.640	34.903	H	13	PLY13	0.000
348	H15	81.485	17.749	35.392	H	13	PLY13	0.000
349	H16	80.247	17.128	34.263	H	13	PLY13	0.000
350	H17	77.952	18.136	36.321	H	13	PLY13	0.000
351	H18	77.842	16.590	35.402	H	13	PLY13	0.000
352	H19	77.972	16.578	37.144	H	13	PLY13	0.000
353	H20	78.072	22.361	35.233	H	13	PLY13	0.000
354	H21	78.891	20.762	35.014	H	13	PLY13	0.000
355	H22	77.783	20.921	36.192	H	13	PLY13	0.000
356	N1	78.761	21.165	41.801	N.3	14	PLY14	0.000
357	O1	78.041	23.832	40.466	O.3	14	PLY14	0.000
358	C2	79.539	23.503	37.038	C.3	14	PLY14	0.000
359	O2	80.170	24.232	39.692	O.3	14	PLY14	0.000
360	C3	78.385	24.038	37.976	C.3	14	PLY14	0.000
361	C5	78.977	23.977	39.445	C.3	14	PLY14	0.000
362	C6	78.517	23.817	41.872	C.3	14	PLY14	0.000
363	C7	79.442	22.544	42.175	C.3	14	PLY14	0.000
364	C8	77.712	20.656	42.807	C.3	14	PLY14	0.000
365	C9	79.807	20.129	41.627	C.3	14	PLY14	0.000

366	C10	77.071	23.139	37.963	C.3	14	PLY14	0.000
367	H04	78.399	21.318	40.849	H	14	PLY14	0.000
368	H05	79.381	24.068	36.111	H	14	PLY14	0.000
369	H06	80.492	23.943	37.355	H	14	PLY14	0.000
370	H10	77.633	23.931	42.510	H	14	PLY14	0.000
371	H11	79.157	24.688	42.064	H	14	PLY14	0.000
372	H12	79.719	22.560	43.230	H	14	PLY14	0.000
373	H13	80.241	22.708	41.450	H	14	PLY14	0.000
374	H14	77.120	19.858	42.355	H	14	PLY14	0.000
375	H15	78.256	20.160	43.612	H	14	PLY14	0.000
376	H16	77.119	21.491	43.182	H	14	PLY14	0.000
377	H17	80.451	20.344	40.772	H	14	PLY14	0.000
378	H18	80.449	20.173	42.508	H	14	PLY14	0.000
379	H19	79.308	19.171	41.476	H	14	PLY14	0.000
380	H20	76.737	23.142	36.918	H	14	PLY14	0.000
381	H21	77.379	22.134	38.277	H	14	PLY14	0.000
382	H22	76.349	23.501	38.705	H	14	PLY14	0.000
383	N1	76.786	28.802	43.176	N.3	15	PLY15	0.000
384	O1	78.175	27.798	40.715	O.3	15	PLY15	0.000
385	C2	78.080	25.547	37.482	C.3	15	PLY15	0.000
386	O2	79.932	26.858	39.585	O.3	15	PLY15	0.000
387	C3	77.603	26.654	38.573	C.3	15	PLY15	0.000
388	C5	78.681	27.011	39.705	C.3	15	PLY15	0.000
389	C6	79.021	28.297	41.787	C.3	15	PLY15	0.000
390	C7	78.207	29.204	42.730	C.3	15	PLY15	0.000
391	C8	76.535	29.792	44.295	C.3	15	PLY15	0.000
392	C9	76.719	27.408	43.744	C.3	15	PLY15	0.000
393	C10	76.274	26.195	39.380	C.3	15	PLY15	0.000
394	H04	76.145	28.862	42.373	H	15	PLY15	0.000
395	H05	77.312	25.481	36.702	H	15	PLY15	0.000
396	H06	78.845	26.097	36.921	H	15	PLY15	0.000

397	H10	79.807	28.858	41.267	H	15	PLY15	0.000
398	H11	79.407	27.452	42.371	H	15	PLY15	0.000
399	H12	78.046	30.161	42.233	H	15	PLY15	0.000
400	H13	78.803	29.513	43.590	H	15	PLY15	0.000
401	H14	76.307	30.705	43.741	H	15	PLY15	0.000
402	H15	75.682	29.416	44.861	H	15	PLY15	0.000
403	H16	77.395	29.958	44.945	H	15	PLY15	0.000
404	H17	76.682	26.741	42.881	H	15	PLY15	0.000
405	H18	77.527	27.389	44.476	H	15	PLY15	0.000
406	H19	75.780	27.245	44.276	H	15	PLY15	0.000
407	H20	75.650	27.032	39.717	H	15	PLY15	0.000
408	H21	75.663	25.632	38.663	H	15	PLY15	0.000
409	H22	76.381	25.420	40.148	H	15	PLY15	0.000
410	N1	79.155	31.252	32.292	N.3	16	PLY16	0.000
411	O1	77.984	30.616	35.256	O.3	16	PLY16	0.000
412	C2	77.221	28.086	37.794	C.3	16	PLY16	0.000
413	O2	76.260	30.457	36.717	O.3	16	PLY16	0.000
414	C3	78.241	29.261	37.317	C.3	16	PLY16	0.000
415	C5	77.412	30.230	36.419	C.3	16	PLY16	0.000
416	C6	77.259	31.192	34.155	C.3	16	PLY16	0.000
417	C7	78.184	32.026	33.220	C.3	16	PLY16	0.000
418	C8	80.186	30.488	33.236	C.3	16	PLY16	0.000
419	C9	79.952	32.171	31.332	C.3	16	PLY16	0.000
420	C10	79.472	28.679	36.541	C.3	16	PLY16	0.000
421	H04	78.552	30.653	31.710	H	16	PLY16	0.000
422	H05	76.417	28.586	38.347	H	16	PLY16	0.000
423	H06	76.556	27.809	36.966	H	16	PLY16	0.000
424	H10	76.594	31.910	34.651	H	16	PLY16	0.000
425	H11	76.684	30.380	33.695	H	16	PLY16	0.000
426	H12	78.693	32.732	33.877	H	16	PLY16	0.000
427	H13	77.525	32.706	32.679	H	16	PLY16	0.000

428	H14	80.882	31.130	33.778	H	16	PLY16	0.000
429	H15	79.522	29.871	33.843	H	16	PLY16	0.000
430	H16	80.821	29.907	32.566	H	16	PLY16	0.000
431	H17	80.360	33.001	31.912	H	16	PLY16	0.000
432	H18	80.729	31.680	30.745	H	16	PLY16	0.000
433	H19	79.314	32.632	30.577	H	16	PLY16	0.000
434	H20	79.989	27.997	37.228	H	16	PLY16	0.000
435	H21	79.187	28.159	35.618	H	16	PLY16	0.000
436	H22	80.200	29.426	36.200	H	16	PLY16	0.000
437	N1	74.348	34.546	37.469	N.3	17	PLY17	0.000
438	O1	76.981	32.472	39.165	O.3	17	PLY17	0.000
439	C2	78.793	30.030	38.623	C.3	17	PLY17	0.000
440	O2	78.132	33.382	37.420	O.3	17	PLY17	0.000
441	C3	79.228	31.554	38.617	C.3	17	PLY17	0.000
442	C5	78.056	32.473	38.253	C.3	17	PLY17	0.000
443	C6	76.026	33.555	39.010	C.3	17	PLY17	0.000
444	C7	75.391	33.493	37.611	C.3	17	PLY17	0.000
445	C8	73.581	34.291	36.102	C.3	17	PLY17	0.000
446	C9	75.023	35.829	37.240	C.3	17	PLY17	0.000
447	C10	80.324	31.781	37.559	C.3	17	PLY17	0.000
448	H04	73.702	34.621	38.268	H	17	PLY17	0.000
449	H05	79.627	29.465	39.057	H	17	PLY17	0.000
450	H06	78.017	29.963	39.395	H	17	PLY17	0.000
451	H10	76.557	34.478	39.276	H	17	PLY17	0.000
452	H11	75.149	33.445	39.660	H	17	PLY17	0.000
453	H12	74.816	32.578	37.467	H	17	PLY17	0.000
454	H13	76.077	33.527	36.763	H	17	PLY17	0.000
455	H14	72.992	33.377	36.182	H	17	PLY17	0.000
456	H15	72.907	35.141	35.982	H	17	PLY17	0.000
457	H16	74.286	34.321	35.270	H	17	PLY17	0.000
458	H17	74.279	36.615	37.382	H	17	PLY17	0.000

459	H18	75.850	36.104	37.896	H	17	PLY17	0.000
460	H19	75.538	35.838	36.278	H	17	PLY17	0.000
461	H20	80.077	31.489	36.531	H	17	PLY17	0.000
462	H21	80.584	32.847	37.552	H	17	PLY17	0.000
463	H22	81.181	31.178	37.884	H	17	PLY17	0.000
464	N1	84.922	31.188	42.476	N.3	18	PLY18	0.000
465	O1	82.761	32.037	40.335	O.3	18	PLY18	0.000
466	C2	79.785	31.875	40.082	C.3	18	PLY18	0.000
467	O2	82.491	33.927	39.031	O.3	18	PLY18	0.000
468	C3	80.592	33.210	40.496	C.3	18	PLY18	0.000
469	C5	82.048	33.192	39.902	C.3	18	PLY18	0.000
470	C6	84.171	31.922	40.069	C.3	18	PLY18	0.000
471	C7	84.857	30.881	41.002	C.3	18	PLY18	0.000
472	C8	86.288	30.773	43.108	C.3	18	PLY18	0.000
473	C9	83.789	30.490	43.196	C.3	18	PLY18	0.000
474	C10	80.768	33.157	42.082	C.3	18	PLY18	0.000
475	H04	84.784	32.198	42.625	H	18	PLY18	0.000
476	H05	80.374	31.002	40.391	H	18	PLY18	0.000
477	H06	78.981	31.758	40.819	H	18	PLY18	0.000
478	H10	84.713	32.875	40.108	H	18	PLY18	0.000
479	H11	84.252	31.523	39.051	H	18	PLY18	0.000
480	H12	85.915	30.937	40.742	H	18	PLY18	0.000
481	H13	84.475	29.873	40.834	H	18	PLY18	0.000
482	H14	86.199	30.900	44.188	H	18	PLY18	0.000
483	H15	86.381	29.687	43.049	H	18	PLY18	0.000
484	H16	87.092	31.400	42.720	H	18	PLY18	0.000
485	H17	83.818	29.404	43.296	H	18	PLY18	0.000
486	H18	83.632	30.961	44.167	H	18	PLY18	0.000
487	H19	82.910	30.796	42.627	H	18	PLY18	0.000
488	H20	79.829	33.039	42.636	H	18	PLY18	0.000
489	H21	81.296	32.286	42.490	H	18	PLY18	0.000

