Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for:

Intermolecular Resonance Energy Transfer between Two Lutein Pigments in Light-Harvesting Complex II studied by Frenkel exciton models

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1. The distance between two LUTs in the conformations sampled.

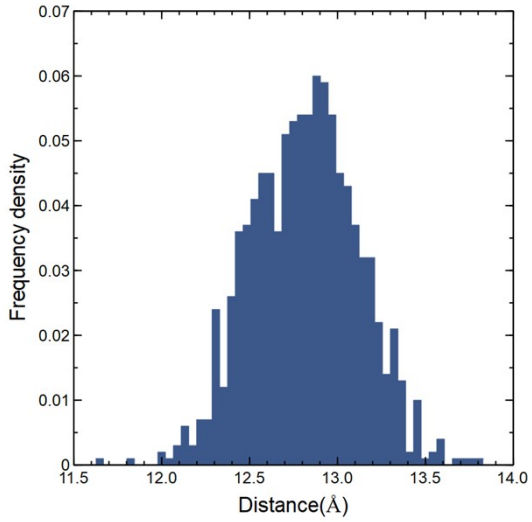

Figure S1. The distance between the C15 (middle carbon of the long chain) of two LUTs.

2. Test results of cam-B3LYP/6-31+G(d) method.

Table S1: The results in the three columns are the excitation energies of the two LUTs in the gas phase, the excitation energies of the two LUTs in a self-consistent converged charge environment, and the excitation energy shifts of the two LUTs caused by the environments. The excitation energies and self-consistent convergent charges here were all calculated by the cam-B3LYP/6-31+G(d) method. (Unit: eV).

	$E_{pigment}^{0}$	$E_{pigment}^{env}$	$\Delta E_{pigment}^{env}$
$E_{LUT1}^{S_2}$	2.8722	2.8435	-0.0287
$E_{LUT2}^{S_2}$	2.8894	2.7668	-0.1226

Table S2: The wavelength of the S_2 state of the two LUTs which are measured by different methods. Unit: eV(nm).

	2DES	TD/B3LYP with B3LYP charges	TD/B3LYP with cam-B3LYP charges	TD/cam-B3LYP with cam-B3LYP charges
$E_{LUT1}^{S_2}$	2.5047(495)	2.3871(519)	2.4227(511)	2.8435(436)
$E_{LUT2}^{S_2}$	2.4311(510)	2.3454(528)	2.2694(546)	2.7668(448)

Table S3: Comparison of the electrostatic potential of residue from two functional optimizations.

Residue name	Residue ID	cam-B3LYP	B3LYP
TYR	24	0.035779	0.021664
LEU	25	-0.073615	-0.05913
SER	32	-0.251675	-0.106098
PRO	33	0.224581	0.084155
TYR	35	-0.256062	-0.087221
LEU	36	0.124823	0.072986
GLY	42	-0.28322	-0.053833
ASH	43	0.04961	0.037177
TYR	44	-0.11761	-0.176728
GLY	45	0.621472	0.06952
TRP	46	-0.146356	0.19958
ASH	47	-0.093335	-0.119712

THR	48	-0.144324	-0.090865
ALA	49	-0.10375	-0.109109
GLY	50	0.012068	0.011607
LEU	51	-0.078772	-0.082836
SER	52	-0.100805	-0.046958
ALA	53	-0.023244	0.054943
THR	57	-0.171319	0.039538
PHE	58	-0.420184	-0.00926
ASN	61	0.23232	-0.019651
ARG	62	-0.113705	-0.030654
GLU	63	-0.053875	-0.073625
LEU	64	0.466088	0.24769
GLU	65	-0.66357	-0.4376
VAL	66	-0.226976	-0.239721
ILE	67	0.01711	-0.0144
HIS	68	-0.08795	-0.092025
CYS	69	0.023792	-0.061813
ARG	70	0.160836	0.041557
TRP	71	0.046838	0.012677
ALA	72	0.00083	0.010718
MET	73	-0.031962	-0.045657
LEU	74	0.000553	-0.02365
GLY	75	-0.1528	-0.145121

ALA	76	0.076789	0.028462
LEU	77	-0.048777	-0.048131
GLY	78	-0.049732	-0.051581
CYS	79	-0.034087	-0.044959
VAL	80	0.147338	0.060395
PHE	81	-0.235424	-0.21842
PRO	82	0.061161	0.023773
GLU	83	-0.040645	0.048596
LEU	84	0.017413	-0.059702
PHE	92	-0.433666	1E-06
GLU	94	0.109061	-0.053889
ALA	95	0.013553	0.003066
VAL	96	-0.062319	-0.116286
TRP	97	0.148393	0.093451
PHE	98	-0.168968	-0.20396
LYS	99	0.165187	0.022106
ALA	100	0.010297	-0.006569
GLY	101	0.000276	-0.036344
SER	102	-0.107181	-0.101068
GLN	103	0.145352	0.137282
ILE	104	-0.280292	-0.095764
LEU	110	-0.178743	-1E-06
TYR	112	-0.04062	1E-06

ILE	124	-0.401859	0
ILE	127	-0.121384	-1E-06
GLN	131	-0.249014	0
MET	135	0.035639	-1E-06
ILE	181	-0.469003	-1E-06
ASN	183	-0.119831	-0.126035
GLY	184	0.173557	-0.132751
ARG	185	0.065316	0.167206
LEU	186	0.007992	-0.01876
ALA	187	0.112425	0.082534
MET	188	-0.127142	-0.143371
PHE	189	0.006847	-0.028107
SER	190	-0.0799	-0.068025
MET	191	-0.022008	-0.052259
PHE	192	0.007167	-0.035287
GLY	193	-0.184984	-0.139925
PHE	194	0.079048	0.01979
PHE	195	-0.078083	0.004322
VAL	196	-0.30553	-0.033342
ALA	198	-0.197097	-2E-06
GLY	204	0.537879	-0.12708
PRO	205	0.130684	-0.042544

3. The influence of environmental components on the excitation energy of LUTs.

Table S4：The excitation energy of LUTs when not considering the ESP charges of each pigment. The difference value refers to the deviation from the excitation energy under the self-consistent convergent charge mentioned in the main text Table 1. (Unit =eV).

	$E_{LUT1}^{S_2}$	Energy shift ($\Delta E_{LUT1}^{S_2}$)	$E_{LUT2}^{S_2}$	Energy shift ($\Delta E_{LUT2}^{S_2}$)	Gap shift ($\Delta E_{LUT1}^{S_2}$-$\Delta E_{LUT2}^{S_2}$)
ESP(LUT1) =0	2.3895	0	2.3990	-0.0478	0.0478
ESP(LUT2) =0	2.4200	-0.0305	2.3512	0	-0.0305
ESP(CLA602) =0	2.3825	0.07	2.3941	-0.0429	0.0499
ESP(CLA603) =0	2.3848	0.0047	2.3309	0.0203	-0.0156
ESP(CLA604) =0	2.3888	0.0007	2.3636	-0.0124	0.0131
ESP(CLA610) =0	2.3971	-0.0076	2.3391	0.0121	-0.0197
ESP(CLA611) =0	2.3682	0.0213	2.3508	0.0004	0.0209
ESP(CLA612) =0	2.3975	-0.008	2.3363	0.0149	-0.0229
ESP(CLA613) =0	2.3872	0.023	2.3469	0.0043	-0.002

Table S5：The excitation energy of LUTs when not considering the ESP charges of each residue. The difference value refers to the deviation from the excitation energy under the self-consistent convergent charge mentioned in the main text Table 1. The form of the first column of the table, i.e. ESP (residue name, residue ID). (Unit =eV).

	$E_{LUT1}^{S_2}$	Energy shift ($\Delta E_{LUT1}^{S_2}$)	$E_{LUT2}^{S_2}$	Energy shift ($\Delta E_{LUT2}^{S_2}$)	Gap shift ($\Delta E_{LUT1}^{S_2}$- $\Delta E_{LUT2}^{S_2}$)
ESP(TRP,46) =0	2.3855	0.004	2.3759	-0.0247	0.0287
ESP(ASH,47) =0	2.3899	-0.0004	2.3312	0.02	-0.0204
ESP(THR,48) =0	2.3895	0	2.3297	0.0215	-0.0215
ESP(ALA,49) =0	2.3904	-0.0009	2.3385	0.0127	-0.0136
ESP(GLY,50) =0	2.3887	0.0008	2.3628	-0.0116	0.0124
ESP(LEU,51) =0	2.3892	0.0003	2.3397	0.0115	-0.0112
ESP(HIS,68) =0	2.38	0.0095	2.4046	-0.0534	0.0629
ESP(CYS,69) =0	2.3968	-0.0073	2.3637	-0.0125	0.0052
ESP(TRP,71) =0	2.3882	0.0013	2.4375	-0.0863	0.0876
ESP(ALA,72) =0	2.4181	-0.0286	2.3844	-0.0332	0.0046
ESP(MET,73) =0	2.395	-0.0055	2.3685	-0.0173	0.0118
ESP(LEU,74) =0	2.4035	-0.014	2.3857	-0.0345	0.0205
ESP(ALA,76) =0	2.4013	-0.0118	2.3498	0.0014	-0.0132
ESP(LEU,77) =0	2.419	-0.0295	2.3609	-0.0097	-0.0198
ESP(GLY,78) =0	2.3952	-0.0057	2.3464	0.0048	-0.0105
ESP(CYS,79) =0	2.3952	-0.0057	2.3515	-0.0003	-0.0054
ESP(PRO,82) =0	2.3802	0.0093	2.304	0.0472	-0.0379
ESP(VAL,96) =0	2.3894	1E-04	2.3772	-0.026	0.0261
ESP(TRP,97) =0	2.3779	0.0116	2.3322	0.019	-0.0074

ESP(PHE,98) =0	2.3949	-0.0054	2.3798	-0.0286	0.0232
ESP(ALA,100) =0	2.385	0.0045	2.3292	0.022	-0.0175
ESP(GLY,101) =0	2.3859	0.0036	2.3328	0.0184	-0.0148
ESP(PHE,161) =0	2.3788	0.0107	2.3511	1E-04	0.0106
ESP(ASH,162) =0	2.3482	0.0413	2.3538	-0.0026	0.0439
ESP(PRO,163) =0	2.4187	-0.0292	2.3465	0.0047	-0.0339
ESP(LEU,164) =0	2.3583	0.0312	2.3535	-0.0023	0.0335
ESP(GLY,165) =0	2.401	-0.0115	2.3494	0.0018	-0.0133
ESP(LEU,166) =0	2.3849	0.0046	2.3501	0.0011	0.0035
ESP(ASN,183) =0	2.4076	-0.0181	2.3561	-0.0049	-0.0132
ESP(GLY,184) =0	2.4158	-0.0263	2.3444	0.0068	-0.0331
ESP(LEU,186) =0	2.4349	-0.0454	2.3447	0.0065	-0.0519
ESP(ALA,187) =0	2.4105	-0.021	2.3724	-0.0212	0.0002
ESP(MET,188) =0	2.4184	-0.0289	2.3214	0.0298	-0.0587
ESP(PHE,189) =0	2.391	-0.0015	2.3616	-0.0104	0.0089
ESP(SER,190) =0	2.4053	-0.0158	2.3588	-0.0076	-0.0082
ESP(MET,191) =0	2.4014	-0.0119	2.4033	-0.0521	0.0402
ESP(PHE,192) =0	2.3838	0.0057	2.3769	-0.0257	0.0314
ESP(GLY,193) =0	2.383	0.0065	2.3597	-0.0085	0.015
ESP(PHE,194) =0	2.4189	-0.0294	2.3522	-0.001	-0.0284
ESP(PHE,195) =0	2.3891	0.0004	2.3805	-0.0293	0.0297
ESP(GLN,197) =0	2.3877	0.0018	2.3372	0.014	-0.0122
ESP(PRO,205) =0	2.3559	0.0336	2.331	0.0202	0.0134

ESP(LEU,206) =0	2.3973	-0.0078	2.3501	0.0011	-0.0089
ESP(ASN,208) =0	2.3873	0.0022	2.348	0.0032	-0.001
ESP(LEU,209) =0	2.3743	0.0152	2.346	0.0052	0.01

4. An ensemble-averaged Hamiltonian.

Table S6: The diagonal terms are the ensemble-averaged excitation energies of the two LUTs and the off-diagonal terms are the ensemble-averaged electronic coupling values. (unit: eV).

	S_2(LUT1)	S_2(LUT2)
S_2(LUT1)	2.35949	0.00505
S_2(LUT2)	0.00505	2.35641

5. Hypothesis test results of Gaussian distribution.

In the text, the stochastic exciton Hamiltonian models can be described as

$$\begin{pmatrix} H_{LUT1} & H_{LUT1LUT2} \\ H_{LUT2LUT1} & H_{LUT2} \end{pmatrix},$$

Table S7. Kolmogorov-Smirnov (K-S) constructive testing results of matrix elements of stochastic exciton Hamiltonian models.

	H_{LUT1}	H_{LUT2}	$H_{LUT1LUT2}$($H_{LUT2LUT1}$)	ΔH ($H_{LUT1} - H_{LUT2}$)
p-values	0.33025	1	0.8499	1

6. Correlation test result.

Table S8. Pearson correlation coefficients test result.

	H_{LUT1}_ H_{LUT2}	H_{LUT1}_ $H_{LUT1LUT2}$	H_{LUT2}_ $H_{LUT1LUT2}$	$H_{LUT1LUT2}$_ ΔH
correlation coefficient	0.00408,	-0.16356	-0.07463	-0.06122

7. The self-consistent convergent charge is used in this paper.

Table S9. Electrostatic potential (ESP) charges of atoms within the 10 Å - radius of LUT1 and LUT2.

Atom	ESP charge	x	y	z	PDB name	Residue name	Residue ID
N	-0.567974	55.76	104.25	21.89	N	TYR	24
H	0.146942	55.56	104.75	22.74	H1	TYR	24
H	0.174402	55.18	105.03	22.10	H2	TYR	24
H	0.223493	56.31	104.02	22.69	H3	TYR	24
C	0.220596	54.93	103.11	21.53	CA	TYR	24
H	0.065051	55.64	102.43	21.34	HA	TYR	24
C	-0.313105	54.01	102.76	22.71	CB	TYR	24
H	0.125978	54.50	102.94	23.56	HB1	TYR	24
H	0.092625	53.78	101.79	22.66	HB2	TYR	24
C	0.140305	52.70	103.53	22.76	CG	TYR	24
C	-0.273067	51.51	102.92	22.37	CD1	TYR	24
H	0.150295	51.51	101.97	22.06	HD1	TYR	24
C	-0.259559	50.31	103.62	22.41	CE1	TYR	24
H	0.159644	49.46	103.17	22.13	HE1	TYR	24
C	0.364338	50.29	104.93	22.83	CZ	TYR	24
O	-0.586887	49.09	105.62	22.84	OH	TYR	24
H	0.393927	49.24	106.55	23.17	HH	TYR	24
C	-0.436554	51.46	105.56	23.23	CE2	TYR	24
H	0.184829	51.44	106.51	23.53	HE2	TYR	24
C	-0.130365	52.66	104.86	23.19	CD2	TYR	24
H	0.112297	53.51	105.31	23.48	HD2	TYR	24
C	0.728436	54.11	103.16	20.23	C	TYR	24
O	-0.693983	53.62	102.12	19.77	O	TYR	24
N	-1.032928	53.96	104.34	19.64	N	LEU	25
H	0.443329	54.34	105.16	20.06	H	LEU	25
C	0.878943	53.22	104.44	18.38	CA	LEU	25
H	-0.003418	52.86	103.53	18.19	HA	LEU	25
C	-0.420968	52.05	105.43	18.51	CB	LEU	25
H	0.074444	51.67	105.58	17.59	HB1	LEU	25

H	0.105286	52.41	106.29	18.87	HB2	LEU	25
C	0.446265	50.90	104.98	19.42	CG	LEU	25
H	-0.034121	51.23	104.89	20.36	HG	LEU	25
C	-0.431847	49.80	106.03	19.42	CD1	LEU	25
H	0.101932	49.06	105.73	20.01	1HD1	LEU	25
H	0.079664	50.16	106.90	19.75	2HD1	LEU	25
H	0.119166	49.45	106.14	18.48	3HD1	LEU	25
C	-0.369552	50.38	103.63	18.95	CD2	LEU	25
H	0.073208	49.63	103.34	19.54	1HD2	LEU	25
H	0.068390	50.05	103.72	18.01	2HD2	LEU	25
H	0.111290	51.11	102.96	18.98	3HD2	LEU	25
C	-0.039398	54.17	104.88	17.27	C	LEU	25
O	-0.228815	53.73	105.32	16.20	O	LEU	25
N	-0.688971	53.34	112.98	24.40	N	SER	32
H	0.370367	54.22	113.45	24.27	H	SER	32
C	0.558365	53.21	111.98	25.45	CA	SER	32
H	-0.117508	52.48	111.37	25.12	HA	SER	32
C	0.095612	54.52	111.22	25.62	CB	SER	32
H	0.046438	54.91	110.97	24.74	HB1	SER	32
H	-0.045407	54.38	110.38	26.16	HB2	SER	32
O	-0.630244	55.47	112.00	26.30	OG	SER	32
H	0.424352	56.32	111.48	26.41	HG	SER	32
C	0.253940	52.78	112.60	26.78	C	SER	32
O	-0.373042	52.92	113.80	26.98	O	SER	32
N	-0.095001	52.25	111.77	27.69	N	PRO	33
C	-0.105980	52.05	110.32	27.59	CD	PRO	33
H	0.069575	52.91	109.83	27.75	HD1	PRO	33
H	0.087382	51.68	110.07	26.69	HD2	PRO	33
C	-0.014691	51.05	110.06	28.68	CG	PRO	33
H	0.015886	51.09	109.10	28.99	HG1	PRO	33
H	0.050222	50.12	110.27	28.39	HG2	PRO	33
C	-0.098726	51.51	110.99	29.77	CB	PRO	33
H	0.082939	52.33	110.63	30.22	HB1	PRO	33
H	0.065103	50.79	111.13	30.44	HB2	PRO	33
C	0.147238	51.81	112.27	29.00	CA	PRO	33
H	0.077089	51.02	112.88	28.92	HA	PRO	33
C	0.044093	52.90	113.11	29.67	C	PRO	33
O	-0.240974	54.08	112.78	29.60	O	PRO	33
N	-0.645471	53.50	113.41	32.73	N	TYR	35
H	0.316795	52.59	113.15	32.41	H	TYR	35
C	0.477837	54.10	112.71	33.86	CA	TYR	35
H	-0.012631	54.69	113.41	34.28	HA	TYR	35
C	-0.402058	53.01	112.27	34.84	CB	TYR	35
H	0.164142	52.57	113.09	35.21	HB1	TYR	35
H	0.083742	53.44	111.76	35.58	HB2	TYR	35
C	0.317875	51.93	111.40	34.24	CG	TYR	35

C	-0.294714	52.12	110.02	34.10	CD1	TYR	35
H	0.160288	52.99	109.62	34.37	HD1	TYR	35
C	-0.188323	51.11	109.21	33.59	CE1	TYR	35
H	0.152734	51.26	108.23	33.49	HE1	TYR	35
C	0.312764	49.90	109.77	33.21	CZ	TYR	35
O	-0.560460	48.91	108.95	32.71	OH	TYR	35
H	0.392952	48.11	109.50	32.48	HH	TYR	35
C	-0.313962	49.69	111.13	33.34	CE2	TYR	35
H	0.181504	48.81	111.53	33.06	HE2	TYR	35
C	-0.280785	50.70	111.94	33.85	CD2	TYR	35
H	0.202614	50.55	112.93	33.94	HD2	TYR	35
C	0.329212	55.02	111.55	33.46	C	TYR	35
O	-0.481276	55.67	110.94	34.31	O	TYR	35
N	-0.439157	55.07	111.24	32.16	N	LEU	36
H	0.336097	54.49	111.74	31.52	H	LEU	36
C	0.781920	55.96	110.20	31.66	CA	LEU	36
H	-0.120537	56.27	109.62	32.41	HA	LEU	36
C	-0.732006	55.25	109.29	30.65	CB	LEU	36
H	0.148084	55.94	108.71	30.22	HB1	LEU	36
H	0.163786	54.83	109.87	29.96	HB2	LEU	36
C	0.651211	54.15	108.36	31.19	CG	LEU	36
H	-0.130359	53.37	108.90	31.50	HG	LEU	36
C	-0.350999	53.69	107.43	30.08	CD1	LEU	36
H	0.055687	52.98	106.82	30.42	1HD1	LEU	36
H	0.043944	53.33	107.97	29.32	2HD1	LEU	36
H	0.089778	54.47	106.88	29.76	3HD1	LEU	36
C	-0.435593	54.69	107.56	32.37	CD2	LEU	36
H	0.071655	53.97	106.96	32.72	1HD2	LEU	36
H	0.110236	55.47	107.01	32.08	2HD2	LEU	36
H	0.128425	54.98	108.19	33.10	3HD2	LEU	36
C	-0.108137	57.08	110.97	30.97	C	LEU	36
O	-0.191049	57.04	111.23	29.77	O	LEU	36
N	-0.685797	61.59	101.39	30.19	N	GLY	42
H	0.384680	62.42	101.58	29.66	H	GLY	42
C	0.550812	60.38	100.96	29.49	CA	GLY	42
H	-0.070294	59.94	100.27	30.06	HA1	GLY	42
H	-0.082378	60.68	100.55	28.63	HA2	GLY	42
C	0.414238	59.39	102.06	29.19	C	GLY	42
O	-0.565094	58.29	101.80	28.69	O	GLY	42
N	-0.390408	59.76	103.29	29.51	N	ASH	43
H	0.279969	60.66	103.45	29.92	H	ASH	43
C	0.087041	58.88	104.42	29.27	CA	ASH	43
H	0.125088	57.99	104.14	29.63	HA	ASH	43
C	-0.256542	59.41	105.65	30.00	CB	ASH	43
H	0.125069	60.28	105.92	29.59	HB1	ASH	43
H	0.092421	59.55	105.41	30.96	HB2	ASH	43

C	0.742512	58.45	106.83	29.94	CG	ASH	43
O	-0.627996	57.70	106.96	28.95	OD1	ASH	43
O	-0.541534	58.47	107.65	30.88	OD2	ASH	43
H	0.445196	57.79	108.37	30.71	HD2	ASH	43
C	0.496339	58.78	104.70	27.76	C	ASH	43
O	-0.539978	59.66	105.33	27.18	O	ASH	43
N	-0.414760	57.71	104.22	27.13	N	TYR	44
H	0.331071	57.06	103.66	27.64	H	TYR	44
C	0.358056	57.48	104.47	25.71	CA	TYR	44
H	-0.003868	58.35	104.81	25.35	HA	TYR	44
C	-0.047047	57.08	103.20	24.96	CB	TYR	44
H	-0.218233	56.63	103.47	24.11	HB1	TYR	44
H	0.104521	56.43	102.70	25.53	HB2	TYR	44
C	0.006439	58.21	102.26	24.61	CG	TYR	44
C	-0.159088	58.87	101.52	25.60	CD1	TYR	44
H	0.159742	58.62	101.66	26.56	HD1	TYR	44
C	-0.219686	59.87	100.60	25.27	CE1	TYR	44
H	0.171788	60.33	100.08	25.99	HE1	TYR	44
C	0.409278	60.22	100.42	23.94	CZ	TYR	44
O	-0.584063	61.19	99.50	23.60	OH	TYR	44
H	0.461583	61.31	99.50	22.60	HH	TYR	44
C	-0.397282	59.58	101.15	22.94	CE2	TYR	44
H	0.181666	59.83	101.02	21.98	HE2	TYR	44
C	-0.092126	58.58	102.06	23.28	CD2	TYR	44
H	0.049084	58.12	102.58	22.56	HD2	TYR	44
C	0.443055	56.35	105.50	25.59	C	TYR	44
O	-0.716858	55.75	105.66	24.51	O	TYR	44
N	-0.221434	56.04	106.18	26.70	N	GLY	45
H	0.340528	56.55	105.98	27.54	H	GLY	45
C	-0.167548	55.00	107.19	26.71	CA	GLY	45
H	0.111183	55.18	107.81	25.95	HA1	GLY	45
H	0.114154	55.09	107.68	27.57	HA2	GLY	45
C	0.469137	53.57	106.67	26.59	C	GLY	45
O	-0.576500	52.68	107.38	26.12	O	GLY	45
N	-0.587851	53.35	105.43	27.03	N	TRP	46
H	0.372042	54.10	104.91	27.43	H	TRP	46
C	0.462125	52.02	104.84	26.94	CA	TRP	46
H	0.004823	51.54	105.51	26.37	HA	TRP	46
C	-0.154064	52.13	103.44	26.30	CB	TRP	46
H	0.074012	52.66	102.85	26.90	HB1	TRP	46
H	0.100327	52.59	103.53	25.41	HB2	TRP	46
C	-0.051716	50.80	102.77	26.06	CG	TRP	46
C	-0.208480	49.60	103.39	25.81	CD1	TRP	46
H	0.126477	49.46	104.37	25.79	HD1	TRP	46
N	-0.386028	48.62	102.44	25.61	NE1	TRP	46
H	0.348269	47.66	102.64	25.41	HE1	TRP	46

C	0.211548	49.17	101.19	25.72	CE2	TRP	46
C	-0.281086	48.57	99.93	25.59	CZ2	TRP	46
H	0.160338	47.60	99.84	25.39	HZ2	TRP	46
C	-0.075186	49.37	98.83	25.75	CH2	TRP	46
H	0.152842	48.97	97.91	25.67	HH2	TRP	46
C	-0.207429	50.75	98.95	26.04	CZ3	TRP	46
H	0.174752	51.31	98.13	26.15	HZ3	TRP	46
C	-0.175920	51.35	100.22	26.17	CE3	TRP	46
H	0.152541	52.32	100.30	26.38	HE3	TRP	46
C	-0.003633	50.55	101.36	26.01	CD2	TRP	46
C	0.451456	51.23	104.74	28.25	C	TRP	46
O	-0.460579	51.58	103.96	29.13	O	TRP	46
N	-0.573686	50.19	105.56	28.37	N	ASH	47
H	0.361610	50.02	106.23	27.64	H	ASH	47
C	0.124733	49.28	105.53	29.52	CA	ASH	47
H	-0.038361	49.17	104.56	29.72	HA	ASH	47
C	0.080987	49.85	106.21	30.77	CB	ASH	47
H	0.048739	49.87	107.20	30.61	HB1	ASH	47
H	0.088026	50.79	105.89	30.91	HB2	ASH	47
C	0.591108	49.02	105.91	32.03	CG	ASH	47
O	-0.540611	49.21	106.58	33.07	OD1	ASH	47
O	-0.606906	48.17	104.99	31.97	OD2	ASH	47
H	0.425302	47.71	104.91	32.85	HD2	ASH	47
C	0.415964	47.97	106.21	29.13	C	ASH	47
O	-0.496617	47.48	107.11	29.82	O	ASH	47
N	-0.370225	47.42	105.76	28.00	N	THR	48
H	0.258060	47.89	105.02	27.51	H	THR	48
C	-0.347274	46.18	106.27	27.46	CA	THR	48
H	0.215680	46.42	107.21	27.21	HA	THR	48
C	0.474464	45.75	105.44	26.25	CB	THR	48
H	0.000316	44.77	105.55	26.08	HB	THR	48
C	-0.452496	46.54	105.82	25.01	CG2	THR	48
H	0.115009	46.24	105.26	24.23	1HG2	THR	48
H	0.107561	46.39	106.79	24.80	2HG2	THR	48
H	0.151031	47.52	105.67	25.17	3HG2	THR	48
O	-0.635615	45.96	104.05	26.56	OG1	THR	48
H	0.387172	45.68	103.50	25.77	HG1	THR	48
C	0.459992	45.03	106.31	28.46	C	THR	48
O	-0.454540	44.14	107.14	28.35	O	THR	48
N	-0.491637	45.05	105.40	29.44	N	ALA	49
H	0.223412	45.80	104.73	29.47	H	ALA	49
C	0.365456	44.00	105.34	30.46	CA	ALA	49
H	0.044209	43.19	105.72	30.02	HA	ALA	49
C	-0.418744	43.76	103.89	30.86	CB	ALA	49
H	0.147902	43.04	103.86	31.56	HB1	ALA	49
H	0.094709	43.47	103.37	30.06	HB2	ALA	49

H	0.044512	44.60	103.51	31.23	HB3	ALA	49
C	0.355926	44.35	106.17	31.69	C	ALA	49
O	-0.474854	43.59	106.22	32.66	O	ALA	49
N	-0.330045	45.52	106.82	31.66	N	GLY	50
H	0.328785	46.11	106.74	30.86	H	GLY	50
C	-0.320820	45.94	107.66	32.77	CA	GLY	50
H	0.212238	45.33	108.45	32.79	HA1	GLY	50
H	0.135568	46.87	107.95	32.57	HA2	GLY	50
C	0.511383	45.91	106.98	34.13	C	GLY	50
O	-0.525502	45.55	107.60	35.13	O	GLY	50
N	-0.443291	46.32	105.72	34.19	N	LEU	51
H	0.178660	46.63	105.27	33.35	H	LEU	51
C	0.004014	46.32	104.98	35.44	CA	LEU	51
H	0.100135	45.51	105.32	35.92	HA	LEU	51
C	-0.040339	46.25	103.48	35.16	CB	LEU	51
H	0.019921	46.26	103.01	36.04	HB1	LEU	51
H	0.013188	47.06	103.23	34.64	HB2	LEU	51
C	0.454431	45.02	103.01	34.39	CG	LEU	51
H	-0.052873	44.97	103.48	33.51	HG	LEU	51
C	-0.562331	45.13	101.51	34.16	CD1	LEU	51
H	0.115595	44.33	101.19	33.65	1HD1	LEU	51
H	0.052453	45.95	101.31	33.64	2HD1	LEU	51
H	0.179178	45.17	101.04	35.04	3HD1	LEU	51
C	-0.460171	43.75	103.36	35.15	CD2	LEU	51
H	0.112815	42.95	103.04	34.63	1HD2	LEU	51
H	0.084234	43.76	102.91	36.05	2HD2	LEU	51
H	0.187527	43.69	104.35	35.28	3HD2	LEU	51
C	0.496492	47.54	105.27	36.32	C	LEU	51
O	-0.522474	47.57	104.88	37.48	O	LEU	51
N	-0.368128	48.54	105.96	35.76	N	SER	52
H	0.238688	48.46	106.25	34.81	H	SER	52
C	0.161946	49.74	106.29	36.53	CA	SER	52
H	0.049529	49.55	105.93	37.44	HA	SER	52
C	0.178167	50.97	105.63	35.91	CB	SER	52
H	-0.035700	51.81	106.00	36.30	HB1	SER	52
H	0.047866	50.98	105.76	34.92	HB2	SER	52
O	-0.612279	50.97	104.23	36.14	OG	SER	52
H	0.380281	51.79	103.82	35.73	HG	SER	52
C	0.422403	49.97	107.80	36.64	C	SER	52
O	-0.509731	51.10	108.25	36.88	O	SER	52
N	-0.583210	48.90	108.58	36.47	N	ALA	53
H	0.390152	48.02	108.15	36.28	H	ALA	53
C	0.397486	48.98	110.03	36.54	CA	ALA	53
H	0.090262	49.61	110.32	35.82	HA	ALA	53
C	-0.571759	47.60	110.64	36.31	CB	ALA	53
H	0.191667	47.66	111.63	36.37	HB1	ALA	53