490	H22	81.328	34.008	42.488	H	18	PLY18	0.000
491	N1	75.972	36.381	45.059	N.3	19	PLY19	0.000
492	O1	78.192	35.356	42.445	O.3	19	PLY19	0.000
493	C2	79.710	34.495	40.104	C.3	19	PLY19	0.000
494	O2	80.171	35.999	43.305	O.3	19	PLY19	0.000
495	C3	79.945	35.930	40.877	C.3	19	PLY19	0.000
496	C5	79.434	35.873	42.329	C.3	19	PLY19	0.000
497	C6	77.628	35.033	43.727	C.3	19	PLY19	0.000
498	C7	77.395	36.255	44.627	C.3	19	PLY19	0.000
499	C8	75.931	37.635	46.003	C.3	19	PLY19	0.000
500	C9	75.482	35.179	45.843	C.3	19	PLY19	0.000
501	C10	78.996	36.984	40.294	C.3	19	PLY19	0.000
502	H04	75.340	36.549	44.263	H	19	PLY19	0.000
503	H05	78.638	34.281	40.191	H	19	PLY19	0.000
504	H06	79.794	34.595	39.014	H	19	PLY19	0.000
505	H10	78.309	34.294	44.168	H	19	PLY19	0.000
506	H11	76.667	34.518	43.603	H	19	PLY19	0.000
507	H12	77.818	37.160	44.188	H	19	PLY19	0.000
508	H13	78.043	36.076	45.486	H	19	PLY19	0.000
509	H14	74.878	37.715	46.277	H	19	PLY19	0.000
510	H15	76.593	37.489	46.858	H	19	PLY19	0.000
511	H16	76.126	38.591	45.514	H	19	PLY19	0.000
512	H17	75.321	34.311	45.201	H	19	PLY19	0.000
513	H18	76.279	35.001	46.566	H	19	PLY19	0.000
514	H19	74.619	35.482	46.438	H	19	PLY19	0.000
515	H20	79.121	37.914	40.863	H	19	PLY19	0.000
516	H21	79.295	37.253	39.274	H	19	PLY19	0.000
517	H22	77.957	36.632	40.284	H	19	PLY19	0.000
518	N1	88.040	37.593	41.061	N.3	20	PLY20	0.000
519	O1	84.296	38.121	41.799	O.3	20	PLY20	0.000
520	C2	81.464	36.393	40.636	C.3	20	PLY20	0.000

521	O2	84.108	36.729	40.023	O.3	20	PLY20	0.000
522	C3	82.045	37.790	40.881	C.3	20	PLY20	0.000
523	C5	83.579	37.495	40.827	C.3	20	PLY20	0.000
524	C6	85.665	37.736	42.091	C.3	20	PLY20	0.000
525	C7	86.688	38.192	40.990	C.3	20	PLY20	0.000
526	C8	88.929	38.440	40.181	C.3	20	PLY20	0.000
527	C9	88.081	36.161	40.491	C.3	20	PLY20	0.000
528	C10	81.613	38.382	42.308	C.3	20	PLY20	0.000
529	H04	88.296	37.621	42.059	H	20	PLY20	0.000
530	H05	81.565	36.149	39.571	H	20	PLY20	0.000
531	H06	82.042	35.639	41.184	H	20	PLY20	0.000
532	H10	85.735	36.642	42.120	H	20	PLY20	0.000
533	H11	86.045	38.053	43.069	H	20	PLY20	0.000
534	H12	86.752	39.243	41.277	H	20	PLY20	0.000
535	H13	86.251	38.089	39.996	H	20	PLY20	0.000
536	H14	88.783	38.332	39.106	H	20	PLY20	0.000
537	H15	88.778	39.511	40.323	H	20	PLY20	0.000
538	H16	89.990	38.238	40.333	H	20	PLY20	0.000
539	H17	89.128	35.928	40.291	H	20	PLY20	0.000
540	H18	87.664	35.452	41.208	H	20	PLY20	0.000
541	H19	87.479	36.127	39.582	H	20	PLY20	0.000
542	H20	81.876	37.792	43.195	H	20	PLY20	0.000
543	H21	82.216	39.245	42.617	H	20	PLY20	0.000
544	H22	80.578	38.738	42.243	H	20	PLY20	0.000
545	N1	84.045	35.719	37.111	N.3	21	PLY21	0.000
546	O1	83.632	38.706	37.599	O.3	21	PLY21	0.000
547	C2	81.556	38.750	39.724	C.3	21	PLY21	0.000
548	O2	84.916	39.863	39.099	O.3	21	PLY21	0.000
549	C3	82.420	40.033	39.285	C.3	21	PLY21	0.000
550	C5	83.824	39.478	38.718	C.3	21	PLY21	0.000
551	C6	84.721	38.323	36.746	C.3	21	PLY21	0.000

552	C7	85.091	36.776	36.957	C.3	21	PLY21	0.000
553	C8	84.802	34.441	36.815	C.3	21	PLY21	0.000
554	C9	82.900	35.933	36.126	C.3	21	PLY21	0.000
555	C10	82.687	41.015	40.487	C.3	21	PLY21	0.000
556	H04	83.666	35.740	38.069	H	21	PLY21	0.000
557	H05	80.607	39.185	40.062	H	21	PLY21	0.000
558	H06	81.357	38.206	38.792	H	21	PLY21	0.000
559	H10	85.571	38.962	37.017	H	21	PLY21	0.000
560	H11	84.506	38.461	35.680	H	21	PLY21	0.000
561	H12	85.779	36.625	37.790	H	21	PLY21	0.000
562	H13	85.744	36.475	36.137	H	21	PLY21	0.000
563	H14	85.033	34.328	35.754	H	21	PLY21	0.000
564	H15	85.723	34.454	37.399	H	21	PLY21	0.000
565	H16	84.174	33.601	37.117	H	21	PLY21	0.000
566	H17	82.362	34.987	36.054	H	21	PLY21	0.000
567	H18	82.282	36.784	36.416	H	21	PLY21	0.000
568	H19	83.270	36.119	35.117	H	21	PLY21	0.000
569	H20	83.087	41.956	40.088	H	21	PLY21	0.000
570	H21	81.776	41.226	41.059	H	21	PLY21	0.000
571	H22	83.443	40.616	41.175	H	21	PLY21	0.000
572	N1	87.096	44.367	40.107	N.3	22	PLY22	0.000
573	O1	84.033	43.251	37.998	O.3	22	PLY22	0.000
574	C2	81.557	40.809	38.180	C.3	22	PLY22	0.000
575	O2	84.078	41.500	36.526	O.3	22	PLY22	0.000
576	C3	81.968	42.202	37.509	C.3	22	PLY22	0.000
577	C5	83.513	42.183	37.357	C.3	22	PLY22	0.000
578	C6	85.497	43.348	38.303	C.3	22	PLY22	0.000
579	C7	85.641	44.184	39.574	C.3	22	PLY22	0.000
580	C8	86.917	44.897	41.569	C.3	22	PLY22	0.000
581	C9	87.963	45.321	39.202	C.3	22	PLY22	0.000
582	C10	81.451	43.404	38.385	C.3	22	PLY22	0.000

583	H04	87.569	43.455	40.177	H	22	PLY22	0.000
584	H05	80.552	40.937	38.601	H	22	PLY22	0.000
585	H06	81.417	40.081	37.372	H	22	PLY22	0.000
586	H10	86.208	43.585	37.502	H	22	PLY22	0.000
587	H11	85.835	42.401	38.741	H	22	PLY22	0.000
588	H12	85.144	43.671	40.399	H	22	PLY22	0.000
589	H13	85.177	45.165	39.460	H	22	PLY22	0.000
590	H14	86.395	45.854	41.545	H	22	PLY22	0.000
591	H15	86.447	44.111	42.161	H	22	PLY22	0.000
592	H16	87.901	45.118	41.985	H	22	PLY22	0.000
593	H17	87.745	45.252	38.135	H	22	PLY22	0.000
594	H18	87.717	46.355	39.448	H	22	PLY22	0.000
595	H19	89.020	45.106	39.367	H	22	PLY22	0.000
596	H20	81.798	44.402	38.091	H	22	PLY22	0.000
597	H21	80.363	43.401	38.524	H	22	PLY22	0.000
598	H22	81.835	43.251	39.402	H	22	PLY22	0.000
599	N1	85.022	41.597	32.298	N.3	23	PLY23	0.000
600	O1	82.393	42.745	33.257	O.3	23	PLY23	0.000
601	C2	81.308	42.257	36.088	C.3	23	PLY23	0.000
602	O2	80.135	42.938	33.078	O.3	23	PLY23	0.000
603	C3	81.222	43.559	35.192	C.3	23	PLY23	0.000
604	C5	81.129	43.052	33.761	C.3	23	PLY23	0.000
605	C6	82.494	42.324	31.893	C.3	23	PLY23	0.000
606	C7	84.012	42.450	31.486	C.3	23	PLY23	0.000
607	C8	85.166	41.959	33.786	C.3	23	PLY23	0.000
608	C9	86.339	41.580	31.567	C.3	23	PLY23	0.000
609	C10	82.536	44.432	35.252	C.3	23	PLY23	0.000
610	H04	84.671	40.631	32.371	H	23	PLY23	0.000
611	H05	80.258	41.964	36.205	H	23	PLY23	0.000
612	H06	81.675	41.421	35.480	H	23	PLY23	0.000
613	H10	81.898	42.941	31.209	H	23	PLY23	0.000