H	0.145810	47.27	110.37	35.41	HB2	ALA	53
H	0.190960	46.97	110.30	37.01	HB3	ALA	53
C	0.036540	49.52	110.47	37.89	C	ALA	53
O	-0.232965	50.28	111.42	37.97	O	ALA	53
N	-0.666234	50.96	106.30	42.78	N	THR	57
H	0.354114	50.51	107.17	42.63	H	THR	57
C	0.320278	50.42	105.09	42.18	CA	THR	57
H	0.053339	50.36	104.42	42.93	HA	THR	57
C	0.460004	49.02	105.34	41.60	CB	THR	57
H	-0.072941	49.05	106.07	40.91	HB	THR	57
C	-0.535629	48.44	104.07	41.01	CG2	THR	57
H	0.165360	47.53	104.26	40.63	1HG2	THR	57
H	0.089642	49.04	103.74	40.27	2HG2	THR	57
H	0.128647	48.37	103.37	41.72	3HG2	THR	57
O	-0.600499	48.15	105.79	42.65	OG1	THR	57
H	0.370616	47.24	105.96	42.27	HG1	THR	57
C	0.399584	51.34	104.60	41.07	C	THR	57
O	-0.426743	51.51	103.40	40.87	O	THR	57
N	-0.473412	51.95	105.55	40.36	N	PHE	58
H	0.335655	51.76	106.51	40.58	H	PHE	58
C	0.102483	52.88	105.26	39.28	CA	PHE	58
H	0.168376	52.37	104.75	38.59	HA	PHE	58
C	-0.670214	53.41	106.57	38.70	CB	PHE	58
H	0.212441	53.90	107.07	39.42	HB1	PHE	58
H	0.316687	52.64	107.12	38.38	HB2	PHE	58
C	0.272170	54.36	106.40	37.55	CG	PHE	58
C	-0.188697	54.24	105.31	36.68	CD1	PHE	58
H	0.132500	53.54	104.62	36.85	HD1	PHE	58
C	-0.186871	55.10	105.18	35.58	CE1	PHE	58
H	0.142124	55.00	104.40	34.97	HE1	PHE	58
C	-0.107154	56.08	106.15	35.34	CZ	PHE	58
H	0.133738	56.69	106.06	34.56	HZ	PHE	58
C	-0.162385	56.20	107.23	36.21	CE2	PHE	58
H	0.171982	56.90	107.92	36.04	HE2	PHE	58
C	-0.201653	55.35	107.35	37.30	CD2	PHE	58
H	0.158726	55.44	108.13	37.92	HD2	PHE	58
C	0.165210	54.04	104.40	39.80	C	PHE	58
O	-0.330966	54.50	103.47	39.11	O	PHE	58
N	-0.726467	52.70	100.88	40.35	N	ASN	61
H	0.433493	52.45	101.85	40.43	H	ASN	61
C	0.525295	52.52	100.19	39.08	CA	ASN	61
H	-0.035027	51.99	99.38	39.32	HA	ASN	61
C	-0.250651	51.73	101.06	38.09	CB	ASN	61
H	-0.012067	51.85	100.69	37.17	HB1	ASN	61
H	0.060807	52.09	102.00	38.13	HB2	ASN	61
C	0.766985	50.23	101.10	38.40	CG	ASN	61

O	-0.564557	49.65	100.10	38.79	OD1	ASN	61
N	-0.946526	49.61	102.26	38.22	ND2	ASN	61
H	0.419213	50.12	103.05	37.88	1HD2	ASN	61
H	0.438361	48.63	102.34	38.40	2HD2	ASN	61
C	0.464188	53.86	99.75	38.48	C	ASN	61
O	-0.592698	53.92	98.72	37.80	O	ASN	61
N	-0.480860	54.92	100.52	38.71	N	ARG	62
H	0.346190	54.83	101.36	39.25	H	ARG	62
C	-0.039786	56.23	100.14	38.19	CA	ARG	62
H	0.124378	56.09	99.98	37.21	HA	ARG	62
C	-0.000873	57.28	101.25	38.38	CB	ARG	62
H	-0.020218	58.19	100.85	38.26	HB1	ARG	62
H	0.079713	57.19	101.60	39.32	HB2	ARG	62
C	0.025511	57.14	102.44	37.42	CG	ARG	62
H	0.044310	56.42	103.05	37.77	HG1	ARG	62
H	-0.004530	56.88	102.09	36.52	HG2	ARG	62
C	-0.098230	58.43	103.24	37.28	CD	ARG	62
H	0.034456	58.28	104.00	36.65	HD1	ARG	62
H	0.089335	59.15	102.65	36.92	HD2	ARG	62
N	-0.476780	58.91	103.80	38.54	NE	ARG	62
H	0.235135	59.75	103.42	38.93	HE	ARG	62
C	0.498778	58.31	104.78	39.21	CZ	ARG	62
N	-0.761989	57.20	105.34	38.75	NH1	ARG	62
H	0.350236	56.80	105.02	37.89	1HH1	ARG	62
H	0.277432	56.75	106.07	39.27	2HH1	ARG	62
N	-0.904043	58.82	105.21	40.36	NH2	ARG	62
H	0.348267	59.66	104.80	40.72	1HH2	ARG	62
H	0.371006	58.37	105.95	40.86	2HH2	ARG	62
C	0.525177	56.70	98.88	38.90	C	ARG	62
O	-0.593269	57.33	98.01	38.29	O	ARG	62
N	-0.495501	56.39	98.77	40.19	N	GLU	63
H	0.344067	55.87	99.50	40.63	H	GLU	63
C	0.078933	56.80	97.61	40.96	CA	GLU	63
H	0.048765	57.77	97.46	40.75	HA	GLU	63
C	0.049234	56.64	97.89	42.46	CB	GLU	63
H	-0.019984	57.07	97.15	42.97	HB1	GLU	63
H	0.041029	55.66	97.92	42.68	HB2	GLU	63
C	-0.023362	57.27	99.21	42.90	CG	GLU	63
H	0.001515	56.69	99.96	42.57	HG1	GLU	63
H	0.014908	58.17	99.28	42.48	HG2	GLU	63
C	0.620281	57.42	99.35	44.42	CD	GLU	63
O	-0.311130	56.48	98.98	45.16	OE1	GLU	63
O	-0.341125	58.47	99.86	44.87	OE2	GLU	63
C	0.547381	56.00	96.39	40.55	C	GLU	63
O	-0.628636	56.54	95.30	40.40	O	GLU	63
N	-0.486414	54.70	96.58	40.36	N	LEU	64

H	0.298765	54.31	97.48	40.51	H	LEU	64
C	0.128648	53.82	95.49	39.93	CA	LEU	64
H	0.047183	53.89	94.80	40.65	HA	LEU	64
C	-0.246297	52.38	96.00	39.80	CB	LEU	64
H	0.048007	51.90	95.36	39.20	HB1	LEU	64
H	0.064829	52.43	96.89	39.35	HB2	LEU	64
C	0.530219	51.52	96.18	41.04	CG	LEU	64
H	-0.088358	52.05	96.61	41.77	HG	LEU	64
C	-0.426890	50.32	97.09	40.73	CD1	LEU	64
H	0.107473	49.76	97.21	41.55	1HD1	LEU	64
H	0.104000	50.65	97.99	40.42	2HD1	LEU	64
H	0.065707	49.77	96.68	40.00	3HD1	LEU	64
C	-0.434718	51.05	94.82	41.54	CD2	LEU	64
H	0.092917	50.48	94.94	42.35	1HD2	LEU	64
H	0.073323	50.51	94.38	40.82	2HD2	LEU	64
H	0.132605	51.84	94.26	41.76	3HD2	LEU	64
C	0.516717	54.27	94.92	38.59	C	LEU	64
O	-0.280026	54.28	93.70	38.37	O	LEU	64
N	-0.492368	54.66	95.82	37.68	N	GLU	65
H	0.363268	54.65	96.79	37.93	H	GLU	65
C	0.167231	55.10	95.44	36.35	CA	GLU	65
H	0.045209	54.37	94.84	36.02	HA	GLU	65
C	0.054576	55.26	96.68	35.46	CB	GLU	65
H	0.046517	56.10	97.14	35.71	HB1	GLU	65
H	0.043029	54.48	97.29	35.63	HB2	GLU	65
C	-0.232687	55.31	96.37	33.98	CG	GLU	65
H	0.087816	54.44	95.97	33.70	HG1	GLU	65
H	0.055374	56.05	95.72	33.81	HG2	GLU	65
C	0.763021	55.55	97.61	33.13	CD	GLU	65
O	-0.774258	55.15	97.61	31.94	OE1	GLU	65
O	-0.530012	56.14	98.59	33.65	OE2	GLU	65
C	0.568177	56.41	94.64	36.34	C	GLU	65
O	-0.602493	56.48	93.59	35.71	O	GLU	65
N	-0.475380	57.42	95.13	37.04	N	VAL	66
H	0.351734	57.30	95.99	37.54	H	VAL	66
C	-0.129286	58.71	94.44	37.09	CA	VAL	66
H	0.064094	58.94	94.32	36.12	HA	VAL	66
C	0.442404	59.77	95.31	37.83	CB	VAL	66
H	0.018127	59.42	95.60	38.72	HB	VAL	66
C	-0.526400	61.05	94.50	38.06	CG1	VAL	66
H	0.124885	61.72	95.08	38.54	1HG1	VAL	66
H	0.096076	60.84	93.70	38.62	2HG1	VAL	66
H	0.093505	61.43	94.21	37.18	3HG1	VAL	66
C	-0.377888	60.08	96.55	37.01	CG2	VAL	66
H	0.073975	60.77	97.10	37.48	1HG2	VAL	66
H	0.075093	60.44	96.28	36.11	2HG2	VAL	66

H	0.106981	59.25	97.09	36.89	3HG2	VAL	66
C	0.498093	58.59	93.08	37.76	C	VAL	66
O	-0.675734	59.20	92.10	37.31	O	VAL	66
N	-0.408937	57.80	93.00	38.82	N	ILE	67
H	0.347740	57.32	93.82	39.15	H	ILE	67
C	0.079969	57.61	91.74	39.52	CA	ILE	67
H	0.010531	58.53	91.40	39.73	HA	ILE	67
C	0.167568	56.82	91.93	40.84	CB	ILE	67
H	0.050747	55.97	92.42	40.65	HB	ILE	67
C	-0.383427	56.47	90.58	41.43	CG2	ILE	67
H	0.128479	55.96	90.71	42.29	1HG2	ILE	67
H	0.062995	55.91	90.06	40.79	2HG2	ILE	67
H	0.067060	57.31	90.07	41.62	3HG2	ILE	67
C	0.060982	57.66	92.74	41.83	CG1	ILE	67
H	0.027972	57.15	92.81	42.69	1HG1	ILE	67
H	-0.005538	57.80	93.66	41.45	2HG1	ILE	67
C	-0.250888	59.05	92.14	42.15	CD	ILE	67
H	0.068368	59.52	92.73	42.80	HD1	ILE	67
H	0.072166	58.93	91.23	42.54	HD2	ILE	67
H	0.035760	59.58	92.08	41.30	HD3	ILE	67
C	0.555809	56.87	90.78	38.60	C	ILE	67
O	-0.678589	57.28	89.63	38.43	O	ILE	67
N	-0.388332	55.77	91.23	38.01	N	HIS	68
H	0.290685	55.44	92.16	38.20	H	HIS	68
C	0.136647	55.04	90.38	37.08	CA	HIS	68
H	-0.016960	54.68	89.61	37.61	HA	HIS	68
C	-0.417223	53.87	91.15	36.44	CB	HIS	68
H	0.120348	53.73	90.80	35.51	HB1	HIS	68
H	0.246021	54.10	92.12	36.40	HB2	HIS	68
C	0.322975	52.58	91.02	37.18	CG	HIS	68
N	-0.549022	52.38	91.54	38.45	ND1	HIS	68
C	0.199162	51.14	91.30	38.83	CE1	HIS	68
H	0.115173	50.74	91.57	39.71	HE1	HIS	68
N	-0.199645	50.52	90.64	37.87	NE2	HIS	68
H	0.472988	49.57	90.33	37.89	HE2	HIS	68
C	-0.255121	51.40	90.45	36.83	CD2	HIS	68
H	0.133249	51.20	89.98	35.97	HD2	HIS	68
C	0.513760	56.02	89.95	35.99	C	HIS	68
O	-0.709522	55.99	88.80	35.52	O	HIS	68
N	-0.340469	56.91	90.86	35.60	N	CYS	69
H	0.328302	56.88	91.76	36.03	H	CYS	69
C	0.105211	57.91	90.60	34.57	CA	CYS	69
H	0.083918	57.36	90.44	33.75	HA	CYS	69
C	-0.061611	58.86	91.80	34.41	CB	CYS	69
H	0.069222	59.75	91.39	34.21	HB1	CYS	69
H	0.204358	58.89	92.21	35.32	HB2	CYS	69

S	-0.600381	58.37	93.00	33.16	SG	CYS	69
H	0.338675	59.04	93.74	33.13	HG	CYS	69
C	0.548843	58.77	89.39	34.86	C	CYS	69
O	-0.672294	58.88	88.48	34.04	O	CYS	69
N	-0.556835	59.38	89.39	36.03	N	ARG	70
H	0.409508	59.23	90.16	36.66	H	ARG	70
C	0.417407	60.25	88.30	36.44	CA	ARG	70
H	-0.076087	60.91	88.20	35.69	HA	ARG	70
C	-0.343475	60.95	88.70	37.74	CB	ARG	70
H	0.031952	61.47	87.92	38.08	HB1	ARG	70
H	0.091806	60.26	88.97	38.41	HB2	ARG	70
C	0.310934	61.90	89.87	37.52	CG	ARG	70
H	-0.099877	61.46	90.52	36.89	HG1	ARG	70
H	-0.031105	62.74	89.53	37.10	HG2	ARG	70
C	0.189405	62.26	90.60	38.79	CD	ARG	70
H	-0.009325	62.65	89.96	39.45	HD1	ARG	70
H	0.005133	61.44	91.02	39.19	HD2	ARG	70
N	-0.767444	63.23	91.65	38.52	NE	ARG	70
H	0.366204	63.60	91.71	37.59	HE	ARG	70
C	0.798955	63.67	92.52	39.42	CZ	ARG	70
N	-1.108164	63.22	92.48	40.66	NH1	ARG	70
H	0.435219	62.55	91.79	40.93	1HH1	ARG	70
H	0.406085	63.56	93.14	41.34	2HH1	ARG	70
N	-1.204966	64.58	93.42	39.07	NH2	ARG	70
H	0.461332	64.93	93.45	38.13	1HH2	ARG	70
H	0.431513	64.92	94.08	39.74	2HH2	ARG	70
C	0.528287	59.52	86.97	36.57	C	ARG	70
O	-0.653142	60.06	85.93	36.21	O	ARG	70
N	-0.484701	58.30	87.01	37.09	N	TRP	71
H	0.373260	57.92	87.88	37.39	H	TRP	71
C	0.331561	57.52	85.79	37.24	CA	TRP	71
H	-0.033078	58.11	85.15	37.73	HA	TRP	71
C	-0.209185	56.25	86.07	38.03	CB	TRP	71
H	0.048919	55.54	85.42	37.76	HB1	TRP	71
H	0.147374	55.93	87.00	37.83	HB2	TRP	71
C	-0.140710	56.42	85.97	39.51	CG	TRP	71
C	-0.209558	56.33	86.98	40.43	CD1	TRP	71
H	0.227636	56.16	87.94	40.20	HD1	TRP	71
N	-0.322691	56.49	86.48	41.70	NE1	TRP	71
H	0.336885	56.46	87.02	42.54	HE1	TRP	71
C	0.116927	56.70	85.13	41.63	CE2	TRP	71
C	-0.264939	56.92	84.20	42.65	CZ2	TRP	71
H	0.137622	56.94	84.48	43.61	HZ2	TRP	71
C	-0.135272	57.10	82.89	42.28	CH2	TRP	71
H	0.115575	57.25	82.20	42.98	HH2	TRP	71
C	-0.228062	57.07	82.50	40.93	CZ3	TRP	71

H	0.152618	57.21	81.54	40.70	HZ3	TRP	71
C	-0.142894	56.86	83.43	39.92	CE3	TRP	71
H	0.095433	56.84	83.14	38.96	HE3	TRP	71
C	0.163789	56.67	84.77	40.27	CD2	TRP	71
C	0.542586	57.14	85.25	35.86	C	TRP	71
O	-0.671783	57.14	84.04	35.65	O	TRP	71
N	-0.507196	56.84	86.16	34.94	N	ALA	72
H	0.392064	56.89	87.13	35.17	H	ALA	72
C	0.348578	56.44	85.78	33.59	CA	ALA	72
H	-0.030592	55.76	85.06	33.71	HA	ALA	72
C	-0.315229	55.83	86.98	32.87	CB	ALA	72
H	0.040540	55.56	86.71	31.95	HB1	ALA	72
H	0.075136	55.03	87.29	33.38	HB2	ALA	72
H	0.156763	56.51	87.71	32.82	HB3	ALA	72
C	0.544718	57.60	85.21	32.77	C	ALA	72
O	-0.651381	57.39	84.41	31.86	O	ALA	72
N	-0.522509	58.82	85.63	33.10	N	MET	73
H	0.405130	58.93	86.29	33.84	H	MET	73
C	0.068365	59.98	85.12	32.39	CA	MET	73
H	0.035513	59.73	85.10	31.42	HA	MET	73
C	0.177329	61.18	86.05	32.57	CB	MET	73
H	-0.041717	62.01	85.57	32.27	HB1	MET	73
H	0.017589	61.26	86.29	33.53	HB2	MET	73
C	-0.000283	61.04	87.33	31.75	CG	MET	73
H	0.096639	60.26	87.80	32.16	HG1	MET	73
H	0.035972	60.79	87.01	30.83	HG2	MET	73
S	-0.371203	62.50	88.37	31.72	SD	MET	73
C	-0.262066	62.25	89.41	33.23	CE	MET	73
H	0.181615	63.01	90.04	33.32	HE1	MET	73
H	0.134654	61.39	89.92	33.14	HE2	MET	73
H	0.123528	62.20	88.82	34.03	HE3	MET	73
C	0.534644	60.30	83.72	32.88	C	MET	73
O	-0.620713	60.63	82.85	32.08	O	MET	73
N	-0.475565	60.19	83.51	34.19	N	LEU	74
H	0.344890	59.94	84.26	34.80	H	LEU	74
C	0.111657	60.45	82.19	34.75	CA	LEU	74
H	0.044652	61.36	81.91	34.45	HA	LEU	74
C	-0.229909	60.42	82.22	36.28	CB	LEU	74
H	0.020862	60.39	81.28	36.60	HB1	LEU	74
H	0.095499	59.58	82.69	36.55	HB2	LEU	74
C	0.524329	61.58	82.91	37.02	CG	LEU	74
H	-0.046271	61.64	83.87	36.73	HG	LEU	74
C	-0.375564	61.33	82.86	38.51	CD1	LEU	74
H	0.073893	62.08	83.31	38.99	1HD1	LEU	74
H	0.059041	60.47	83.33	38.73	2HD1	LEU	74
H	0.072868	61.27	81.91	38.81	3HD1	LEU	74

C	-0.593206	62.90	82.24	36.70	CD2	LEU	74
H	0.138750	63.64	82.70	37.19	1HD2	LEU	74
H	0.115025	62.86	81.28	36.98	2HD2	LEU	74
H	0.164516	63.07	82.29	35.71	3HD2	LEU	74
C	0.488181	59.35	81.25	34.23	C	LEU	74
O	-0.613803	59.62	80.12	33.82	O	LEU	74
N	-0.353602	58.11	81.76	34.23	N	GLY	75
H	0.335831	57.97	82.69	34.55	H	GLY	75
C	-0.000691	56.97	80.98	33.77	CA	GLY	75
H	0.017482	56.15	81.51	33.99	HA1	GLY	75
H	0.033678	56.97	80.13	34.30	HA2	GLY	75
C	0.458793	56.96	80.65	32.29	C	GLY	75
O	-0.623841	56.47	79.59	31.89	O	GLY	75
N	-0.417525	57.48	81.55	31.46	N	ALA	76
H	0.352094	57.85	82.40	31.83	H	ALA	76
C	0.222411	57.50	81.31	30.03	CA	ALA	76
H	0.027387	56.57	81.07	29.75	HA	ALA	76
C	-0.249956	57.94	82.57	29.29	CB	ALA	76
H	-0.017494	57.96	82.39	28.30	HB1	ALA	76
H	0.103047	57.30	83.32	29.48	HB2	ALA	76
H	0.123464	58.86	82.84	29.59	HB3	ALA	76
C	0.540739	58.47	80.17	29.76	C	ALA	76
O	-0.645718	58.13	79.19	29.09	O	ALA	76
N	-0.507703	59.69	80.31	30.27	N	LEU	77
H	0.350555	59.91	81.13	30.80	H	LEU	77
C	0.199855	60.71	79.30	30.09	CA	LEU	77
H	-0.001386	60.82	79.19	29.10	HA	LEU	77
C	-0.210921	62.03	79.77	30.71	CB	LEU	77
H	0.117054	61.84	79.99	31.67	HB1	LEU	77
H	0.096605	62.31	80.59	30.22	HB2	LEU	77
C	0.288017	63.21	78.79	30.69	CG	LEU	77
H	-0.063043	62.97	77.96	31.19	HG	LEU	77
C	-0.249848	63.52	78.38	29.25	CD1	LEU	77
H	0.046990	64.28	77.74	29.24	1HD1	LEU	77
H	0.014403	62.71	77.94	28.84	2HD1	LEU	77
H	0.055606	63.75	79.19	28.71	3HD1	LEU	77
C	-0.344437	64.43	79.43	31.36	CD2	LEU	77
H	0.046793	65.19	78.79	31.34	1HD2	LEU	77
H	0.133239	64.67	80.27	30.86	2HD2	LEU	77
H	0.103504	64.20	79.66	32.30	3HD2	LEU	77
C	0.492331	60.26	77.97	30.71	C	LEU	77
O	-0.626976	60.43	76.90	30.13	O	LEU	77
N	-0.318085	59.65	78.06	31.89	N	GLY	78
H	0.333609	59.52	78.96	32.32	H	GLY	78
C	-0.103873	59.18	76.87	32.57	CA	GLY	78
H	0.084340	58.87	77.16	33.48	HA1	GLY	78

H	0.078746	59.97	76.26	32.67	HA2	GLY	78
C	0.472647	58.06	76.12	31.89	C	GLY	78
O	-0.582098	57.98	74.89	31.98	O	GLY	78
N	-0.448968	57.17	76.83	31.20	N	CYS	79
H	0.364800	57.27	77.83	31.16	H	CYS	79
C	0.142377	56.05	76.19	30.52	CA	CYS	79
H	0.070313	55.71	75.52	31.19	HA	CYS	79
C	-0.094705	54.97	77.22	30.16	CB	CYS	79
H	0.075496	54.41	76.75	29.48	HB1	CYS	79
H	0.152741	55.48	77.96	29.71	HB2	CYS	79
S	-0.617130	54.00	77.82	31.55	SG	CYS	79
H	0.398653	53.33	78.48	31.22	HG	CYS	79
C	0.489749	56.50	75.47	29.26	C	CYS	79
O	-0.587799	55.95	74.43	28.89	O	CYS	79
N	-0.413748	57.51	76.02	28.61	N	VAL	80
H	0.345863	57.93	76.85	28.97	H	VAL	80
C	0.032897	58.02	75.47	27.37	CA	VAL	80
H	0.037943	57.20	75.02	27.01	HA	VAL	80
C	0.259328	58.60	76.60	26.47	CB	VAL	80
H	0.033697	59.31	77.10	26.96	HB	VAL	80
C	-0.475372	59.22	76.02	25.22	CG1	VAL	80
H	0.127001	59.58	76.76	24.65	1HG1	VAL	80
H	0.099619	59.96	75.39	25.47	2HG1	VAL	80
H	0.097798	58.52	75.52	24.70	3HG1	VAL	80
C	-0.226494	57.51	77.57	26.09	CG2	VAL	80
H	0.041796	57.89	78.29	25.51	1HG2	VAL	80
H	0.056426	56.79	77.09	25.59	2HG2	VAL	80
H	0.030104	57.12	77.98	26.92	3HG2	VAL	80
C	0.499595	59.09	74.38	27.51	C	VAL	80
O	-0.631337	59.06	73.38	26.80	O	VAL	80
N	-0.534404	60.02	74.57	28.44	N	PHE	81
H	0.380106	59.96	75.37	29.04	H	PHE	81
C	0.246655	61.13	73.64	28.61	CA	PHE	81
H	0.004094	61.61	73.78	27.74	HA	PHE	81
C	-0.254491	61.98	74.02	29.83	CB	PHE	81
H	0.094983	61.54	73.68	30.66	HB1	PHE	81
H	0.151442	62.05	75.02	29.88	HB2	PHE	81
C	0.083175	63.38	73.47	29.78	CG	PHE	81
C	-0.183905	64.28	73.92	28.82	CD1	PHE	81
H	0.140372	64.01	74.67	28.21	HD1	PHE	81
C	-0.119626	65.54	73.35	28.70	CE1	PHE	81
H	0.124905	66.18	73.69	28.01	HE1	PHE	81
C	-0.130292	65.92	72.31	29.55	CZ	PHE	81
H	0.124657	66.83	71.90	29.47	HZ	PHE	81
C	-0.123195	65.03	71.86	30.52	CE2	PHE	81
H	0.122770	65.30	71.11	31.13	HE2	PHE	81

C	-0.171497	63.76	72.43	30.63	CD2	PHE	81
H	0.125116	63.13	72.10	31.32	HD2	PHE	81
C	0.408222	60.78	72.15	28.66	C	PHE	81
O	-0.570993	61.32	71.37	27.88	O	PHE	81
N	-0.157319	59.89	71.74	29.57	N	PRO	82
C	-0.136718	59.36	72.44	30.75	CD	PRO	82
H	0.139797	58.54	72.97	30.51	HD1	PRO	82
H	0.075243	60.05	73.06	31.13	HD2	PRO	82
C	0.136025	59.04	71.29	31.70	CG	PRO	82
H	-0.005276	58.34	71.54	32.37	HG1	PRO	82
H	-0.015007	59.86	70.97	32.17	HG2	PRO	82
C	-0.144377	58.53	70.26	30.77	CB	PRO	82
H	0.079756	57.60	70.48	30.46	HB1	PRO	82
H	0.021051	58.52	69.36	31.21	HB2	PRO	82
C	0.058994	59.54	70.32	29.63	CA	PRO	82
H	0.048361	60.35	69.76	29.78	HA	PRO	82
C	0.504215	58.96	69.79	28.30	C	PRO	82
O	-0.435674	59.36	68.73	27.82	O	PRO	82
N	-0.241673	58.03	70.54	27.72	N	GLU	83
H	0.271740	57.74	71.40	28.14	H	GLU	83
C	-0.124607	57.42	70.12	26.45	CA	GLU	83
H	0.048121	57.01	69.23	26.62	HA	GLU	83
C	0.206397	56.33	71.12	26.03	CB	GLU	83
H	0.060669	56.74	72.03	25.98	HB1	GLU	83
H	-0.024924	55.62	71.12	26.74	HB2	GLU	83
C	-0.299304	55.67	70.82	24.69	CG	GLU	83
H	0.085847	55.39	69.87	24.68	HG1	GLU	83
H	0.068298	56.34	70.98	23.96	HG2	GLU	83
C	0.712141	54.45	71.70	24.41	CD	GLU	83
O	-0.523653	54.43	72.87	24.84	OE1	GLU	83
O	-0.501908	53.51	71.21	23.74	OE2	GLU	83
C	0.517948	58.51	70.00	25.38	C	GLU	83
O	-0.569329	58.44	69.14	24.49	O	GLU	83
N	-0.663430	59.53	70.85	25.47	N	LEU	84
H	0.442615	59.55	71.52	26.21	H	LEU	84
C	0.641301	60.63	70.81	24.51	CA	LEU	84
H	-0.054395	60.21	70.86	23.61	HA	LEU	84
C	-0.989811	61.57	72.00	24.72	CB	LEU	84
H	0.283097	61.92	71.96	25.66	HB1	LEU	84
H	0.243049	61.04	72.84	24.60	HB2	LEU	84
C	0.659978	62.77	72.05	23.77	CG	LEU	84
H	-0.110676	63.33	71.23	23.88	HG	LEU	84
C	-0.304517	62.29	72.11	22.34	CD1	LEU	84
H	0.034193	63.08	72.14	21.72	1HD1	LEU	84
H	0.066494	61.75	71.29	22.14	2HD1	LEU	84
H	0.059186	61.73	72.92	22.20	3HD1	LEU	84

C	-0.291123	63.63	73.27	24.09	CD2	LEU	84
H	0.029899	64.41	73.30	23.47	1HD2	LEU	84
H	0.054982	63.08	74.10	23.98	2HD2	LEU	84
H	0.068910	63.96	73.20	25.03	3HD2	LEU	84
C	0.167684	61.41	69.51	24.67	C	LEU	84
O	-0.298797	61.66	68.80	23.69	O	LEU	84
N	-1.007450	59.53	66.55	23.43	N	ARG	87
H	0.427486	59.60	67.47	23.84	H	ARG	87
C	0.776721	59.55	66.41	21.98	CA	ARG	87
H	-0.033079	58.83	65.75	21.77	HA	ARG	87
C	-0.236001	59.26	67.75	21.31	CB	ARG	87
H	0.028741	59.53	67.70	20.35	HB1	ARG	87
H	0.111192	59.80	68.46	21.76	HB2	ARG	87
C	-0.381165	57.81	68.14	21.38	CG	ARG	87
H	0.152453	57.54	68.19	22.34	HG1	ARG	87
H	0.111060	57.27	67.43	20.92	HG2	ARG	87
C	0.422675	57.53	69.48	20.72	CD	ARG	87
H	-0.045963	58.15	69.62	19.95	HD1	ARG	87
H	0.003813	57.64	70.22	21.39	HD2	ARG	87
N	-0.868590	56.16	69.50	20.23	NE	ARG	87
H	0.405842	55.43	69.73	20.88	HE	ARG	87
C	0.920385	55.82	69.23	18.98	CZ	ARG	87
N	-1.031552	56.75	68.94	18.08	NH1	ARG	87
H	0.470270	57.72	68.93	18.36	1HH1	ARG	87
H	0.438369	56.50	68.74	17.14	2HH1	ARG	87
N	-1.057156	54.54	69.21	18.63	NH2	ARG	87
H	0.408583	53.83	69.39	19.31	1HH2	ARG	87
H	0.456473	54.28	69.00	17.69	2HH2	ARG	87
C	-0.127915	60.88	65.87	21.51	C	ARG	87
O	-0.345192	61.10	65.68	20.32	O	ARG	87
N	-0.766842	57.98	62.45	30.48	N	PHE	92
H	0.359565	57.61	62.74	29.60	H	PHE	92
C	0.487820	57.45	63.05	31.69	CA	PHE	92
H	0.016935	58.08	62.87	32.45	HA	PHE	92
C	-0.431544	57.26	64.56	31.50	CB	PHE	92
H	0.103817	56.83	64.93	32.32	HB1	PHE	92
H	0.175883	56.67	64.71	30.71	HB2	PHE	92
C	0.193229	58.54	65.30	31.27	CG	PHE	92
C	-0.143977	59.20	65.92	32.32	CD1	PHE	92
H	0.118389	58.82	65.87	33.25	HD1	PHE	92
C	-0.170069	60.38	66.62	32.11	CE1	PHE	92
H	0.140814	60.85	67.07	32.87	HE1	PHE	92
C	-0.178871	60.92	66.71	30.82	CZ	PHE	92
H	0.123657	61.76	67.21	30.66	HZ	PHE	92
C	-0.068332	60.27	66.09	29.76	CE2	PHE	92
H	0.137751	60.65	66.14	28.84	HE2	PHE	92