614	H11	82.170	41.278	31.834	H	23	PLY23	0.000
615	H12	84.150	43.516	31.676	H	23	PLY23	0.000
616	H13	84.056	42.093	30.456	H	23	PLY23	0.000
617	H14	85.336	43.034	33.860	H	23	PLY23	0.000
618	H15	84.225	41.728	34.287	H	23	PLY23	0.000
619	H16	86.017	41.487	34.279	H	23	PLY23	0.000
620	H17	87.022	40.975	32.166	H	23	PLY23	0.000
621	H18	86.242	41.221	30.541	H	23	PLY23	0.000
622	H19	86.616	42.631	31.477	H	23	PLY23	0.000
623	H20	82.711	45.058	34.369	H	23	PLY23	0.000
624	H21	82.532	45.033	36.170	H	23	PLY23	0.000
625	H22	83.447	43.822	35.290	H	23	PLY23	0.000
626	N1	80.878	46.991	40.067	N.3	24	PLY24	0.000
627	O1	80.537	46.986	37.148	O.3	24	PLY24	0.000
628	C2	79.839	44.430	35.598	C.3	24	PLY24	0.000
629	O2	81.458	47.535	35.176	O.3	24	PLY24	0.000
630	C3	79.534	45.913	35.190	C.3	24	PLY24	0.000
631	C5	80.675	46.795	35.803	C.3	24	PLY24	0.000
632	C6	81.156	48.183	37.673	C.3	24	PLY24	0.000
633	C7	80.809	48.282	39.170	C.3	24	PLY24	0.000
634	C8	80.235	47.317	41.433	C.3	24	PLY24	0.000
635	C9	82.275	46.498	40.257	C.3	24	PLY24	0.000
636	C10	78.265	46.277	35.950	C.3	24	PLY24	0.000
637	H04	80.238	46.250	39.746	H	24	PLY24	0.000
638	H05	79.827	44.497	36.693	H	24	PLY24	0.000
639	H06	78.959	43.785	35.478	H	24	PLY24	0.000
640	H10	80.908	49.020	37.008	H	24	PLY24	0.000
641	H11	82.252	48.139	37.662	H	24	PLY24	0.000
642	H12	79.781	48.619	39.317	H	24	PLY24	0.000
643	H13	81.363	49.095	39.642	H	24	PLY24	0.000
644	H14	79.152	47.323	41.297	H	24	PLY24	0.000

645	H15	80.466	46.577	42.201	H	24	PLY24	0.000
646	H16	80.586	48.276	41.817	H	24	PLY24	0.000
647	H17	82.273	45.571	40.832	H	24	PLY24	0.000
648	H18	82.739	46.425	39.272	H	24	PLY24	0.000
649	H19	82.773	47.194	40.934	H	24	PLY24	0.000
650	H20	77.350	46.139	35.361	H	24	PLY24	0.000
651	H21	78.114	45.698	36.870	H	24	PLY24	0.000
652	H22	78.284	47.316	36.300	H	24	PLY24	0.000
653	N1	83.558	51.271	31.531	N.3	25	PLY25	0.000
654	O1	80.484	49.067	31.823	O.3	25	PLY25	0.000
655	C2	79.421	45.976	33.588	C.3	25	PLY25	0.000
656	O2	81.701	47.223	32.404	O.3	25	PLY25	0.000
657	C3	79.247	47.329	32.839	C.3	25	PLY25	0.000
658	C5	80.695	47.879	32.470	C.3	25	PLY25	0.000
659	C6	81.556	49.588	31.083	C.3	25	PLY25	0.000
660	C7	82.616	50.171	32.076	C.3	25	PLY25	0.000
661	C8	84.166	50.853	30.237	C.3	25	PLY25	0.000
662	C9	84.499	51.625	32.727	C.3	25	PLY25	0.000
663	C10	78.463	48.490	33.705	C.3	25	PLY25	0.000
664	H04	83.000	52.112	31.324	H	25	PLY25	0.000
665	H05	78.558	45.341	33.355	H	25	PLY25	0.000
666	H06	80.198	45.364	33.114	H	25	PLY25	0.000
667	H10	81.152	50.412	30.483	H	25	PLY25	0.000
668	H11	82.054	48.880	30.410	H	25	PLY25	0.000
669	H12	83.206	49.452	32.646	H	25	PLY25	0.000
670	H13	82.090	50.733	32.849	H	25	PLY25	0.000
671	H14	83.371	50.573	29.545	H	25	PLY25	0.000
672	H15	84.722	51.678	29.791	H	25	PLY25	0.000
673	H16	84.783	49.961	30.360	H	25	PLY25	0.000
674	H17	85.230	52.321	32.313	H	25	PLY25	0.000
675	H18	83.949	52.059	33.564	H	25	PLY25	0.000

676	H19	85.158	50.803	33.006	H	25	PLY25	0.000
677	H20	78.943	48.676	34.674	H	25	PLY25	0.000
678	H21	78.440	49.434	33.147	H	25	PLY25	0.000
679	H22	77.411	48.225	33.870	H	25	PLY25	0.000
680	N1	77.605	41.691	27.661	N.3	26	PLY26	0.000
681	O1	78.150	43.776	29.855	O.3	26	PLY26	0.000
682	C2	78.322	47.170	31.562	C.3	26	PLY26	0.000
683	O2	77.001	44.570	31.659	O.3	26	PLY26	0.000
684	C3	78.501	46.130	30.357	C.3	26	PLY26	0.000
685	C5	77.804	44.769	30.675	C.3	26	PLY26	0.000
686	C6	77.618	42.442	30.076	C.3	26	PLY26	0.000
687	C7	78.239	41.568	29.032	C.3	26	PLY26	0.000
688	C8	78.381	40.792	26.703	C.3	26	PLY26	0.000
689	C9	77.608	43.161	27.066	C.3	26	PLY26	0.000
690	C10	80.031	45.928	30.049	C.3	26	PLY26	0.000
691	H04	76.632	41.359	27.724	H	26	PLY26	0.000
692	H05	78.445	48.154	31.093	H	26	PLY26	0.000
693	H06	77.288	47.081	31.918	H	26	PLY26	0.000
694	H10	76.522	42.413	30.042	H	26	PLY26	0.000
695	H11	77.983	41.983	31.003	H	26	PLY26	0.000
696	H12	78.157	40.535	29.372	H	26	PLY26	0.000
697	H13	79.286	41.807	28.838	H	26	PLY26	0.000
698	H14	78.462	39.787	27.121	H	26	PLY26	0.000
699	H15	77.805	40.711	25.781	H	26	PLY26	0.000
700	H16	79.381	41.204	26.557	H	26	PLY26	0.000
701	H17	77.225	43.280	26.051	H	26	PLY26	0.000
702	H18	77.078	43.793	27.779	H	26	PLY26	0.000
703	H19	78.655	43.464	27.021	H	26	PLY26	0.000
704	H20	80.508	45.372	30.865	H	26	PLY26	0.000
705	H21	80.225	45.221	29.232	H	26	PLY26	0.000
706	H22	80.489	46.874	29.736	H	26	PLY26	0.000

707	N1	71.618	43.764	28.549	N.3	27	PLY27	0.000
708	O1	75.243	45.051	28.937	O.3	27	PLY27	0.000
709	C2	77.917	46.621	28.981	C.3	27	PLY27	0.000
710	O2	74.712	46.644	30.477	O.3	27	PLY27	0.000
711	C3	76.401	47.166	28.783	C.3	27	PLY27	0.000
712	C5	75.322	46.311	29.500	C.3	27	PLY27	0.000
713	C6	74.117	44.156	29.192	C.3	27	PLY27	0.000
714	C7	72.899	44.633	28.485	C.3	27	PLY27	0.000
715	C8	70.467	44.396	27.772	C.3	27	PLY27	0.000
716	C9	71.168	43.736	30.002	C.3	27	PLY27	0.000
717	C10	76.150	47.028	27.161	C.3	27	PLY27	0.000
718	H04	71.737	42.788	28.241	H	27	PLY27	0.000
719	H05	78.071	45.819	28.249	H	27	PLY27	0.000
720	H06	78.577	47.355	28.503	H	27	PLY27	0.000
721	H10	73.919	44.241	30.267	H	27	PLY27	0.000
722	H11	74.378	43.104	29.019	H	27	PLY27	0.000
723	H12	73.122	44.648	27.417	H	27	PLY27	0.000
724	H13	72.669	45.655	28.789	H	27	PLY27	0.000
725	H14	69.591	43.750	27.835	H	27	PLY27	0.000
726	H15	70.224	45.426	28.037	H	27	PLY27	0.000
727	H16	70.719	44.348	26.711	H	27	PLY27	0.000
728	H17	70.174	43.335	30.207	H	27	PLY27	0.000
729	H18	71.924	43.230	30.604	H	27	PLY27	0.000
730	H19	71.143	44.782	30.309	H	27	PLY27	0.000
731	H20	75.146	47.299	26.810	H	27	PLY27	0.000
732	H21	76.964	47.621	26.726	H	27	PLY27	0.000
733	H22	76.279	45.963	26.930	H	27	PLY27	0.000
734	N1	77.028	52.777	23.842	N.3	28	PLY28	0.000
735	O1	76.769	50.531	27.028	O.3	28	PLY28	0.000
736	C2	76.341	48.688	29.219	C.3	28	PLY28	0.000
737	O2	74.652	49.987	26.247	O.3	28	PLY28	0.000