C	-0.165075	59.09	65.39	29.99	CD2	PHE	92
H	0.122186	58.62	64.94	29.22	HD2	PHE	92
C	0.103831	56.08	62.41	31.89	C	PHE	92
O	-0.159166	55.52	61.85	30.96	O	PHE	92
N	-0.552624	53.55	64.14	32.57	N	GLU	94
H	0.424558	54.26	64.46	33.19	H	GLU	94
C	0.431406	52.77	65.12	31.83	CA	GLU	94
H	0.031752	52.43	64.68	30.99	HA	GLU	94
C	-0.246481	51.60	65.58	32.68	CB	GLU	94
H	0.105573	51.85	66.44	33.14	HB1	GLU	94
H	0.155165	51.39	64.88	33.37	HB2	GLU	94
C	-0.212709	50.36	65.83	31.90	CG	GLU	94
H	0.050763	50.55	66.54	31.22	HG1	GLU	94
H	0.167706	49.64	66.15	32.52	HG2	GLU	94
C	0.598554	49.88	64.58	31.19	CD	GLU	94
O	-0.467097	49.42	63.65	31.88	OE1	GLU	94
O	-0.455200	49.98	64.54	29.94	OE2	GLU	94
C	0.497630	53.68	66.30	31.49	C	GLU	94
O	-0.515532	54.08	67.03	32.39	O	GLU	94
N	-0.584579	53.99	66.49	30.21	N	ALA	95
H	0.321444	53.61	65.87	29.52	H	ALA	95
C	0.288258	54.88	67.57	29.77	CA	ALA	95
H	0.046041	55.45	67.71	30.58	HA	ALA	95
C	-0.306010	55.67	67.12	28.55	CB	ALA	95
H	0.087264	56.28	67.86	28.26	HB1	ALA	95
H	0.117329	56.22	66.32	28.79	HB2	ALA	95
H	0.089286	55.04	66.89	27.81	HB3	ALA	95
C	0.492238	54.21	68.91	29.47	C	ALA	95
O	-0.526814	54.82	69.96	29.68	O	ALA	95
N	-0.432453	52.98	68.89	28.96	N	VAL	96
H	0.284886	52.54	68.01	28.79	H	VAL	96
C	-0.225313	52.26	70.12	28.65	CA	VAL	96
H	0.132178	52.83	70.63	28.00	HA	VAL	96
C	0.356028	50.91	69.79	27.99	CB	VAL	96
H	-0.011216	50.44	69.07	28.50	HB	VAL	96
C	-0.416348	50.01	71.02	28.01	CG1	VAL	96
H	0.145472	49.13	70.79	27.58	1HG1	VAL	96
H	0.072711	49.85	71.31	28.95	2HG1	VAL	96
H	0.088715	50.44	71.76	27.50	3HG1	VAL	96
C	-0.275320	51.15	69.33	26.57	CG2	VAL	96
H	0.071600	50.28	69.11	26.14	1HG2	VAL	96
H	0.064569	51.62	70.05	26.06	2HG2	VAL	96
H	0.057611	51.73	68.51	26.59	3HG2	VAL	96
C	0.643547	52.06	70.92	29.93	C	VAL	96
O	-0.666494	51.50	70.42	30.91	O	VAL	96
N	-0.559673	52.49	72.18	29.91	N	TRP	97

H	0.318312	52.88	72.54	29.06	H	TRP	97
C	0.089324	52.43	73.03	31.08	CA	TRP	97
H	0.197426	53.08	72.57	31.69	HA	TRP	97
C	-0.382544	52.85	74.47	30.74	CB	TRP	97
H	0.180861	53.67	74.43	30.16	HB1	TRP	97
H	0.169750	53.07	74.96	31.58	HB2	TRP	97
C	-0.036953	51.82	75.27	30.01	CG	TRP	97
C	-0.292732	51.67	75.39	28.66	CD1	TRP	97
H	0.192703	52.27	74.97	27.98	HD1	TRP	97
N	-0.318552	50.58	76.18	28.37	NE1	TRP	97
H	0.344426	50.26	76.41	27.45	HE1	TRP	97
C	0.065970	50.00	76.58	29.54	CE2	TRP	97
C	-0.264003	48.86	77.39	29.76	CZ2	TRP	97
H	0.183974	48.34	77.76	28.99	HZ2	TRP	97
C	-0.130110	48.50	77.63	31.06	CH2	TRP	97
H	0.110028	47.70	78.20	31.24	HH2	TRP	97
C	-0.185674	49.23	77.10	32.14	CZ3	TRP	97
H	0.141756	48.94	77.29	33.07	HZ3	TRP	97
C	-0.278881	50.36	76.30	31.92	CE3	TRP	97
H	0.257771	50.88	75.92	32.69	HE3	TRP	97
C	0.227555	50.75	76.03	30.60	CD2	TRP	97
C	0.509279	51.09	73.05	31.82	C	TRP	97
O	-0.501063	51.06	72.94	33.05	O	TRP	97
N	-0.534024	49.98	73.16	31.10	N	PHE	98
H	0.283407	50.04	73.21	30.10	H	PHE	98
C	0.355126	48.69	73.21	31.76	CA	PHE	98
H	-0.023446	48.90	73.71	32.60	HA	PHE	98
C	-0.257894	47.68	73.98	30.89	CB	PHE	98
H	0.105626	48.06	74.88	30.67	HB1	PHE	98
H	0.033118	46.83	74.11	31.41	HB2	PHE	98
C	0.141810	47.32	73.31	29.60	CG	PHE	98
C	-0.162095	46.38	72.28	29.57	CD1	PHE	98
H	0.098846	45.96	71.97	30.43	HD1	PHE	98
C	-0.154584	46.00	71.68	28.37	CE1	PHE	98
H	0.134736	45.33	70.94	28.36	HE1	PHE	98
C	-0.105944	46.58	72.10	27.17	CZ	PHE	98
H	0.148402	46.31	71.67	26.30	HZ	PHE	98
C	-0.167806	47.53	73.13	27.18	CE2	PHE	98
H	0.154545	47.94	73.44	26.32	HE2	PHE	98
C	-0.171240	47.89	73.73	28.40	CD2	PHE	98
H	0.097450	48.57	74.46	28.41	HD2	PHE	98
C	0.436976	48.14	71.85	32.19	C	PHE	98
O	-0.586017	46.97	71.73	32.58	O	PHE	98
N	-0.495895	49.00	70.83	32.13	N	LYS	99
H	0.399190	49.93	70.98	31.80	H	LYS	99
C	0.353625	48.59	69.48	32.54	CA	LYS	99

H	-0.016674	47.68	69.57	32.93	HA	LYS	99
C	-0.356140	48.56	68.54	31.34	CB	LYS	99
H	0.017997	48.27	67.63	31.64	HB1	LYS	99
H	0.112239	49.48	68.48	30.95	HB2	LYS	99
C	0.249844	47.61	68.99	30.25	CG	LYS	99
H	-0.083852	48.13	69.10	29.39	HG1	LYS	99
H	-0.004094	47.21	69.87	30.51	HG2	LYS	99
C	-0.034859	46.51	68.00	30.03	CD	LYS	99
H	-0.005459	45.78	68.44	29.49	HD1	LYS	99
H	0.015146	46.14	67.72	30.92	HD2	LYS	99
C	-0.100006	47.01	66.77	29.29	CE	LYS	99
H	0.039313	46.27	66.10	29.23	HE1	LYS	99
H	0.078222	47.78	66.38	29.79	HE2	LYS	99
N	0.258399	47.46	67.11	27.90	NZ	LYS	99
H	-0.170251	47.78	66.28	27.45	HZ1	LYS	99
H	-0.074095	46.69	67.50	27.39	HZ2	LYS	99
H	-0.044929	48.20	67.78	27.95	HZ3	LYS	99
C	0.434066	49.56	68.95	33.59	C	LYS	99
O	-0.598279	49.24	67.99	34.30	O	LYS	99
N	-0.426201	50.72	69.59	33.69	N	ALA	100
H	0.354199	50.89	70.37	33.08	H	ALA	100
C	0.231176	51.77	69.21	34.64	CA	ALA	100
H	-0.024545	52.07	68.32	34.30	HA	ALA	100
C	-0.267675	52.90	70.24	34.60	CB	ALA	100
H	0.004545	53.62	69.98	35.25	HB1	ALA	100
H	0.112372	53.29	70.29	33.68	HB2	ALA	100
H	0.152030	52.54	71.14	34.85	HB3	ALA	100
C	0.474290	51.29	69.03	36.07	C	ALA	100
O	-0.664313	51.62	68.05	36.72	O	ALA	100
N	-0.284638	50.50	69.97	36.57	N	GLY	101
H	0.304904	50.26	70.76	36.00	H	GLY	101
C	-0.048896	50.00	69.87	37.93	CA	GLY	101
H	0.097518	49.34	70.62	38.05	HA1	GLY	101
H	0.024240	50.78	70.01	38.54	HA2	GLY	101
C	0.527716	49.33	68.55	38.27	C	GLY	101
O	-0.636092	49.58	67.98	39.34	O	GLY	101
N	-0.437411	48.50	68.04	37.37	N	SER	102
H	0.342887	48.35	68.53	36.51	H	SER	102
C	0.149779	47.78	66.80	37.61	CA	SER	102
H	-0.006721	47.30	67.00	38.46	HA	SER	102
C	0.153812	46.83	66.51	36.45	CB	SER	102
H	0.010067	46.29	67.32	36.22	HB1	SER	102
H	-0.013165	46.22	65.75	36.66	HB2	SER	102
O	-0.544549	47.56	66.15	35.29	OG	SER	102
H	0.361183	46.92	65.97	34.54	HG	SER	102
C	0.461975	48.65	65.56	37.87	C	SER	102

O	-0.578925	48.15	64.54	38.35	O	SER	102
N	-0.463387	49.94	65.63	37.56	N	GLN	103
H	0.372630	50.32	66.47	37.17	H	GLN	103
C	0.162726	50.81	64.47	37.79	CA	GLN	103
H	0.030542	50.44	63.76	37.19	HA	GLN	103
C	0.108168	52.26	64.80	37.41	CB	GLN	103
H	-0.036346	52.82	63.98	37.57	HB1	GLN	103
H	-0.018021	52.58	65.54	38.00	HB2	GLN	103
C	-0.325591	52.46	65.21	35.98	CG	GLN	103
H	0.079142	51.87	66.00	35.80	HG1	GLN	103
H	0.099262	52.19	64.45	35.39	HG2	GLN	103
C	0.861419	53.89	65.59	35.70	CD	GLN	103
O	-0.654136	54.64	64.80	35.12	OE1	GLN	103
N	-1.061338	54.29	66.79	36.12	NE2	GLN	103
H	0.481149	53.65	67.39	36.59	1HE2	GLN	103
H	0.471521	55.23	67.09	35.95	2HE2	GLN	103
C	0.547544	50.77	64.02	39.25	C	GLN	103
O	-0.518002	50.91	62.82	39.54	O	GLN	103
N	-0.803642	50.59	64.97	40.17	N	ILE	104
H	0.434548	50.48	65.92	39.87	H	ILE	104
C	0.483301	50.54	64.64	41.58	CA	ILE	104
H	0.011523	51.43	64.22	41.75	HA	ILE	104
C	0.010510	50.36	65.92	42.45	CB	ILE	104
H	0.011348	50.93	66.66	42.09	HB	ILE	104
C	-0.251389	48.91	66.39	42.40	CG2	ILE	104
H	0.040446	48.81	67.21	42.96	1HG2	ILE	104
H	0.129942	48.66	66.60	41.46	2HG2	ILE	104
H	0.026400	48.32	65.67	42.76	3HG2	ILE	104
C	0.218126	50.76	65.63	43.90	CG1	ILE	104
H	-0.048770	50.20	64.87	44.23	1HG1	ILE	104
H	-0.056272	50.57	66.45	44.44	2HG1	ILE	104
C	-0.366964	52.25	65.25	44.08	CD	ILE	104
H	0.083753	52.43	65.08	45.05	HD1	ILE	104
H	0.092647	52.45	64.43	43.55	HD2	ILE	104
H	0.067247	52.82	66.01	43.76	HD3	ILE	104
C	0.150403	49.42	63.65	41.89	C	ILE	104
O	-0.328921	49.46	62.97	42.93	O	ILE	104
N	-0.734377	54.65	62.48	41.25	N	LEU	110
H	0.338443	54.68	62.65	42.23	H	LEU	110
C	0.623876	55.37	63.35	40.34	CA	LEU	110
H	-0.051488	55.05	63.09	39.43	HA	LEU	110
C	-0.485831	55.04	64.81	40.65	CB	LEU	110
H	0.089636	55.58	65.08	41.45	HB1	LEU	110
H	0.169389	54.07	64.86	40.88	HB2	LEU	110
C	0.410828	55.32	65.84	39.55	CG	LEU	110
H	-0.008664	54.98	65.50	38.67	HG	LEU	110

C	-0.398141	54.59	67.13	39.87	CD1	LEU	110
H	0.092594	54.76	67.80	39.16	1HD1	LEU	110
H	0.088669	53.61	66.95	39.93	2HD1	LEU	110
H	0.073212	54.92	67.48	40.75	3HD1	LEU	110
C	-0.293899	56.82	66.07	39.39	CD2	LEU	110
H	0.088478	56.98	66.74	38.66	1HD2	LEU	110
H	0.065865	57.20	66.41	40.25	2HD2	LEU	110
H	0.038629	57.27	65.21	39.15	3HD2	LEU	110
C	0.078592	56.88	63.14	40.38	C	LEU	110
O	-0.185812	57.54	63.48	41.36	O	LEU	110
N	-0.764821	60.51	64.04	38.86	N	TYR	112
H	0.338837	60.73	63.89	39.83	H	TYR	112
C	0.728258	61.24	65.04	38.11	CA	TYR	112
H	-0.058227	60.57	65.70	37.78	HA	TYR	112
C	-0.475615	62.26	65.73	39.01	CB	TYR	112
H	0.142375	63.07	65.14	39.10	HB1	TYR	112
H	0.169305	61.85	65.86	39.92	HB2	TYR	112
C	0.034902	62.73	67.07	38.51	CG	TYR	112
C	-0.150949	61.98	68.23	38.76	CD1	TYR	112
H	0.161246	61.13	68.17	39.27	HD1	TYR	112
C	-0.280465	62.41	69.48	38.30	CE1	TYR	112
H	0.152289	61.87	70.30	38.48	HE1	TYR	112
C	0.394022	63.60	69.57	37.58	CZ	TYR	112
O	-0.552558	64.05	70.78	37.13	OH	TYR	112
H	0.401706	64.92	70.66	36.64	HH	TYR	112
C	-0.364292	64.36	68.43	37.33	CE2	TYR	112
H	0.165144	65.21	68.50	36.81	HE2	TYR	112
C	-0.075757	63.92	67.19	37.79	CD2	TYR	112
H	0.133877	64.46	66.38	37.61	HD2	TYR	112
C	0.067087	61.95	64.39	36.91	C	TYR	112
O	-0.166363	62.69	63.42	37.06	O	TYR	112
N	-0.875080	50.01	66.43	47.53	N	ILE	124
H	0.412034	49.30	65.75	47.36	H	ILE	124
C	0.684220	49.79	67.81	47.09	CA	ILE	124
H	-0.002648	50.62	68.03	46.57	HA	ILE	124
C	-0.184501	48.53	67.98	46.20	CB	ILE	124
H	0.074851	48.62	67.40	45.39	HB	ILE	124
C	-0.096647	47.28	67.56	46.94	CG2	ILE	124
H	0.068111	46.49	67.67	46.34	1HG2	ILE	124
H	0.018144	47.36	66.60	47.21	2HG2	ILE	124
H	-0.014848	47.18	68.13	47.75	3HG2	ILE	124
C	0.168219	48.35	69.44	45.79	CG1	ILE	124
H	-0.020683	48.25	69.99	46.62	1HG1	ILE	124
H	0.001974	47.52	69.52	45.24	2HG1	ILE	124
C	-0.316889	49.51	70.03	44.98	CD	ILE	124
H	0.086638	49.31	70.98	44.76	HD1	ILE	124

H	0.050730	50.35	69.97	45.51	HD2	ILE	124
H	0.079583	49.62	69.50	44.13	HD3	ILE	124
C	0.118232	49.67	68.72	48.32	C	ILE	124
O	-0.251440	50.09	69.88	48.28	O	ILE	124
N	-0.883288	53.10	69.60	49.40	N	ILE	127
H	0.409004	52.52	68.86	49.07	H	ILE	127
C	0.696230	53.69	70.54	48.45	CA	ILE	127
H	0.013210	54.68	70.47	48.57	HA	ILE	127
C	-0.344748	53.31	70.19	47.00	CB	ILE	127
H	0.088982	52.31	70.13	46.91	HB	ILE	127
C	-0.181745	53.79	71.30	46.06	CG2	ILE	127
H	0.089749	53.54	71.07	45.12	1HG2	ILE	127
H	0.032506	53.36	72.16	46.32	2HG2	ILE	127
H	0.057376	54.79	71.38	46.13	3HG2	ILE	127
C	0.372070	53.89	68.83	46.62	CG1	ILE	127
H	-0.112528	53.50	68.14	47.23	1HG1	ILE	127
H	-0.060808	54.88	68.87	46.75	2HG1	ILE	127
C	-0.149758	53.61	68.41	45.18	CD	ILE	127
H	0.034017	54.02	67.52	45.01	HD1	ILE	127
H	0.033593	52.62	68.36	45.04	HD2	ILE	127
H	0.018286	54.00	69.09	44.56	HD3	ILE	127
C	0.176473	53.13	71.92	48.76	C	ILE	127
O	-0.288622	53.87	72.90	48.87	O	ILE	127
N	-0.810117	55.11	75.41	50.27	N	GLN	131
H	0.430779	54.50	74.65	50.03	H	GLN	131
C	0.618641	55.08	76.62	49.47	CA	GLN	131
H	0.037464	56.04	76.78	49.25	HA	GLN	131
C	-0.145741	54.25	76.42	48.21	CB	GLN	131
H	0.027310	53.28	76.39	48.46	HB1	GLN	131
H	0.095013	54.51	75.55	47.79	HB2	GLN	131
C	-0.192438	54.45	77.54	47.19	CG	GLN	131
H	0.030895	55.40	77.51	46.86	HG1	GLN	131
H	0.029010	54.28	78.41	47.63	HG2	GLN	131
C	0.832044	53.54	77.43	45.99	CD	GLN	131
O	-0.609145	53.45	76.39	45.34	OE1	GLN	131
N	-1.051982	52.85	78.52	45.67	NE2	GLN	131
H	0.458627	52.95	79.35	46.22	1HE2	GLN	131
H	0.471361	52.23	78.51	44.89	2HE2	GLN	131
C	0.082622	54.55	77.81	50.25	C	GLN	131
O	-0.304343	54.99	78.95	50.03	O	GLN	131
N	-0.901365	57.40	80.54	50.43	N	MET	135
H	0.442833	56.80	79.75	50.35	H	MET	135
C	0.812335	57.10	81.76	49.69	CA	MET	135
H	-0.023523	57.97	82.00	49.23	HA	MET	135
C	-0.287246	56.01	81.53	48.64	CB	MET	135
H	0.073518	55.71	82.42	48.29	HB1	MET	135

H	0.088563	55.24	81.07	49.08	HB2	MET	135
C	-0.109137	56.44	80.70	47.45	CG	MET	135
H	0.147696	55.67	80.76	46.81	HG1	MET	135
H	0.137333	56.49	79.77	47.81	HG2	MET	135
S	-0.312721	57.99	81.24	46.69	SD	MET	135
C	-0.164160	57.52	82.87	46.07	CE	MET	135
H	0.134783	58.31	83.29	45.62	HE1	MET	135
H	0.087583	56.77	82.77	45.42	HE2	MET	135
H	0.069469	57.23	83.44	46.84	HE3	MET	135
C	0.042723	56.68	82.88	50.63	C	MET	135
O	-0.238685	57.05	84.04	50.45	O	MET	135
N	-0.918024	69.08	87.91	53.40	N	LEU	148
H	0.440225	68.08	87.94	53.34	H	LEU	148
C	0.764434	69.87	88.27	52.23	CA	LEU	148
H	-0.044992	70.78	87.93	52.49	HA	LEU	148
C	-0.246288	69.31	87.60	50.98	CB	LEU	148
H	0.050568	69.74	88.01	50.18	HB1	LEU	148
H	0.070390	68.32	87.77	50.96	HB2	LEU	148
C	0.317357	69.53	86.08	50.93	CG	LEU	148
H	-0.000685	69.05	85.64	51.69	HG	LEU	148
C	-0.341790	68.98	85.52	49.63	CD1	LEU	148
H	0.090581	69.13	84.53	49.60	1HD1	LEU	148
H	0.073024	68.00	85.71	49.57	2HD1	LEU	148
H	0.102297	69.45	85.95	48.85	3HD1	LEU	148
C	-0.473465	71.01	85.80	51.04	CD2	LEU	148
H	0.132495	71.16	84.81	51.00	1HD2	LEU	148
H	0.095705	71.49	86.23	50.28	2HD2	LEU	148
H	0.106257	71.36	86.15	51.91	3HD2	LEU	148
C	0.019928	70.04	89.76	51.98	C	LEU	148
O	-0.238016	70.45	90.16	50.89	O	LEU	148
N	-0.724883	62.86	97.22	44.06	N	LEU	155
H	0.348963	63.04	98.20	43.97	H	LEU	155
C	0.540553	62.96	96.36	42.90	CA	LEU	155
H	-0.074189	62.49	95.54	43.22	HA	LEU	155
C	-0.441759	62.30	97.02	41.69	CB	LEU	155
H	0.102404	62.50	96.45	40.89	HB1	LEU	155
H	0.091132	62.72	97.92	41.57	HB2	LEU	155
C	0.515551	60.79	97.23	41.73	CG	LEU	155
H	-0.059766	60.53	97.74	42.54	HG	LEU	155
C	-0.439891	60.36	98.02	40.49	CD1	LEU	155
H	0.070452	59.37	98.15	40.51	1HD1	LEU	155
H	0.081026	60.82	98.90	40.49	2HD1	LEU	155
H	0.142384	60.61	97.51	39.67	3HD1	LEU	155
C	-0.548033	60.09	95.87	41.77	CD2	LEU	155
H	0.093713	59.10	96.01	41.80	1HD2	LEU	155
H	0.152949	60.34	95.35	40.96	2HD2	LEU	155

H	0.158260	60.38	95.38	42.59	3HD2	LEU	155
C	0.476975	64.37	95.94	42.50	C	LEU	155
O	-0.493710	64.55	94.90	41.87	O	LEU	155
N	-0.718638	65.36	96.75	42.85	N	TYR	156
H	0.344425	65.16	97.56	43.39	H	TYR	156
C	0.476314	66.74	96.46	42.47	CA	TYR	156
H	-0.018860	66.72	95.57	42.02	HA	TYR	156
C	0.263877	67.21	97.57	41.53	CB	TYR	156
H	-0.091797	68.11	97.33	41.16	HB1	TYR	156
H	-0.084281	67.27	98.42	42.04	HB2	TYR	156
C	-0.166740	66.27	97.79	40.36	CG	TYR	156
C	-0.112562	66.26	96.91	39.27	CD1	TYR	156
H	0.171244	66.89	96.14	39.26	HD1	TYR	156
C	-0.269730	65.38	97.10	38.19	CE1	TYR	156
H	0.209823	65.39	96.47	37.42	HE1	TYR	156
C	0.459999	64.50	98.18	38.21	CZ	TYR	156
O	-0.564121	63.65	98.38	37.15	OH	TYR	156
H	0.395992	63.09	99.19	37.32	HH	TYR	156
C	-0.400136	64.49	99.06	39.28	CE2	TYR	156
H	0.168549	63.85	99.83	39.30	HE2	TYR	156
C	-0.090999	65.37	98.86	40.35	CD2	TYR	156
H	0.127571	65.36	99.49	41.12	HD2	TYR	156
C	0.314506	67.70	96.34	43.66	C	TYR	156
O	-0.561001	68.62	97.14	43.83	O	TYR	156
N	-0.090162	67.51	95.30	44.49	N	PRO	157
C	-0.211667	66.55	94.21	44.25	CD	PRO	157
H	0.154202	66.89	93.57	43.56	HD1	PRO	157
H	0.127739	65.66	94.57	43.94	HD2	PRO	157
C	0.114855	66.45	93.57	45.60	CG	PRO	157
H	0.004321	66.13	92.63	45.54	HG1	PRO	157
H	-0.009156	65.85	94.09	46.21	HG2	PRO	157
C	-0.114342	67.82	93.61	46.09	CB	PRO	157
H	0.067445	68.36	92.89	45.65	HB1	PRO	157
H	0.009951	67.84	93.49	47.08	HB2	PRO	157
C	0.086780	68.30	95.00	45.68	CA	PRO	157
H	0.037768	68.14	95.74	46.34	HA	PRO	157
C	0.477247	69.81	95.03	45.49	C	PRO	157
O	-0.512894	70.53	95.69	46.23	O	PRO	157
N	-0.340855	70.29	94.29	44.50	N	GLY	158
H	0.302003	69.67	93.78	43.90	H	GLY	158
C	-0.225625	71.72	94.20	44.29	CA	GLY	158
H	0.166743	72.11	95.12	44.33	HA1	GLY	158
H	0.126981	71.90	93.81	43.39	HA2	GLY	158
C	0.471522	72.28	93.32	45.39	C	GLY	158
O	-0.562195	71.59	92.44	45.90	O	GLY	158
N	-0.388487	73.54	93.54	45.75	N	GLY	159

H	0.294318	74.06	94.27	45.30	H	GLY	159
C	-0.204902	74.17	92.75	46.80	CA	GLY	159
H	0.183613	73.70	92.96	47.65	HA1	GLY	159
H	0.131201	75.12	93.04	46.86	HA2	GLY	159
C	0.542635	74.10	91.26	46.53	C	GLY	159
O	-0.619429	74.66	90.77	45.56	O	GLY	159
N	-0.379320	73.43	90.54	47.42	N	SER	160
H	0.296345	73.00	91.00	48.20	H	SER	160
C	-0.062296	73.29	89.10	47.27	CA	SER	160
H	0.089833	74.23	88.74	47.26	HA	SER	160
C	0.325303	72.49	88.52	48.43	CB	SER	160
H	-0.036072	72.39	87.53	48.33	HB1	SER	160
H	0.021334	71.59	88.94	48.49	HB2	SER	160
O	-0.659180	73.15	88.75	49.66	OG	SER	160
H	0.392896	72.61	88.36	50.41	HG	SER	160
C	0.517775	72.59	88.78	45.96	C	SER	160
O	-0.590555	72.75	87.68	45.43	O	SER	160
N	-0.487807	71.83	89.73	45.44	N	PHE	161
H	0.373321	71.75	90.62	45.90	H	PHE	161
C	0.365582	71.10	89.50	44.21	CA	PHE	161
H	0.000752	71.15	88.50	44.15	HA	PHE	161
C	-0.576540	69.67	90.02	44.34	CB	PHE	161
H	0.147779	69.21	89.91	43.46	HB1	PHE	161
H	0.201130	69.71	90.99	44.58	HB2	PHE	161
C	0.297803	68.87	89.30	45.39	CG	PHE	161
C	-0.332893	68.84	89.75	46.70	CD1	PHE	161
H	0.167474	69.32	90.60	46.94	HD1	PHE	161
C	-0.069537	68.15	89.05	47.70	CE1	PHE	161
H	0.110811	68.14	89.39	48.64	HE1	PHE	161
C	-0.220745	67.48	87.88	47.38	CZ	PHE	161
H	0.129197	66.98	87.38	48.09	HZ	PHE	161
C	-0.101231	67.50	87.42	46.07	CE2	PHE	161
H	0.129068	67.02	86.57	45.83	HE2	PHE	161
C	-0.183661	68.19	88.13	45.08	CD2	PHE	161
H	0.159230	68.20	87.79	44.14	HD2	PHE	161
C	0.383487	71.76	89.98	42.92	C	PHE	161
O	-0.461385	71.12	90.02	41.87	O	PHE	161
N	-0.605990	73.04	90.34	43.00	N	ASH	162
H	0.430752	73.49	90.34	43.90	H	ASH	162
C	0.243859	73.82	90.72	41.82	CA	ASH	162
H	-0.073351	73.39	90.28	41.04	HA	ASH	162
C	0.001349	73.80	92.24	41.57	CB	ASH	162
H	0.040322	74.25	92.69	42.33	HB1	ASH	162
H	0.103398	72.84	92.54	41.52	HB2	ASH	162
C	0.605581	74.52	92.64	40.25	CG	ASH	162
O	-0.645590	74.63	91.78	39.33	OD1	ASH	162

O	-0.513232	74.96	93.81	40.13	OD2	ASH	162
H	0.430000	75.39	93.91	39.23	HD2	ASH	162
C	0.377514	75.25	90.24	42.04	C	ASH	162
O	-0.522304	76.20	91.02	41.96	O	ASH	162
N	-0.267735	75.41	88.94	42.32	N	PRO	163
C	-0.113746	74.33	87.95	42.33	CD	PRO	163
H	0.024302	74.05	87.71	41.40	HD1	PRO	163
H	0.140153	73.54	88.29	42.84	HD2	PRO	163
C	0.237668	74.98	86.78	43.03	CG	PRO	163
H	-0.035812	74.52	85.92	42.80	HG1	PRO	163
H	-0.000611	74.97	86.90	44.02	HG2	PRO	163
C	-0.165260	76.36	86.81	42.50	CB	PRO	163
H	0.067067	76.39	86.46	41.56	HB1	PRO	163
H	0.005962	76.97	86.26	43.07	HB2	PRO	163
C	0.137481	76.70	88.29	42.56	CA	PRO	163
H	0.090454	77.08	88.60	43.43	HA	PRO	163
C	0.517838	77.77	88.66	41.54	C	PRO	163
O	-0.502458	78.85	89.11	41.90	O	PRO	163
N	-0.512973	77.46	88.47	40.27	N	LEU	164
H	0.266613	76.56	88.10	40.03	H	LEU	164
C	0.173565	78.40	88.78	39.21	CA	LEU	164
H	0.037822	79.25	88.36	39.52	HA	LEU	164
C	-0.279837	77.92	88.17	37.89	CB	LEU	164
H	0.084496	78.59	88.40	37.18	HB1	LEU	164
H	0.034921	77.03	88.57	37.66	HB2	LEU	164
C	0.413835	77.77	86.65	37.91	CG	LEU	164
H	-0.055748	77.07	86.39	38.58	HG	LEU	164
C	-0.343546	77.34	86.15	36.53	CD1	LEU	164
H	0.108080	77.24	85.16	36.55	1HD1	LEU	164
H	-0.025067	76.46	86.57	36.28	2HD1	LEU	164
H	0.121857	78.03	86.40	35.86	3HD1	LEU	164
C	-0.515444	79.08	86.01	38.32	CD2	LEU	164
H	0.133826	78.98	85.02	38.34	1HD2	LEU	164
H	0.136009	79.79	86.26	37.67	2HD2	LEU	164
H	0.153139	79.34	86.34	39.23	3HD2	LEU	164
C	0.352429	78.63	90.27	39.02	C	LEU	164
O	-0.506591	79.40	90.67	38.16	O	LEU	164
N	-0.239572	77.95	91.08	39.83	N	GLY	165
H	0.321162	77.33	90.69	40.51	H	GLY	165
C	-0.277897	78.09	92.52	39.74	CA	GLY	165
H	0.125675	79.02	92.75	40.04	HA1	GLY	165
H	0.138552	77.43	92.92	40.38	HA2	GLY	165
C	0.489405	77.85	93.11	38.36	C	GLY	165
O	-0.568630	78.52	94.06	37.97	O	GLY	165
N	-0.492730	76.89	92.57	37.63	N	LEU	166
H	0.325885	76.35	91.81	38.00	H	LEU	166