738	C3	75.235	49.720	28.665	C.3	28	PLY28	0.000
739	C5	75.491	50.029	27.136	C.3	28	PLY28	0.000
740	C6	77.193	51.019	25.672	C.3	28	PLY28	0.000
741	C7	76.740	52.394	25.328	C.3	28	PLY28	0.000
742	C8	76.433	54.189	23.538	C.3	28	PLY28	0.000
743	C9	76.436	51.801	22.809	C.3	28	PLY28	0.000
744	C10	75.526	51.110	29.336	C.3	28	PLY28	0.000
745	H04	78.019	52.813	23.561	H	28	PLY28	0.000
746	H05	77.310	49.105	28.920	H	28	PLY28	0.000
747	H06	76.194	48.733	30.306	H	28	PLY28	0.000
748	H10	76.773	50.290	24.968	H	28	PLY28	0.000
749	H11	78.279	50.959	25.527	H	28	PLY28	0.000
750	H12	77.257	53.139	25.935	H	28	PLY28	0.000
751	H13	75.681	52.510	25.564	H	28	PLY28	0.000
752	H14	76.878	54.877	24.258	H	28	PLY28	0.000
753	H15	76.554	54.561	22.519	H	28	PLY28	0.000
754	H16	75.347	54.182	23.640	H	28	PLY28	0.000
755	H17	75.380	52.075	22.825	H	28	PLY28	0.000
756	H18	76.757	51.970	21.780	H	28	PLY28	0.000
757	H19	76.495	50.774	23.172	H	28	PLY28	0.000
758	H20	75.058	51.254	30.318	H	28	PLY28	0.000
759	H21	76.611	51.259	29.394	H	28	PLY28	0.000
760	H22	75.136	51.866	28.644	H	28	PLY28	0.000
761	N1	68.973	51.556	24.715	N.3	29	PLY29	0.000
762	O1	71.096	49.943	26.382	O.3	29	PLY29	0.000
763	C2	73.771	49.214	29.007	C.3	29	PLY29	0.000
764	O2	72.277	47.982	26.827	O.3	29	PLY29	0.000
765	C3	72.401	49.853	28.464	C.3	29	PLY29	0.000
766	C5	72.076	49.189	27.060	C.3	29	PLY29	0.000
767	C6	70.559	49.425	25.119	C.3	29	PLY29	0.000
768	C7	70.054	50.618	24.156	C.3	29	PLY29	0.000

769	C8	67.554	50.952	24.548	C.3	29	PLY29	0.000
770	C9	69.007	52.927	24.001	C.3	29	PLY29	0.000
771	C10	72.429	51.367	28.332	C.3	29	PLY29	0.000
772	H04	68.975	51.765	25.723	H	29	PLY29	0.000
773	H05	73.787	49.060	30.093	H	29	PLY29	0.000
774	H06	73.688	48.157	28.725	H	29	PLY29	0.000
775	H10	69.745	48.705	25.270	H	29	PLY29	0.000
776	H11	71.372	48.862	24.644	H	29	PLY29	0.000
777	H12	69.618	50.030	23.347	H	29	PLY29	0.000
778	H13	70.943	51.140	23.799	H	29	PLY29	0.000
779	H14	66.792	51.695	24.787	H	29	PLY29	0.000
780	H15	67.473	50.666	23.499	H	29	PLY29	0.000
781	H16	67.358	50.093	25.191	H	29	PLY29	0.000
782	H17	69.683	53.517	24.622	H	29	PLY29	0.000
783	H18	69.426	52.853	22.997	H	29	PLY29	0.000
784	H19	68.055	53.451	23.900	H	29	PLY29	0.000
785	H20	72.876	51.958	29.140	H	29	PLY29	0.000
786	H21	72.958	51.591	27.397	H	29	PLY29	0.000
787	H22	71.462	51.854	28.156	H	29	PLY29	0.000
788	N1	73.126	47.158	34.053	N.3	30	PLY30	0.000
789	O1	72.562	49.149	32.096	O.3	30	PLY30	0.000
790	C2	71.198	49.279	29.415	C.3	30	PLY30	0.000
791	O2	72.570	51.412	31.721	O.3	30	PLY30	0.000
792	C3	70.739	50.027	30.745	C.3	30	PLY30	0.000
793	C5	72.083	50.296	31.519	C.3	30	PLY30	0.000
794	C6	73.793	49.277	32.848	C.3	30	PLY30	0.000
795	C7	74.250	47.862	33.390	C.3	30	PLY30	0.000
796	C8	72.440	48.048	35.086	C.3	30	PLY30	0.000
797	C9	73.559	45.738	34.520	C.3	30	PLY30	0.000
798	C10	69.810	49.215	31.648	C.3	30	PLY30	0.000
799	H04	72.436	46.903	33.332	H	30	PLY30	0.000

800	H05	71.545	48.272	29.677	H	30	PLY30	0.000
801	H06	70.344	49.048	28.766	H	30	PLY30	0.000
802	H10	73.684	50.068	33.600	H	30	PLY30	0.000
803	H11	74.575	49.720	32.219	H	30	PLY30	0.000
804	H12	75.099	47.998	34.063	H	30	PLY30	0.000
805	H13	74.559	47.286	32.517	H	30	PLY30	0.000
806	H14	71.635	47.492	35.570	H	30	PLY30	0.000
807	H15	73.116	48.432	35.851	H	30	PLY30	0.000
808	H16	71.846	48.854	34.654	H	30	PLY30	0.000
809	H17	73.630	45.178	33.587	H	30	PLY30	0.000
810	H18	74.606	45.811	34.820	H	30	PLY30	0.000
811	H19	72.885	45.374	35.296	H	30	PLY30	0.000
812	H20	68.776	49.141	31.289	H	30	PLY30	0.000
813	H21	70.218	48.263	32.010	H	30	PLY30	0.000
814	H22	69.791	49.720	32.622	H	30	PLY30	0.000
815	N1	72.325	56.312	30.920	N.3	31	PLY31	0.000
816	O1	69.844	54.720	30.885	O.3	31	PLY31	0.000
817	C2	70.012	51.442	30.370	C.3	31	PLY31	0.000
818	O2	68.045	53.838	29.781	O.3	31	PLY31	0.000
819	C3	69.188	52.336	31.302	C.3	31	PLY31	0.000
820	C5	68.953	53.700	30.564	C.3	31	PLY31	0.000
821	C6	69.786	56.001	30.188	C.3	31	PLY31	0.000
822	C7	70.943	56.974	30.703	C.3	31	PLY31	0.000
823	C8	73.010	57.312	31.820	C.3	31	PLY31	0.000
824	C9	73.030	56.235	29.599	C.3	31	PLY31	0.000
825	C10	69.981	52.608	32.657	C.3	31	PLY31	0.000
826	H04	72.239	55.440	31.462	H	31	PLY31	0.000
827	H05	69.487	51.351	29.411	H	31	PLY31	0.000
828	H06	70.887	52.066	30.146	H	31	PLY31	0.000
829	H10	68.898	56.586	30.457	H	31	PLY31	0.000
830	H11	69.779	55.858	29.100	H	31	PLY31	0.000

831	H12	70.690	57.253	31.727	H	31	PLY31	0.000
832	H13	71.151	57.833	30.063	H	31	PLY31	0.000
833	H14	74.025	56.971	32.032	H	31	PLY31	0.000
834	H15	72.960	58.279	31.319	H	31	PLY31	0.000
835	H16	72.534	57.406	32.797	H	31	PLY31	0.000
836	H17	73.886	55.607	29.849	H	31	PLY31	0.000
837	H18	72.477	55.749	28.793	H	31	PLY31	0.000
838	H19	73.280	57.258	29.315	H	31	PLY31	0.000
839	H20	70.014	51.760	33.352	H	31	PLY31	0.000
840	H21	70.958	53.085	32.510	H	31	PLY31	0.000
841	H22	69.397	53.380	33.173	H	31	PLY31	0.000
842	N1	65.571	54.824	28.700	N.3	32	PLY32	0.000
843	O1	64.423	53.222	31.144	O.3	32	PLY32	0.000
844	C2	67.815	51.576	31.637	C.3	32	PLY32	0.000
845	O2	65.856	52.285	29.615	O.3	32	PLY32	0.000
846	C3	66.392	52.262	32.031	C.3	32	PLY32	0.000
847	C5	65.548	52.509	30.770	C.3	32	PLY32	0.000
848	C6	63.668	53.963	30.185	C.3	32	PLY32	0.000
849	C7	64.360	55.196	29.593	C.3	32	PLY32	0.000
850	C8	66.426	56.050	28.562	C.3	32	PLY32	0.000
851	C9	65.076	54.418	27.294	C.3	32	PLY32	0.000
852	C10	66.589	53.599	32.803	C.3	32	PLY32	0.000
853	H04	66.164	54.056	29.047	H	32	PLY32	0.000
854	H05	68.013	50.816	32.402	H	32	PLY32	0.000
855	H06	67.710	50.840	30.831	H	32	PLY32	0.000
856	H10	62.727	54.333	30.608	H	32	PLY32	0.000
857	H11	63.263	53.330	29.386	H	32	PLY32	0.000
858	H12	64.773	55.680	30.479	H	32	PLY32	0.000
859	H13	63.756	55.901	29.020	H	32	PLY32	0.000
860	H14	67.116	55.899	27.730	H	32	PLY32	0.000
861	H15	65.743	56.829	28.220	H	32	PLY32	0.000

862	H16	66.895	56.428	29.472	H	32	PLY32	0.000
863	H17	64.374	53.595	27.438	H	32	PLY32	0.000
864	H18	64.578	55.318	26.930	H	32	PLY32	0.000
865	H19	65.892	54.225	26.596	H	32	PLY32	0.000
866	H20	65.671	54.081	33.160	H	32	PLY32	0.000
867	H21	67.241	53.540	33.683	H	32	PLY32	0.000
868	H22	67.164	54.209	32.096	H	32	PLY32	0.000
869	N1	67.447	46.257	35.132	N.3	33	PLY33	0.000
870	O1	64.936	47.840	33.714	O.3	33	PLY33	0.000
871	C2	65.545	51.331	33.052	C.3	33	PLY33	0.000
872	O2	64.281	49.634	34.884	O.3	33	PLY33	0.000
873	C3	64.860	49.971	32.527	C.3	33	PLY33	0.000
874	C5	64.691	49.120	33.840	C.3	33	PLY33	0.000
875	C6	64.917	46.974	34.960	C.3	33	PLY33	0.000
876	C7	66.282	47.053	35.706	C.3	33	PLY33	0.000
877	C8	67.966	47.053	33.907	C.3	33	PLY33	0.000
878	C9	67.035	44.834	34.659	C.3	33	PLY33	0.000
879	C10	65.765	49.105	31.500	C.3	33	PLY33	0.000
880	H04	68.171	46.131	35.854	H	33	PLY33	0.000
881	H05	64.754	52.007	33.401	H	33	PLY33	0.000
882	H06	66.132	51.181	33.967	H	33	PLY33	0.000
883	H10	64.699	45.916	34.766	H	33	PLY33	0.000
884	H11	64.107	47.228	35.654	H	33	PLY33	0.000
885	H12	66.167	46.599	36.691	H	33	PLY33	0.000
886	H13	66.572	48.097	35.827	H	33	PLY33	0.000
887	H14	67.926	48.097	34.222	H	33	PLY33	0.000
888	H15	69.012	46.804	33.722	H	33	PLY33	0.000
889	H16	67.310	46.741	33.093	H	33	PLY33	0.000
890	H17	66.459	44.330	35.436	H	33	PLY33	0.000
891	H18	66.448	44.817	33.740	H	33	PLY33	0.000
892	H19	67.886	44.223	34.354	H	33	PLY33	0.000

893	H20	66.772	49.018	31.929	H	33	PLY33	0.000
894	H21	65.405	48.085	31.320	H	33	PLY33	0.000
895	H22	65.935	49.565	30.519	H	33	PLY33	0.000
896	N1	62.494	48.146	26.771	N.3	34	PLY34	0.000
897	O1	63.604	48.785	29.240	O.3	34	PLY34	0.000
898	C2	63.510	50.315	31.709	C.3	34	PLY34	0.000
899	O2	63.285	46.958	30.668	O.3	34	PLY34	0.000
900	C3	62.463	49.158	31.347	C.3	34	PLY34	0.000
901	C5	63.083	48.108	30.369	C.3	34	PLY34	0.000
902	C6	64.448	48.060	28.375	C.3	34	PLY34	0.000
903	C7	63.604	47.314	27.425	C.3	34	PLY34	0.000
904	C8	61.315	47.112	26.647	C.3	34	PLY34	0.000
905	C9	62.787	48.749	25.434	C.3	34	PLY34	0.000
906	C10	61.356	49.909	30.570	C.3	34	PLY34	0.000
907	H04	62.181	48.907	27.390	H	34	PLY34	0.000
908	H05	63.755	50.773	30.743	H	34	PLY34	0.000
909	H06	63.031	51.115	32.288	H	34	PLY34	0.000
910	H10	65.108	47.375	28.921	H	34	PLY34	0.000
911	H11	65.060	48.838	27.902	H	34	PLY34	0.000
912	H12	63.215	46.434	27.938	H	34	PLY34	0.000
913	H13	64.299	46.972	26.656	H	34	PLY34	0.000
914	H14	60.463	47.722	26.343	H	34	PLY34	0.000
915	H15	61.560	46.346	25.909	H	34	PLY34	0.000
916	H16	61.021	46.738	27.629	H	34	PLY34	0.000
917	H17	63.713	49.320	25.524	H	34	PLY34	0.000
918	H18	62.802	47.939	24.704	H	34	PLY34	0.000
919	H19	62.031	49.483	25.151	H	34	PLY34	0.000
920	H20	61.727	50.487	29.714	H	34	PLY34	0.000
921	H21	60.455	49.348	30.293	H	34	PLY34	0.000
922	H22	60.982	50.685	31.249	H	34	PLY34	0.000
923	N1	59.884	43.117	35.092	N.3	35	PLY35	0.000

924	O1	59.497	46.353	34.543	O.3	35	PLY35	0.000
925	C2	61.997	48.552	32.731	C.3	35	PLY35	0.000
926	O2	61.399	47.477	35.141	O.3	35	PLY35	0.000
927	C3	60.560	47.852	32.906	C.3	35	PLY35	0.000
928	C5	60.616	47.144	34.267	C.3	35	PLY35	0.000
929	C6	59.421	45.636	35.757	C.3	35	PLY35	0.000
930	C7	60.452	44.417	35.695	C.3	35	PLY35	0.000
931	C8	60.882	42.026	35.567	C.3	35	PLY35	0.000
932	C9	59.748	43.205	33.538	C.3	35	PLY35	0.000
933	C10	60.325	46.702	31.864	C.3	35	PLY35	0.000
934	H04	58.935	42.914	35.437	H	35	PLY35	0.000
935	H05	62.103	49.321	33.506	H	35	PLY35	0.000
936	H06	62.665	47.716	32.970	H	35	PLY35	0.000
937	H10	58.390	45.288	35.896	H	35	PLY35	0.000
938	H11	59.691	46.227	36.642	H	35	PLY35	0.000
939	H12	60.633	44.235	36.756	H	35	PLY35	0.000
940	H13	61.382	44.642	35.172	H	35	PLY35	0.000
941	H14	61.242	42.170	36.587	H	35	PLY35	0.000
942	H15	60.322	41.090	35.520	H	35	PLY35	0.000
943	H16	61.736	41.982	34.890	H	35	PLY35	0.000
944	H17	58.993	43.945	33.267	H	35	PLY35	0.000
945	H18	60.690	43.416	33.030	H	35	PLY35	0.000
946	H19	59.414	42.214	33.228	H	35	PLY35	0.000
947	H20	61.215	46.067	31.954	H	35	PLY35	0.000
948	H21	59.502	45.997	32.034	H	35	PLY35	0.000
949	H22	60.165	47.078	30.846	H	35	PLY35	0.000
950	N1	63.689	52.139	37.455	N.3	36	PLY36	0.000
951	O1	60.846	50.526	35.461	O.3	36	PLY36	0.000
952	C2	59.303	48.881	32.825	C.3	36	PLY36	0.000
953	O2	60.397	51.838	33.628	O.3	36	PLY36	0.000
954	C3	58.950	49.916	34.045	C.3	36	PLY36	0.000

955	C5	60.212	50.806	34.281	C.3	36	PLY36	0.000
956	C6	61.843	51.514	35.714	C.3	36	PLY36	0.000
957	C7	62.639	51.106	37.010	C.3	36	PLY36	0.000
958	C8	64.912	52.176	36.493	C.3	36	PLY36	0.000
959	C9	64.236	51.658	38.825	C.3	36	PLY36	0.000
960	C10	58.516	49.198	35.298	C.3	36	PLY36	0.000
961	H04	63.314	53.098	37.462	H	36	PLY36	0.000
962	H05	58.442	48.205	32.746	H	36	PLY36	0.000
963	H06	59.265	49.347	31.833	H	36	PLY36	0.000
964	H10	61.231	52.389	35.965	H	36	PLY36	0.000
965	H11	62.536	51.690	34.881	H	36	PLY36	0.000
966	H12	63.113	50.131	36.886	H	36	PLY36	0.000
967	H13	61.854	50.941	37.750	H	36	PLY36	0.000
968	H14	64.609	51.633	35.597	H	36	PLY36	0.000
969	H15	65.162	53.223	36.316	H	36	PLY36	0.000
970	H16	65.646	51.612	37.070	H	36	PLY36	0.000
971	H17	64.425	50.584	38.828	H	36	PLY36	0.000
972	H18	65.059	52.304	39.135	H	36	PLY36	0.000
973	H19	63.430	51.787	39.548	H	36	PLY36	0.000
974	H20	58.269	49.733	36.224	H	36	PLY36	0.000
975	H21	57.562	48.691	35.110	H	36	PLY36	0.000
976	H22	59.281	48.496	35.652	H	36	PLY36	0.000
977	N1	53.360	48.147	33.092	N.3	37	PLY37	0.000
978	O1	54.956	50.273	34.599	O.3	37	PLY37	0.000
979	C2	57.713	50.815	33.407	C.3	37	PLY37	0.000
980	O2	56.124	50.776	36.504	O.3	37	PLY37	0.000
981	C3	56.858	51.769	34.319	C.3	37	PLY37	0.000
982	C5	55.937	50.902	35.283	C.3	37	PLY37	0.000
983	C6	54.222	49.207	35.243	C.3	37	PLY37	0.000
984	C7	53.010	48.904	34.366	C.3	37	PLY37	0.000
985	C8	54.450	48.810	32.194	C.3	37	PLY37	0.000