C	-0.050032	76.60	93.05	36.28	CA	LEU	166
H	0.114839	77.49	93.06	35.84	HA	LEU	166
C	-0.047576	75.61	92.12	35.58	CB	LEU	166
H	0.031649	75.39	92.52	34.69	HB1	LEU	166
H	0.016367	74.78	92.07	36.14	HB2	LEU	166
C	0.473502	76.08	90.68	35.33	CG	LEU	166
H	-0.079075	76.13	90.19	36.20	HG	LEU	166
C	-0.477762	75.09	89.96	34.42	CD1	LEU	166
H	0.085564	75.41	89.03	34.26	1HD1	LEU	166
H	0.051026	74.19	89.94	34.86	2HD1	LEU	166
H	0.159983	75.03	90.45	33.55	3HD1	LEU	166
C	-0.603282	77.45	90.71	34.69	CD2	LEU	166
H	0.131026	77.76	89.78	34.52	1HD2	LEU	166
H	0.123473	77.40	91.21	33.82	2HD2	LEU	166
H	0.221480	78.09	91.17	35.30	3HD2	LEU	166
C	0.441830	76.03	94.46	36.27	C	LEU	166
O	-0.518876	76.03	95.12	35.23	O	LEU	166
N	-0.454016	75.55	94.93	37.42	N	ALA	167
H	0.223675	75.59	94.36	38.24	H	ALA	167
C	0.389104	74.97	96.26	37.49	CA	ALA	167
H	0.000736	74.95	96.55	36.53	HA	ALA	167
C	-0.467212	73.58	96.17	38.10	CB	ALA	167
H	0.101974	73.17	97.08	38.15	HB1	ALA	167
H	0.102600	73.00	95.58	37.53	HB2	ALA	167
H	0.121615	73.64	95.78	39.02	HB3	ALA	167
C	0.454883	75.80	97.30	38.24	C	ALA	167
O	-0.502361	75.27	98.33	38.67	O	ALA	167
N	-0.635395	77.10	97.05	38.41	N	ASH	168
H	0.423992	77.49	96.21	38.04	H	ASH	168
C	0.454153	77.94	98.00	39.13	CA	ASH	168
H	0.095310	77.44	98.18	39.97	HA	ASH	168
C	-0.577234	79.30	97.37	39.44	CB	ASH	168
H	0.206812	79.85	98.04	39.93	HB1	ASH	168
H	0.196436	79.75	97.14	38.57	HB2	ASH	168
C	0.681343	79.18	96.11	40.28	CG	ASH	168
O	-0.572966	78.38	96.11	41.24	OD1	ASH	168
O	-0.457059	79.89	95.12	39.98	OD2	ASH	168
H	0.410501	79.70	94.37	40.62	HD2	ASH	168
C	0.017093	78.13	99.31	38.37	C	ASH	168
O	-0.244248	78.22	100.37	38.98	O	ASH	168
N	-0.825901	73.87	99.57	34.12	N	PHE	173
H	0.390861	74.61	100.12	34.51	H	PHE	173
C	0.735659	72.72	99.26	34.94	CA	PHE	173
H	0.023078	72.65	98.27	35.00	HA	PHE	173
C	-0.767549	72.92	99.86	36.34	CB	PHE	173
H	0.174853	72.93	100.86	36.26	HB1	PHE	173

H	0.278773	73.79	99.55	36.70	HB2	PHE	173
C	0.258783	71.85	99.50	37.32	CG	PHE	173
C	-0.196925	71.15	98.30	37.21	CD1	PHE	173
H	0.120482	71.33	97.69	36.44	HD1	PHE	173
C	-0.170962	70.21	97.93	38.17	CE1	PHE	173
H	0.147486	69.72	97.06	38.08	HE1	PHE	173
C	-0.102110	69.96	98.77	39.25	CZ	PHE	173
H	0.141348	69.28	98.50	39.95	HZ	PHE	173
C	-0.154915	70.64	99.97	39.37	CE2	PHE	173
H	0.144358	70.46	100.57	40.14	HE2	PHE	173
C	-0.186772	71.58	100.33	38.41	CD2	PHE	173
H	0.153005	72.07	101.19	38.49	HD2	PHE	173
C	0.139718	71.45	99.83	34.30	C	PHE	173
O	-0.303271	70.44	99.13	34.16	O	PHE	173
N	-0.726461	70.59	97.64	31.22	N	LEU	176
H	0.367238	71.41	98.02	31.65	H	LEU	176
C	0.493729	70.15	96.30	31.59	CA	LEU	176
H	-0.055816	70.20	95.75	30.76	HA	LEU	176
C	-0.112476	71.08	95.71	32.66	CB	LEU	176
H	-0.042505	70.60	94.94	33.09	HB1	LEU	176
H	0.017749	71.23	96.43	33.35	HB2	LEU	176
C	0.466033	72.45	95.21	32.19	CG	LEU	176
H	-0.031050	72.89	95.90	31.61	HG	LEU	176
C	-0.602198	73.38	94.97	33.37	CD1	LEU	176
H	0.172528	74.26	94.64	33.04	1HD1	LEU	176
H	0.110656	73.51	95.82	33.88	2HD1	LEU	176
H	0.177847	72.97	94.28	33.97	3HD1	LEU	176
C	-0.521896	72.26	93.94	31.38	CD2	LEU	176
H	0.127572	73.15	93.61	31.07	1HD2	LEU	176
H	0.117223	71.83	93.24	31.95	2HD2	LEU	176
H	0.120392	71.68	94.13	30.59	3HD2	LEU	176
C	0.511652	68.71	96.34	32.09	C	LEU	176
O	-0.602335	67.93	95.41	31.84	O	LEU	176
N	-0.541714	68.35	97.42	32.78	N	LYS	177
H	0.347446	69.02	98.15	32.94	H	LYS	177
C	0.030953	66.99	97.56	33.29	CA	LYS	177
H	0.136775	66.85	96.77	33.88	HA	LYS	177
C	-0.082302	66.84	98.85	34.10	CB	LYS	177
H	0.023559	65.87	99.08	34.15	HB1	LYS	177
H	0.020726	67.33	99.58	33.61	HB2	LYS	177
C	0.236565	67.38	98.79	35.50	CG	LYS	177
H	-0.017669	68.37	98.64	35.47	HG1	LYS	177
H	-0.045475	66.94	98.04	35.99	HG2	LYS	177
C	0.125305	67.09	100.10	36.21	CD	LYS	177
H	-0.044352	66.10	100.26	36.21	HD1	LYS	177
H	-0.058331	67.55	100.84	35.73	HD2	LYS	177

C	-0.275886	67.58	100.07	37.64	CE	LYS	177
H	0.092926	68.54	99.78	37.64	HE1	LYS	177
H	0.118111	67.03	99.40	38.15	HE2	LYS	177
N	0.459234	67.47	101.39	38.32	NZ	LYS	177
H	-0.124316	67.81	101.31	39.26	HZ1	LYS	177
H	-0.153857	68.02	102.06	37.82	HZ2	LYS	177
H	-0.181866	66.51	101.68	38.33	HZ3	LYS	177
C	0.556360	65.98	97.57	32.15	C	LYS	177
O	-0.598463	64.93	96.94	32.24	O	LYS	177
N	-0.442397	66.31	98.29	31.07	N	VAL	178
H	0.291257	67.18	98.79	31.07	H	VAL	178
C	-0.183946	65.45	98.37	29.89	CA	VAL	178
H	0.108765	64.58	98.73	30.23	HA	VAL	178
C	0.421801	66.05	99.31	28.81	CB	VAL	178
H	-0.011239	66.97	99.01	28.57	HB	VAL	178
C	-0.508979	65.19	99.28	27.54	CG1	VAL	178
H	0.134470	65.59	99.89	26.86	1HG1	VAL	178
H	0.116550	65.16	98.35	27.19	2HG1	VAL	178
H	0.114528	64.26	99.58	27.76	3HG1	VAL	178
C	-0.370974	66.13	100.74	29.34	CG2	VAL	178
H	0.083657	66.51	101.33	28.63	1HG2	VAL	178
H	0.083018	65.21	101.05	29.58	2HG2	VAL	178
H	0.082311	66.71	100.76	30.15	3HG2	VAL	178
C	0.544012	65.29	96.97	29.31	C	VAL	178
O	-0.648521	64.19	96.54	28.99	O	VAL	178
N	-0.596889	66.41	96.26	29.18	N	LYS	179
H	0.356899	67.28	96.67	29.46	H	LYS	179
C	0.383649	66.41	94.91	28.65	CA	LYS	179
H	-0.063321	66.04	94.99	27.73	HA	LYS	179
C	-0.351220	67.84	94.36	28.63	CB	LYS	179
H	0.028223	67.80	93.37	28.45	HB1	LYS	179
H	0.141293	68.26	94.52	29.52	HB2	LYS	179
C	0.311533	68.72	94.98	27.58	CG	LYS	179
H	-0.143657	68.78	95.97	27.75	HG1	LYS	179
H	-0.012615	68.32	94.83	26.68	HG2	LYS	179
C	0.190307	70.10	94.38	27.63	CD	LYS	179
H	-0.045679	70.03	93.39	27.59	HD1	LYS	179
H	-0.076667	70.54	94.65	28.48	HD2	LYS	179
C	-0.281620	70.95	94.86	26.46	CE	LYS	179
H	0.066864	70.89	95.86	26.39	HE1	LYS	179
H	0.075774	70.61	94.45	25.61	HE2	LYS	179
N	0.353706	72.38	94.49	26.64	NZ	LYS	179
H	-0.168080	72.91	94.82	25.86	HZ1	LYS	179
H	-0.173954	72.73	94.90	27.48	HZ2	LYS	179
H	0.135247	72.45	93.49	26.70	HZ3	LYS	179
C	0.585840	65.53	93.97	29.48	C	LYS	179

O	-0.727141	64.85	93.11	28.93	O	LYS	179
N	-0.495103	65.56	94.15	30.80	N	GLU	180
H	0.356908	66.15	94.87	31.18	H	GLU	180
C	0.254842	64.77	93.33	31.71	CA	GLU	180
H	-0.045890	65.00	92.38	31.49	HA	GLU	180
C	-0.013557	65.16	93.63	33.16	CB	GLU	180
H	0.089070	64.78	94.53	33.41	HB1	GLU	180
H	0.010655	66.15	93.67	33.23	HB2	GLU	180
C	-0.294072	64.65	92.60	34.17	CG	GLU	180
H	0.049902	65.07	91.72	33.97	HG1	GLU	180
H	0.080150	63.66	92.53	34.07	HG2	GLU	180
C	0.789955	64.96	92.97	35.62	CD	GLU	180
O	-0.668266	65.28	92.06	36.41	OE1	GLU	180
O	-0.552526	64.87	94.17	35.97	OE2	GLU	180
C	0.511879	63.28	93.58	31.49	C	GLU	180
O	-0.653552	62.50	92.63	31.34	O	GLU	180
N	-0.426188	62.88	94.85	31.48	N	ILE	181
H	0.327470	63.56	95.57	31.61	H	ILE	181
C	0.165278	61.49	95.23	31.26	CA	ILE	181
H	-0.022906	60.99	94.74	31.98	HA	ILE	181
C	0.006957	61.29	96.78	31.38	CB	ILE	181
H	0.058236	62.06	97.25	30.94	HB	ILE	181
C	-0.340131	59.99	97.21	30.69	CG2	ILE	181
H	0.107244	59.88	98.20	30.77	1HG2	ILE	181
H	0.102274	60.03	96.96	29.72	2HG2	ILE	181
H	0.070721	59.22	96.75	31.13	3HG2	ILE	181
C	0.319892	61.21	97.21	32.84	CG1	ILE	181
H	-0.089177	61.34	98.20	32.89	1HG1	ILE	181
H	-0.092201	61.94	96.76	33.35	2HG1	ILE	181
C	-0.217341	59.90	96.87	33.51	CD	ILE	181
H	0.028858	59.92	97.18	34.46	HD1	ILE	181
H	0.051805	59.15	97.33	33.03	HD2	ILE	181
H	0.034659	59.76	95.88	33.48	HD3	ILE	181
C	0.559264	61.02	94.76	29.88	C	ILE	181
O	-0.671502	59.89	94.32	29.72	O	ILE	181
N	-0.495826	61.88	94.88	28.87	N	LYS	182
H	0.362775	62.80	95.25	29.04	H	LYS	182
C	0.298974	61.50	94.46	27.52	CA	LYS	182
H	-0.013200	60.61	94.88	27.38	HA	LYS	182
C	-0.268023	62.50	94.99	26.50	CB	LYS	182
H	0.011181	62.20	94.71	25.58	HB1	LYS	182
H	0.093741	63.40	94.59	26.69	HB2	LYS	182
C	0.427120	62.62	96.51	26.53	CG	LYS	182
H	-0.055160	63.54	96.75	26.84	HG1	LYS	182
H	-0.112023	61.95	96.87	27.18	HG2	LYS	182
C	-0.146929	62.39	97.15	25.17	CD	LYS	182

H	-0.008401	62.47	98.15	25.27	HD1	LYS	182
H	0.056691	61.47	96.92	24.85	HD2	LYS	182
C	-0.131082	63.39	96.68	24.16	CE	LYS	182
H	0.053824	63.22	95.72	23.95	HE1	LYS	182
H	0.087937	64.31	96.78	24.54	HE2	LYS	182
N	0.728890	63.35	97.45	22.89	NZ	LYS	182
H	-0.609136	64.03	97.10	22.25	HZ1	LYS	182
H	-0.057862	62.44	97.36	22.48	HZ2	LYS	182
H	-0.110015	63.53	98.42	23.07	HZ3	LYS	182
C	0.513547	61.35	92.93	27.40	C	LYS	182
O	-0.660911	60.36	92.45	26.86	O	LYS	182
N	-0.417957	62.33	92.18	27.90	N	ASN	183
H	0.340083	63.13	92.61	28.30	H	ASN	183
C	0.184710	62.23	90.72	27.87	CA	ASN	183
H	0.011531	62.14	90.45	26.92	HA	ASN	183
C	-0.385653	63.50	90.09	28.47	CB	ASN	183
H	0.086726	63.25	89.21	28.88	HB1	ASN	183
H	0.194626	63.86	90.70	29.17	HB2	ASN	183
C	0.884617	64.58	89.84	27.43	CG	ASN	183
O	-0.763932	64.58	88.82	26.74	OD1	ASN	183
N	-1.042328	65.50	90.79	27.31	ND2	ASN	183
H	0.493481	65.46	91.61	27.89	1HD2	ASN	183
H	0.455903	66.24	90.69	26.64	2HD2	ASN	183
C	0.469565	61.02	90.32	28.72	C	ASN	183
O	-0.678372	60.28	89.39	28.37	O	ASN	183
N	-0.281801	60.82	91.03	29.83	N	GLY	184
H	0.333653	61.45	91.78	30.05	H	GLY	184
C	-0.102459	59.71	90.75	30.72	CA	GLY	184
H	0.121499	59.82	91.34	31.52	HA1	GLY	184
H	0.038983	59.80	89.79	31.01	HA2	GLY	184
C	0.594412	58.35	90.97	30.10	C	GLY	184
O	-0.727371	57.45	90.14	30.23	O	GLY	184
N	-0.577492	58.19	92.11	29.43	N	ARG	185
H	0.414541	58.96	92.75	29.37	H	ARG	185
C	0.271073	56.93	92.44	28.77	CA	ARG	185
H	-0.042078	56.23	92.38	29.48	HA	ARG	185
C	-0.147593	56.99	93.86	28.19	CB	ARG	185
H	-0.017903	56.24	93.98	27.54	HB1	ARG	185
H	0.066143	57.87	93.98	27.72	HB2	ARG	185
C	0.289511	56.88	94.94	29.26	CG	ARG	185
H	-0.047189	57.51	94.72	30.00	HG1	ARG	185
H	-0.046016	55.94	94.94	29.62	HG2	ARG	185
C	0.031036	57.19	96.33	28.74	CD	ARG	185
H	0.046483	56.59	96.55	27.97	HD1	ARG	185
H	0.019347	58.15	96.38	28.44	HD2	ARG	185
N	-0.710747	56.99	97.33	29.78	NE	ARG	185