986	C9	52.147	48.004	32.199	C.3	37	PLY37	0.000
987	C10	56.010	52.503	33.252	C.3	37	PLY37	0.000
988	H04	53.658	47.212	33.407	H	37	PLY37	0.000
989	H05	57.021	50.102	32.942	H	37	PLY37	0.000
990	H06	58.120	51.377	32.557	H	37	PLY37	0.000
991	H10	53.892	49.452	36.260	H	37	PLY37	0.000
992	H11	54.830	48.303	35.116	H	37	PLY37	0.000
993	H12	52.423	49.787	34.107	H	37	PLY37	0.000
994	H13	52.431	48.264	35.033	H	37	PLY37	0.000
995	H14	54.367	49.895	32.274	H	37	PLY37	0.000
996	H15	55.475	48.635	32.526	H	37	PLY37	0.000
997	H16	54.260	48.563	31.149	H	37	PLY37	0.000
998	H17	51.577	47.207	32.677	H	37	PLY37	0.000
999	H18	51.628	48.963	32.166	H	37	PLY37	0.000
1000	H19	52.350	47.698	31.172	H	37	PLY37	0.000
1001	H20	56.481	53.341	32.723	H	37	PLY37	0.000
1002	H21	55.676	51.719	32.561	H	37	PLY37	0.000
1003	H22	55.088	52.852	33.733	H	37	PLY37	0.000
1004	N1	60.092	57.483	32.398	N.3	38	PLY38	0.000
1005	O1	58.038	55.396	33.656	O.3	38	PLY38	0.000
1006	C2	57.710	52.810	35.120	C.3	38	PLY38	0.000
1007	O2	55.816	55.633	34.066	O.3	38	PLY38	0.000
1008	C3	57.226	54.215	35.643	C.3	38	PLY38	0.000
1009	C5	56.864	55.118	34.354	C.3	38	PLY38	0.000
1010	C6	57.903	55.964	32.329	C.3	38	PLY38	0.000
1011	C7	59.344	56.305	31.750	C.3	38	PLY38	0.000
1012	C8	61.544	57.417	31.900	C.3	38	PLY38	0.000
1013	C9	60.113	57.526	33.920	C.3	38	PLY38	0.000
1014	C10	58.496	54.844	36.452	C.3	38	PLY38	0.000
1015	H04	59.618	58.359	32.135	H	38	PLY38	0.000
1016	H05	58.454	53.095	34.365	H	38	PLY38	0.000

1017	H06	58.193	52.219	35.908	H	38	PLY38	0.000
1018	H10	57.418	56.946	32.390	H	38	PLY38	0.000
1019	H11	57.249	55.438	31.622	H	38	PLY38	0.000
1020	H12	59.300	56.560	30.690	H	38	PLY38	0.000
1021	H13	59.890	55.365	31.839	H	38	PLY38	0.000
1022	H14	61.662	57.774	30.876	H	38	PLY38	0.000
1023	H15	62.014	58.113	32.597	H	38	PLY38	0.000
1024	H16	61.912	56.391	31.936	H	38	PLY38	0.000
1025	H17	60.888	56.845	34.278	H	38	PLY38	0.000
1026	H18	60.363	58.517	34.302	H	38	PLY38	0.000
1027	H19	59.158	57.339	34.412	H	38	PLY38	0.000
1028	H20	58.626	54.380	37.437	H	38	PLY38	0.000
1029	H21	59.411	54.748	35.855	H	38	PLY38	0.000
1030	H22	58.264	55.888	36.696	H	38	PLY38	0.000
1031	N1	57.940	51.631	41.561	N.3	39	PLY39	0.000
1032	O1	56.995	54.078	39.621	O.3	39	PLY39	0.000
1033	C2	55.986	54.008	36.633	C.3	39	PLY39	0.000
1034	O2	57.526	56.180	39.040	O.3	39	PLY39	0.000
1035	C3	55.692	55.080	37.783	C.3	39	PLY39	0.000
1036	C5	56.844	55.189	38.854	C.3	39	PLY39	0.000
1037	C6	57.775	54.228	40.858	C.3	39	PLY39	0.000
1038	C7	57.338	53.037	41.802	C.3	39	PLY39	0.000
1039	C8	56.984	50.664	42.244	C.3	39	PLY39	0.000
1040	C9	59.375	51.542	42.093	C.3	39	PLY39	0.000
1041	C10	54.480	54.549	38.403	C.3	39	PLY39	0.000
1042	H04	57.926	51.463	40.545	H	39	PLY39	0.000
1043	H05	56.292	53.121	37.202	H	39	PLY39	0.000
1044	H06	55.076	53.830	36.047	H	39	PLY39	0.000
1045	H10	57.411	55.130	41.367	H	39	PLY39	0.000
1046	H11	58.825	54.308	40.550	H	39	PLY39	0.000
1047	H12	56.274	52.933	41.584	H	39	PLY39	0.000

1048	H13	57.553	53.326	42.832	H	39	PLY39	0.000
1049	H14	57.303	49.681	41.895	H	39	PLY39	0.000
1050	H15	57.002	50.845	43.320	H	39	PLY39	0.000
1051	H16	55.968	50.776	41.863	H	39	PLY39	0.000
1052	H17	59.478	51.768	43.155	H	39	PLY39	0.000
1053	H18	59.760	50.526	41.985	H	39	PLY39	0.000
1054	H19	60.149	52.083	41.546	H	39	PLY39	0.000
1055	H20	54.154	55.182	39.238	H	39	PLY39	0.000
1056	H21	53.644	54.638	37.698	H	39	PLY39	0.000
1057	H22	54.553	53.501	38.720	H	39	PLY39	0.000
1058	N1	51.770	55.176	33.929	N.3	40	PLY40	0.000
1059	O1	52.484	56.951	36.393	O.3	40	PLY40	0.000
1060	C2	55.423	56.462	37.031	C.3	40	PLY40	0.000
1061	O2	52.389	56.833	38.681	O.3	40	PLY40	0.000
1062	C3	54.451	57.644	37.708	C.3	40	PLY40	0.000
1063	C5	52.946	57.224	37.673	C.3	40	PLY40	0.000
1064	C6	51.140	56.366	36.254	C.3	40	PLY40	0.000
1065	C7	50.855	56.065	34.747	C.3	40	PLY40	0.000
1066	C8	52.978	55.942	33.403	C.3	40	PLY40	0.000
1067	C9	50.974	54.736	32.730	C.3	40	PLY40	0.000
1068	C10	54.562	58.930	36.780	C.3	40	PLY40	0.000
1069	H04	52.160	54.438	34.533	H	40	PLY40	0.000
1070	H05	54.857	56.180	36.135	H	40	PLY40	0.000
1071	H06	56.347	56.903	36.637	H	40	PLY40	0.000
1072	H10	50.348	56.959	36.728	H	40	PLY40	0.000
1073	H11	51.266	55.416	36.788	H	40	PLY40	0.000
1074	H12	50.793	57.049	34.280	H	40	PLY40	0.000
1075	H13	49.840	55.673	34.671	H	40	PLY40	0.000
1076	H14	52.790	56.892	32.899	H	40	PLY40	0.000
1077	H15	53.639	56.132	34.250	H	40	PLY40	0.000
1078	H16	53.573	55.281	32.771	H	40	PLY40	0.000

1079	H17	50.141	54.115	33.063	H	40	PLY40	0.000
1080	H18	50.638	55.608	32.166	H	40	PLY40	0.000
1081	H19	51.637	54.115	32.126	H	40	PLY40	0.000
1082	H20	54.662	58.566	35.750	H	40	PLY40	0.000
1083	H21	53.654	59.544	36.772	H	40	PLY40	0.000
1084	H22	55.538	59.416	36.899	H	40	PLY40	0.000
1085	N1	50.084	62.119	38.963	N.3	41	PLY41	0.000
1086	O1	52.216	59.716	39.191	O.3	41	PLY41	0.000
1087	C2	55.014	58.024	39.200	C.3	41	PLY41	0.000
1088	O2	52.263	58.462	41.096	O.3	41	PLY41	0.000
1089	C3	54.393	59.109	40.179	C.3	41	PLY41	0.000
1090	C5	52.868	58.995	40.194	C.3	41	PLY41	0.000
1091	C6	50.790	59.597	39.030	C.3	41	PLY41	0.000
1092	C7	50.213	60.774	38.282	C.3	41	PLY41	0.000
1093	C8	49.264	62.937	37.912	C.3	41	PLY41	0.000
1094	C9	51.451	62.704	39.186	C.3	41	PLY41	0.000
1095	C10	54.871	60.522	39.699	C.3	41	PLY41	0.000
1096	H04	49.595	62.041	39.866	H	41	PLY41	0.000
1097	H05	56.096	58.202	39.218	H	41	PLY41	0.000
1098	H06	54.880	57.046	39.678	H	41	PLY41	0.000
1099	H10	50.360	59.615	40.039	H	41	PLY41	0.000
1100	H11	50.620	58.670	38.468	H	41	PLY41	0.000
1101	H12	49.177	60.518	38.053	H	41	PLY41	0.000
1102	H13	50.647	60.866	37.285	H	41	PLY41	0.000
1103	H14	48.813	63.854	38.291	H	41	PLY41	0.000
1104	H15	49.940	63.140	37.080	H	41	PLY41	0.000
1105	H16	48.435	62.309	37.581	H	41	PLY41	0.000
1106	H17	51.925	62.887	38.220	H	41	PLY41	0.000
1107	H18	51.280	63.667	39.670	H	41	PLY41	0.000
1108	H19	51.997	62.124	39.930	H	41	PLY41	0.000
1109	H20	55.961	60.651	39.696	H	41	PLY41	0.000

1110	H21	54.540	60.870	38.713	H	41	PLY41	0.000
1111	H22	54.458	61.250	40.408	H	41	PLY41	0.000
1112	N1	60.256	59.788	42.078	N.3	42	PLY42	0.000
1113	O1	57.199	60.549	42.090	O.3	42	PLY42	0.000
1114	C2	54.979	58.879	41.608	C.3	42	PLY42	0.000
1115	O2	55.755	62.252	42.259	O.3	42	PLY42	0.000
1116	C3	54.998	59.973	42.808	C.3	42	PLY42	0.000
1117	C5	56.018	61.075	42.486	C.3	42	PLY42	0.000
1118	C6	58.297	61.519	41.832	C.3	42	PLY42	0.000
1119	C7	59.449	60.674	41.159	C.3	42	PLY42	0.000
1120	C8	61.500	59.306	41.406	C.3	42	PLY42	0.000
1121	C9	59.463	58.526	42.395	C.3	42	PLY42	0.000
1122	C10	55.570	59.195	44.016	C.3	42	PLY42	0.000
1123	H04	60.487	60.265	42.960	H	42	PLY42	0.000
1124	H05	56.017	58.527	41.558	H	42	PLY42	0.000
1125	H06	54.481	57.986	42.006	H	42	PLY42	0.000
1126	H10	58.688	62.069	42.697	H	42	PLY42	0.000
1127	H11	58.012	62.200	41.021	H	42	PLY42	0.000
1128	H12	60.135	61.403	40.725	H	42	PLY42	0.000
1129	H13	59.007	60.076	40.361	H	42	PLY42	0.000
1130	H14	62.274	60.073	41.352	H	42	PLY42	0.000
1131	H15	61.869	58.420	41.925	H	42	PLY42	0.000
1132	H16	61.168	59.018	40.408	H	42	PLY42	0.000
1133	H17	59.091	58.124	41.452	H	42	PLY42	0.000
1134	H18	59.982	57.829	43.054	H	42	PLY42	0.000
1135	H19	58.592	58.878	42.949	H	42	PLY42	0.000
1136	H20	55.790	59.866	44.856	H	42	PLY42	0.000
1137	H21	54.879	58.388	44.289	H	42	PLY42	0.000
1138	H22	56.533	58.749	43.739	H	42	PLY42	0.000
1139	N1	55.840	65.239	42.177	N.3	43	PLY43	0.000
1140	O1	53.557	64.028	43.923	O.3	43	PLY43	0.000

1141	C2	53.523	60.378	43.076	C.3	43	PLY43	0.000
1142	O2	52.547	63.068	42.212	O.3	43	PLY43	0.000
1143	C3	53.235	61.584	44.085	C.3	43	PLY43	0.000
1144	C5	53.118	62.935	43.266	C.3	43	PLY43	0.000
1145	C6	53.498	65.292	43.222	C.3	43	PLY43	0.000
1146	C7	54.330	65.357	41.944	C.3	43	PLY43	0.000
1147	C8	56.287	66.477	43.021	C.3	43	PLY43	0.000
1148	C9	56.582	65.279	40.822	C.3	43	PLY43	0.000
1149	C10	54.246	61.854	45.208	C.3	43	PLY43	0.000
1150	H04	55.989	64.349	42.675	H	43	PLY43	0.000
1151	H05	52.883	59.517	43.304	H	43	PLY43	0.000
1152	H06	53.067	60.720	42.139	H	43	PLY43	0.000
1153	H10	53.930	66.053	43.884	H	43	PLY43	0.000
1154	H11	52.455	65.600	43.083	H	43	PLY43	0.000
1155	H12	54.048	66.293	41.461	H	43	PLY43	0.000
1156	H13	54.114	64.608	41.181	H	43	PLY43	0.000
1157	H14	55.685	66.489	43.931	H	43	PLY43	0.000
1158	H15	57.369	66.486	43.160	H	43	PLY43	0.000
1159	H16	55.948	67.367	42.489	H	43	PLY43	0.000
1160	H17	55.882	64.957	40.049	H	43	PLY43	0.000
1161	H18	56.938	66.297	40.656	H	43	PLY43	0.000
1162	H19	57.375	64.535	40.914	H	43	PLY43	0.000
1163	H20	54.013	62.684	45.888	H	43	PLY43	0.000
1164	H21	54.388	61.048	45.938	H	43	PLY43	0.000
1165	H22	55.238	62.172	44.863	H	43	PLY43	0.000
1166	N1	55.869	60.718	49.397	N.3	44	PLY44	0.000
1167	O1	52.912	60.904	48.072	O.3	44	PLY44	0.000
1168	C2	51.755	61.348	44.763	C.3	44	PLY44	0.000
1169	O2	52.079	62.800	47.297	O.3	44	PLY44	0.000
1170	C3	51.556	60.597	46.132	C.3	44	PLY44	0.000
1171	C5	52.110	61.535	47.229	C.3	44	PLY44	0.000

1172	C6	53.462	61.662	49.229	C.3	44	PLY44	0.000
1173	C7	54.488	60.816	49.972	C.3	44	PLY44	0.000
1174	C8	56.217	61.931	48.635	C.3	44	PLY44	0.000
1175	C9	55.899	59.423	48.669	C.3	44	PLY44	0.000
1176	C10	52.226	59.281	46.062	C.3	44	PLY44	0.000
1177	H04	56.554	60.568	50.152	H	44	PLY44	0.000
1178	H05	51.059	60.862	44.069	H	44	PLY44	0.000
1179	H06	51.498	62.404	44.915	H	44	PLY44	0.000
1180	H10	52.652	61.906	49.928	H	44	PLY44	0.000
1181	H11	53.891	62.637	48.965	H	44	PLY44	0.000
1182	H12	54.004	59.843	50.060	H	44	PLY44	0.000
1183	H13	54.507	61.159	51.008	H	44	PLY44	0.000
1184	H14	56.019	62.832	49.218	H	44	PLY44	0.000
1185	H15	57.267	61.881	48.342	H	44	PLY44	0.000
1186	H16	55.604	61.862	47.735	H	44	PLY44	0.000
1187	H17	56.910	59.219	48.313	H	44	PLY44	0.000
1188	H18	55.604	58.576	49.291	H	44	PLY44	0.000
1189	H19	55.273	59.590	47.791	H	44	PLY44	0.000
1190	H20	52.024	58.620	46.915	H	44	PLY44	0.000
1191	H21	51.875	58.768	45.158	H	44	PLY44	0.000
1192	H22	53.313	59.427	46.059	H	44	PLY44	0.000
1193	N1	49.236	55.252	45.928	N.3	45	PLY45	0.000
1194	O1	49.489	57.849	47.592	O.3	45	PLY45	0.000
1195	C2	50.010	60.488	46.207	C.3	45	PLY45	0.000
1196	O2	50.691	59.078	49.096	O.3	45	PLY45	0.000
1197	C3	49.223	60.261	47.554	C.3	45	PLY45	0.000
1198	C5	49.904	59.027	48.192	C.3	45	PLY45	0.000
1199	C6	49.855	56.552	48.191	C.3	45	PLY45	0.000
1200	C7	49.127	55.367	47.481	C.3	45	PLY45	0.000
1201	C8	50.676	55.226	45.398	C.3	45	PLY45	0.000
1202	C9	48.498	56.357	45.232	C.3	45	PLY45	0.000

1203	C10	47.807	59.942	47.056	C.3	45	PLY45	0.000
1204	H04	48.728	54.400	45.648	H	45	PLY45	0.000
1205	H05	49.818	59.627	45.555	H	45	PLY45	0.000
1206	H06	49.489	61.265	45.634	H	45	PLY45	0.000
1207	H10	49.588	56.473	49.253	H	45	PLY45	0.000
1208	H11	50.941	56.397	48.159	H	45	PLY45	0.000
1209	H12	48.087	55.358	47.809	H	45	PLY45	0.000
1210	H13	49.626	54.514	47.943	H	45	PLY45	0.000
1211	H14	51.254	54.395	45.804	H	45	PLY45	0.000
1212	H15	50.659	55.134	44.311	H	45	PLY45	0.000
1213	H16	51.123	56.190	45.645	H	45	PLY45	0.000
1214	H17	49.184	57.205	45.247	H	45	PLY45	0.000
1215	H18	48.309	55.970	44.229	H	45	PLY45	0.000
1216	H19	47.604	56.523	45.834	H	45	PLY45	0.000
1217	H20	47.776	59.318	46.155	H	45	PLY45	0.000
1218	H21	47.275	59.325	47.790	H	45	PLY45	0.000
1219	H22	47.147	60.813	46.956	H	45	PLY45	0.000
1220	N1	47.716	62.923	55.236	N.3	46	PLY46	0.000
1221	O1	48.623	62.563	52.075	O.3	46	PLY46	0.000
1222	C2	49.329	61.479	48.574	C.3	46	PLY46	0.000
1223	O2	49.918	63.350	50.411	O.3	46	PLY46	0.000
1224	C3	48.386	61.645	49.814	C.3	46	PLY46	0.000
1225	C5	49.024	62.663	50.797	C.3	46	PLY46	0.000
1226	C6	49.129	63.432	53.088	C.3	46	PLY46	0.000
1227	C7	48.980	62.718	54.478	C.3	46	PLY46	0.000
1228	C8	47.721	64.371	55.731	C.3	46	PLY46	0.000
1229	C9	47.563	62.034	56.456	C.3	46	PLY46	0.000
1230	C10	48.284	60.196	50.548	C.3	46	PLY46	0.000
1231	H04	46.932	62.740	54.594	H	46	PLY46	0.000
1232	H05	49.352	62.394	47.969	H	46	PLY46	0.000
1233	H06	50.357	61.466	48.957	H	46	PLY46	0.000

1234	H10	48.543	64.357	53.164	H	46	PLY46	0.000
1235	H11	50.182	63.597	52.826	H	46	PLY46	0.000
1236	H12	49.782	62.998	55.162	H	46	PLY46	0.000
1237	H13	49.087	61.673	54.184	H	46	PLY46	0.000
1238	H14	48.497	64.410	56.497	H	46	PLY46	0.000
1239	H15	48.015	64.924	54.838	H	46	PLY46	0.000
1240	H16	46.756	64.721	56.100	H	46	PLY46	0.000
1241	H17	48.475	62.044	57.056	H	46	PLY46	0.000
1242	H18	46.790	62.526	57.048	H	46	PLY46	0.000
1243	H19	47.181	61.060	56.145	H	46	PLY46	0.000
1244	H20	47.816	59.473	49.868	H	46	PLY46	0.000
1245	H21	49.261	59.837	50.893	H	46	PLY46	0.000
1246	H22	47.646	60.251	51.439	H	46	PLY46	0.000
1247	N1	51.358	65.454	49.230	N.3	47	PLY47	0.000
1248	O1	48.552	64.599	48.123	O.3	47	PLY47	0.000
1249	C2	46.911	61.984	49.466	C.3	47	PLY47	0.000
1250	O2	47.276	63.876	46.464	O.3	47	PLY47	0.000
1251	C3	46.519	63.376	48.867	C.3	47	PLY47	0.000
1252	C5	47.479	63.973	47.676	C.3	47	PLY47	0.000
1253	C6	49.498	65.388	47.306	C.3	47	PLY47	0.000
1254	C7	50.422	66.228	48.236	C.3	47	PLY47	0.000
1255	C8	51.347	66.060	50.660	C.3	47	PLY47	0.000
1256	C9	52.729	65.372	48.654	C.3	47	PLY47	0.000
1257	C10	46.556	64.446	49.981	C.3	47	PLY47	0.000
1258	H04	51.077	64.464	49.275	H	47	PLY47	0.000
1259	H05	46.303	61.906	50.377	H	47	PLY47	0.000
1260	H06	46.436	61.156	48.925	H	47	PLY47	0.000
1261	H10	48.950	65.995	46.576	H	47	PLY47	0.000
1262	H11	50.144	64.640	46.829	H	47	PLY47	0.000
1263	H12	49.776	66.890	48.815	H	47	PLY47	0.000
1264	H13	51.107	66.809	47.616	H	47	PLY47	0.000

1265	H14	52.246	65.761	51.200	H	47	PLY47	0.000
1266	H15	51.287	67.143	50.779	H	47	PLY47	0.000
1267	H16	50.432	65.679	51.116	H	47	PLY47	0.000
1268	H17	53.294	64.918	49.470	H	47	PLY47	0.000
1269	H18	52.730	64.734	47.769	H	47	PLY47	0.000
1270	H19	53.044	66.373	48.357	H	47	PLY47	0.000
1271	H20	45.937	64.160	50.840	H	47	PLY47	0.000
1272	H21	47.554	64.722	50.344	H	47	PLY47	0.000
1273	H22	46.118	65.419	49.725	H	47	PLY47	0.000
1274	N1	41.601	65.789	53.645	N.3	48	PLY48	0.000
1275	O1	43.146	64.979	50.943	O.3	48	PLY48	0.000
1276	C2	44.984	63.303	48.267	C.3	48	PLY48	0.000
1277	O2	43.087	65.691	48.782	O.3	48	PLY48	0.000
1278	C3	43.643	63.329	49.201	C.3	48	PLY48	0.000
1279	C5	43.328	64.837	49.586	C.3	48	PLY48	0.000
1280	C6	42.919	66.315	51.388	C.3	48	PLY48	0.000
1281	C7	42.881	66.307	52.941	C.3	48	PLY48	0.000
1282	C8	41.610	66.347	55.066	C.3	48	PLY48	0.000
1283	C9	41.634	64.236	53.622	C.3	48	PLY48	0.000
1284	C10	43.708	62.357	50.374	C.3	48	PLY48	0.000
1285	H04	40.865	66.270	53.108	H	48	PLY48	0.000
1286	H05	44.984	62.432	47.600	H	48	PLY48	0.000
1287	H06	44.854	64.191	47.635	H	48	PLY48	0.000
1288	H10	41.981	66.797	51.087	H	48	PLY48	0.000
1289	H11	43.755	66.972	51.118	H	48	PLY48	0.000
1290	H12	43.047	67.298	53.366	H	48	PLY48	0.000
1291	H13	43.700	65.716	53.355	H	48	PLY48	0.000
1292	H14	42.286	65.718	55.646	H	48	PLY48	0.000
1293	H15	41.926	67.391	55.067	H	48	PLY48	0.000
1294	H16	40.617	66.250	55.508	H	48	PLY48	0.000
1295	H17	40.829	63.685	54.110	H	48	PLY48	0.000

1296	H18	41.664	63.878	52.592	H	48	PLY48	0.000
1297	H19	42.535	63.935	54.158	H	48	PLY48	0.000
1298	H20	43.867	61.350	49.970	H	48	PLY48	0.000
1299	H21	44.518	62.577	51.080	H	48	PLY48	0.000
1300	H22	42.792	62.468	50.968	H	48	PLY48	0.000
1301	N1	40.504	57.744	46.787	N.3	49	PLY49	0.000
1302	O1	40.443	60.327	48.404	O.3	49	PLY49	0.000
1303	C2	42.491	62.898	48.161	C.3	49	PLY49	0.000
1304	O2	40.590	61.096	50.540	O.3	49	PLY49	0.000
1305	C3	40.950	62.685	48.657	C.3	49	PLY49	0.000
1306	C5	40.799	61.295	49.345	C.3	49	PLY49	0.000
1307	C6	39.994	59.104	48.909	C.3	49	PLY49	0.000
1308	C7	39.435	58.338	47.707	C.3	49	PLY49	0.000
1309	C8	41.286	58.925	46.088	C.3	49	PLY49	0.000
1310	C9	39.773	56.853	45.751	C.3	49	PLY49	0.000
1311	C10	40.089	62.818	47.342	C.3	49	PLY49	0.000
1312	H04	41.153	57.123	47.290	H	49	PLY49	0.000
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1315	H10	39.261	59.216	49.717	H	49	PLY49	0.000
1316	H11	40.776	58.536	49.428	H	49	PLY49	0.000
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1318	H13	38.748	57.610	48.142	H	49	PLY49	0.000
1319	H14	41.948	59.262	46.887	H	49	PLY49	0.000
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1321	H16	40.568	59.686	45.782	H	49	PLY49	0.000
1322	H17	39.121	56.160	46.284	H	49	PLY49	0.000
1323	H18	39.127	57.471	45.126	H	49	PLY49	0.000
1324	H19	40.485	56.332	45.109	H	49	PLY49	0.000
1325	H20	39.021	62.581	47.422	H	49	PLY49	0.000
1326	H21	40.215	63.728	46.744	H	49	PLY49	0.000

1327	H22	40.322	61.987	46.665	H	49	PLY49	0.000
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1331	O2	37.179	64.298	48.079	O.3	50	TIL50	0.000
1332	C3	38.859	63.960	49.854	C.3	50	TIL50	0.000
1333	C4	38.103	62.664	50.125	C.3	50	TIL50	0.000
1334	C5	38.215	64.700	48.634	C.3	50	TIL50	0.000
1335	C6	38.161	66.927	47.710	C.3	50	TIL50	0.000
1336	C7	38.610	68.320	48.076	C.3	50	TIL50	0.000
1337	C8	37.654	68.403	50.324	C.3	50	TIL50	0.000
1338	C9	38.795	70.273	49.541	C.3	50	TIL50	0.000
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1355	H19	39.724	70.690	49.149	H	50	TIL50	0.000
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1358 H22 39.530 65.716 51.000 H 50 TIL50 0.000

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@<TRIPOS>SUBSTRUCTURE

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3	PLY3	59	GROUP	1 X	PLY
4	PLY4	86	GROUP	1 X	PLY

5	PLY5	113	GROUP	1 X	PLY
6	PLY6	140	GROUP	1 X	PLY
7	PLY7	167	GROUP	1 X	PLY
8	PLY8	194	GROUP	1 X	PLY
9	PLY9	221	GROUP	1 X	PLY
10	PLY10	248	GROUP	1 X	PLY
11	PLY11	275	GROUP	1 X	PLY
12	PLY12	302	GROUP	1 X	PLY
13	PLY13	329	GROUP	1 X	PLY
14	PLY14	356	GROUP	1 X	PLY
15	PLY15	383	GROUP	1 X	PLY
16	PLY16	410	GROUP	1 X	PLY
17	PLY17	437	GROUP	1 X	PLY
18	PLY18	464	GROUP	1 X	PLY
19	PLY19	491	GROUP	1 X	PLY
20	PLY20	518	GROUP	1 X	PLY
21	PLY21	545	GROUP	1 X	PLY
22	PLY22	572	GROUP	1 X	PLY
23	PLY23	599	GROUP	1 X	PLY
24	PLY24	626	GROUP	1 X	PLY
25	PLY25	653	GROUP	1 X	PLY
26	PLY26	680	GROUP	1 X	PLY
27	PLY27	707	GROUP	1 X	PLY
28	PLY28	734	GROUP	1 X	PLY
29	PLY29	761	GROUP	1 X	PLY
30	PLY30	788	GROUP	1 X	PLY
31	PLY31	815	GROUP	1 X	PLY
32	PLY32	842	GROUP	1 X	PLY
33	PLY33	869	GROUP	1 X	PLY
34	PLY34	896	GROUP	1 X	PLY
35	PLY35	923	GROUP	1 X	PLY

36	PLY36	950	GROUP	1 X	PLY
37	PLY37	977	GROUP	1 X	PLY
38	PLY38	1004	GROUP	1 X	PLY
39	PLY39	1031	GROUP	1 X	PLY
40	PLY40	1058	GROUP	1 X	PLY
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42	PLY42	1112	GROUP	1 X	PLY
43	PLY43	1139	GROUP	1 X	PLY
44	PLY44	1166	GROUP	1 X	PLY
45	PLY45	1193	GROUP	1 X	PLY
46	PLY46	1220	GROUP	1 X	PLY
47	PLY47	1247	GROUP	1 X	PLY
48	PLY48	1274	GROUP	1 X	PLY
49	PLY49	1301	GROUP	1 X	PLY
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