H	0.358719	56.62	97.01	30.66	HE	ARG	185
C	0.817452	57.25	98.63	29.66	CZ	ARG	185
N	-1.120453	57.74	99.10	28.52	NH1	ARG	185
H	0.405256	57.91	98.48	27.75	1HH1	ARG	185
H	0.442530	57.94	100.08	28.43	2HH1	ARG	185
N	-1.249112	57.02	99.45	30.67	NH2	ARG	185
H	0.486053	56.65	99.10	31.53	1HH2	ARG	185
H	0.451069	57.22	100.43	30.58	2HH2	ARG	185
C	0.554450	56.62	91.42	27.67	C	ARG	185
O	-0.680931	55.46	91.04	27.49	O	ARG	185
N	-0.453281	57.65	90.99	26.94	N	LEU	186
H	0.350607	58.57	91.34	27.12	H	LEU	186
C	0.126632	57.46	89.99	25.89	CA	LEU	186
H	0.019968	56.79	90.38	25.26	HA	LEU	186
C	-0.203970	58.77	89.74	25.15	CB	LEU	186
H	0.131384	59.46	89.49	25.83	HB1	LEU	186
H	0.051652	59.04	90.59	24.70	HB2	LEU	186
C	0.287820	58.75	88.64	24.07	CG	LEU	186
H	-0.033382	58.52	87.76	24.49	HG	LEU	186
C	-0.290882	57.69	88.93	23.01	CD1	LEU	186
H	0.042761	57.70	88.20	22.32	1HD1	LEU	186
H	0.051975	56.79	88.98	23.43	2HD1	LEU	186
H	0.079731	57.90	89.80	22.56	3HD1	LEU	186
C	-0.320330	60.12	88.53	23.45	CD2	LEU	186
H	0.082934	60.12	87.82	22.75	1HD2	LEU	186
H	0.052613	60.37	89.41	23.03	2HD2	LEU	186
H	0.065183	60.79	88.30	24.16	3HD2	LEU	186
C	0.575580	56.95	88.69	26.52	C	LEU	186
O	-0.668123	56.05	88.04	25.98	O	LEU	186
N	-0.526689	57.53	88.32	27.66	N	ALA	187
H	0.375211	58.26	88.89	28.04	H	ALA	187
C	0.371567	57.13	87.11	28.38	CA	ALA	187
H	-0.046058	57.23	86.38	27.71	HA	ALA	187
C	-0.298453	58.06	86.87	29.58	CB	ALA	187
H	0.040537	57.77	86.04	30.06	HB1	ALA	187
H	0.077915	59.00	86.77	29.26	HB2	ALA	187
H	0.137010	58.00	87.65	30.20	HB3	ALA	187
C	0.668444	55.68	87.17	28.85	C	ALA	187
O	-0.704338	54.96	86.19	28.73	O	ALA	187
N	-0.585529	55.26	88.32	29.39	N	MET	188
H	0.430672	55.90	89.08	29.48	H	MET	188
C	-0.022161	53.88	88.47	29.86	CA	MET	188
H	0.029982	53.74	87.73	30.53	HA	MET	188
C	0.274926	53.66	89.83	30.53	CB	MET	188
H	-0.075668	52.68	89.93	30.71	HB1	MET	188
H	0.034153	53.96	90.54	29.89	HB2	MET	188

C	0.026345	54.41	90.02	31.84	CG	MET	188
H	0.063572	55.37	89.98	31.58	HG1	MET	188
H	0.037473	54.17	89.22	32.38	HG2	MET	188
S	-0.436084	53.99	91.58	32.69	SD	MET	188
C	-0.196430	54.99	92.78	31.77	CE	MET	188
H	0.146507	54.85	93.69	32.14	HE1	MET	188
H	0.157363	55.96	92.53	31.84	HE2	MET	188
H	0.095292	54.72	92.77	30.80	HE3	MET	188
C	0.512095	52.92	88.33	28.67	C	MET	188
O	-0.637967	51.94	87.58	28.72	O	MET	188
N	-0.430064	53.23	89.06	27.61	N	PHE	189
H	0.333633	54.04	89.65	27.65	H	PHE	189
C	0.128050	52.44	89.06	26.39	CA	PHE	189
H	0.044459	51.55	89.46	26.58	HA	PHE	189
C	-0.096838	53.19	89.89	25.34	CB	PHE	189
H	0.111861	54.03	89.41	25.09	HB1	PHE	189
H	0.078235	53.41	90.78	25.73	HB2	PHE	189
C	0.003951	52.42	90.12	24.08	CG	PHE	189
C	-0.113734	51.63	91.25	23.93	CD1	PHE	189
H	0.127041	51.55	91.90	24.69	HD1	PHE	189
C	-0.169937	50.95	91.50	22.73	CE1	PHE	189
H	0.117415	50.39	92.32	22.64	HE1	PHE	189
C	-0.094393	51.05	90.61	21.68	CZ	PHE	189
H	0.101597	50.56	90.78	20.83	HZ	PHE	189
C	-0.141352	51.83	89.47	21.82	CE2	PHE	189
H	0.128373	51.91	88.82	21.07	HE2	PHE	189
C	-0.191759	52.51	89.24	23.02	CD2	PHE	189
H	0.149734	53.07	88.41	23.11	HD2	PHE	189
C	0.524227	52.30	87.61	25.92	C	PHE	189
O	-0.610443	51.20	87.14	25.59	O	PHE	189
N	-0.430119	53.42	86.90	25.89	N	SER	190
H	0.357394	54.28	87.34	26.17	H	SER	190
C	0.076431	53.45	85.51	25.46	CA	SER	190
H	0.073851	52.93	85.51	24.60	HA	SER	190
C	0.303116	54.90	85.08	25.23	CB	SER	190
H	-0.102332	54.94	84.14	24.91	HB1	SER	190
H	0.010584	55.43	85.17	26.08	HB2	SER	190
O	-0.559685	55.51	85.90	24.25	OG	SER	190
H	0.311780	56.45	85.61	24.11	HG	SER	190
C	0.492629	52.76	84.57	26.44	C	SER	190
O	-0.636769	52.19	83.55	26.03	O	SER	190
N	-0.424385	52.80	84.88	27.73	N	MET	191
H	0.355419	53.29	85.70	28.03	H	MET	191
C	0.176067	52.14	84.03	28.70	CA	MET	191
H	-0.009598	52.44	83.10	28.52	HA	MET	191
C	0.093696	52.54	84.41	30.12	CB	MET	191

H	-0.028471	51.80	84.17	30.74	HB1	MET	191
H	0.040727	52.69	85.40	30.16	HB2	MET	191
C	0.037140	53.82	83.71	30.60	CG	MET	191
H	0.010444	53.95	84.06	31.53	HG1	MET	191
H	0.097990	54.53	84.07	30.01	HG2	MET	191
S	-0.302396	53.73	81.88	30.56	SD	MET	191
C	-0.237596	52.27	81.55	31.59	CE	MET	191
H	0.162589	52.11	80.57	31.64	HE1	MET	191
H	-0.001288	52.42	81.92	32.50	HE2	MET	191
H	0.146871	51.47	81.99	31.17	HE3	MET	191
C	0.468501	50.62	84.17	28.52	C	MET	191
O	-0.653445	49.89	83.19	28.68	O	MET	191
N	-0.277828	50.17	85.37	28.18	N	PHE	192
H	0.303032	50.82	86.13	28.09	H	PHE	192
C	-0.031472	48.75	85.62	27.93	CA	PHE	192
H	0.035823	48.23	85.41	28.76	HA	PHE	192
C	-0.121279	48.53	87.08	27.55	CB	PHE	192
H	0.104111	48.93	87.24	26.65	HB1	PHE	192
H	0.170833	48.98	87.66	28.23	HB2	PHE	192
C	0.102236	47.08	87.48	27.50	CG	PHE	192
C	-0.141484	46.34	87.65	28.66	CD1	PHE	192
H	0.155716	46.78	87.48	29.54	HD1	PHE	192
C	-0.161820	45.01	88.06	28.61	CE1	PHE	192
H	0.097529	44.49	88.18	29.46	HE1	PHE	192
C	-0.113590	44.40	88.30	27.39	CZ	PHE	192
H	0.092241	43.44	88.59	27.35	HZ	PHE	192
C	-0.153074	45.12	88.13	26.22	CE2	PHE	192
H	0.114249	44.68	88.30	25.34	HE2	PHE	192
C	-0.196353	46.46	87.72	26.28	CD2	PHE	192
H	0.134873	46.97	87.60	25.43	HD2	PHE	192
C	0.494192	48.40	84.72	26.75	C	PHE	192
O	-0.631563	47.33	84.13	26.69	O	PHE	192
N	-0.322455	49.34	84.63	25.80	N	GLY	193
H	0.321213	50.19	85.15	25.90	H	GLY	193
C	-0.177401	49.14	83.79	24.63	CA	GLY	193
H	0.120183	49.93	83.92	24.02	HA1	GLY	193
H	0.111549	48.31	84.08	24.17	HA2	GLY	193
C	0.496171	49.03	82.33	25.03	C	GLY	193
O	-0.604678	48.16	81.60	24.54	O	GLY	193
N	-0.347886	49.91	81.88	25.92	N	PHE	194
H	0.294530	50.62	82.50	26.27	H	PHE	194
C	0.011224	49.86	80.50	26.40	CA	PHE	194
H	0.037816	50.01	79.93	25.59	HA	PHE	194
C	-0.117136	50.95	80.25	27.45	CB	PHE	194
H	0.033874	50.72	79.42	27.96	HB1	PHE	194
H	0.122021	50.98	81.02	28.08	HB2	PHE	194

C	0.228957	52.34	80.06	26.88	CG	PHE	194
C	-0.232947	53.41	79.75	27.72	CD1	PHE	194
H	0.128186	53.25	79.65	28.70	HD1	PHE	194
C	-0.089871	54.70	79.56	27.21	CE1	PHE	194
H	0.131612	55.45	79.33	27.82	HE1	PHE	194
C	-0.260250	54.92	79.70	25.84	CZ	PHE	194
H	0.143162	55.84	79.57	25.47	HZ	PHE	194
C	-0.055742	53.87	80.01	24.99	CE2	PHE	194
H	0.050306	54.03	80.11	24.01	HE2	PHE	194
C	-0.212530	52.58	80.19	25.51	CD2	PHE	194
H	0.099044	51.83	80.42	24.89	HD2	PHE	194
C	0.555537	48.48	80.24	27.03	C	PHE	194
O	-0.633309	47.85	79.21	26.75	O	PHE	194
N	-0.589352	48.01	81.16	27.87	N	PHE	195
H	0.406731	48.56	81.98	28.05	H	PHE	195
C	0.553841	46.71	81.01	28.52	CA	PHE	195
H	-0.151982	46.82	80.14	29.01	HA	PHE	195
C	-0.581789	46.45	82.18	29.48	CB	PHE	195
H	0.094973	45.52	82.09	29.84	HB1	PHE	195
H	0.223016	46.54	83.04	28.98	HB2	PHE	195
C	0.451082	47.39	82.23	30.65	CG	PHE	195
C	-0.456845	48.03	81.08	31.11	CD1	PHE	195
H	0.267808	47.88	80.21	30.64	HD1	PHE	195
C	-0.047740	48.88	81.13	32.22	CE1	PHE	195
H	0.112329	49.34	80.29	32.53	HE1	PHE	195
C	-0.210801	49.10	82.32	32.88	CZ	PHE	195
H	0.086182	49.71	82.35	33.67	HZ	PHE	195
C	-0.098121	48.47	83.48	32.44	CE2	PHE	195
H	0.099362	48.63	84.34	32.91	HE2	PHE	195
C	-0.262572	47.62	83.43	31.32	CD2	PHE	195
H	0.140486	47.17	84.27	31.01	HD2	PHE	195
C	0.515044	45.54	80.90	27.56	C	PHE	195
O	-0.640877	44.70	79.99	27.69	O	PHE	195
N	-0.422642	45.47	81.80	26.58	N	VAL	196
H	0.370686	46.17	82.51	26.51	H	VAL	196
C	-0.067489	44.37	81.77	25.62	CA	VAL	196
H	0.049344	43.57	81.63	26.21	HA	VAL	196
C	0.369574	44.27	83.11	24.84	CB	VAL	196
H	0.008883	45.16	83.33	24.43	HB	VAL	196
C	-0.459981	43.23	83.01	23.74	CG1	VAL	196
H	0.093134	43.18	83.88	23.25	1HG1	VAL	196
H	0.078483	43.49	82.28	23.10	2HG1	VAL	196
H	0.095131	42.34	82.81	24.14	3HG1	VAL	196
C	-0.237632	43.88	84.23	25.79	CG2	VAL	196
H	0.037203	43.82	85.09	25.28	1HG2	VAL	196
H	0.034727	42.99	84.02	26.20	2HG2	VAL	196

H	0.066407	44.56	84.32	26.51	3HG2	VAL	196
C	0.478337	44.45	80.60	24.65	C	VAL	196
O	-0.623011	43.43	79.98	24.34	O	VAL	196
N	-0.508640	45.65	80.28	24.17	N	GLN	197
H	0.402232	46.45	80.81	24.45	H	GLN	197
C	0.199682	45.84	79.16	23.23	CA	GLN	197
H	-0.017508	45.20	79.34	22.48	HA	GLN	197
C	0.163342	47.28	79.11	22.71	CB	GLN	197
H	-0.057566	47.37	78.33	22.09	HB1	GLN	197
H	0.001630	47.90	78.99	23.49	HB2	GLN	197
C	-0.256846	47.68	80.37	21.97	CG	GLN	197
H	0.077813	47.64	81.14	22.61	HG1	GLN	197
H	0.032608	47.02	80.52	21.23	HG2	GLN	197
C	0.908888	49.07	80.32	21.37	CD	GLN	197
O	-0.791571	49.66	81.36	21.05	OE1	GLN	197
N	-1.059868	49.60	79.11	21.21	NE2	GLN	197
H	0.479399	49.08	78.29	21.47	1HE2	GLN	197
H	0.532745	50.51	79.01	20.82	2HE2	GLN	197
C	0.493740	45.49	77.83	23.89	C	GLN	197
O	-0.586924	44.93	76.94	23.25	O	GLN	197
N	-0.503925	45.82	77.70	25.17	N	ALA	198
H	0.354776	46.30	78.44	25.64	H	ALA	198
C	0.260278	45.50	76.47	25.89	CA	ALA	198
H	0.043496	45.97	75.72	25.44	HA	ALA	198
C	-0.311177	45.98	76.56	27.34	CB	ALA	198
H	0.071054	45.76	75.71	27.82	HB1	ALA	198
H	0.089331	46.97	76.70	27.35	HB2	ALA	198
H	0.109363	45.54	77.33	27.79	HB3	ALA	198
C	0.579240	43.98	76.29	25.85	C	ALA	198
O	-0.588721	43.48	75.26	25.41	O	ALA	198
N	-0.545855	43.27	77.32	26.31	N	ILE	199
H	0.350706	43.74	78.13	26.64	H	ILE	199
C	0.003484	41.82	77.28	26.33	CA	ILE	199
H	0.046958	41.64	76.47	26.90	HA	ILE	199
C	0.236957	41.25	78.58	26.95	CB	ILE	199
H	-0.002361	41.66	79.37	26.49	HB	ILE	199
C	-0.441600	39.75	78.66	26.75	CG2	ILE	199
H	0.108792	39.41	79.51	27.15	1HG2	ILE	199
H	0.074072	39.54	78.64	25.77	2HG2	ILE	199
H	0.094227	39.32	77.88	27.20	3HG2	ILE	199
C	0.241936	41.59	78.64	28.44	CG1	ILE	199
H	-0.061984	42.57	78.49	28.55	1HG1	ILE	199
H	-0.067026	41.09	77.91	28.90	2HG1	ILE	199
C	-0.178241	41.23	79.96	29.09	CD	ILE	199
H	0.039610	41.48	79.93	30.06	HD1	ILE	199
H	0.033490	41.73	80.70	28.64	HD2	ILE	199

H	0.008962	40.25	80.12	29.00	HD3	ILE	199
C	0.453300	41.18	77.07	24.96	C	ILE	199
O	-0.522068	40.21	76.34	24.83	O	ILE	199
N	-0.481024	41.73	77.70	23.92	N	VAL	200
H	0.342775	42.55	78.26	24.06	H	VAL	200
C	0.014852	41.15	77.58	22.60	CA	VAL	200
H	0.085078	40.19	77.47	22.85	HA	VAL	200
C	0.260094	41.46	78.86	21.76	CB	VAL	200
H	0.006492	42.45	79.00	21.71	HB	VAL	200
C	-0.416863	40.94	78.70	20.33	CG1	VAL	200
H	0.112620	41.15	79.53	19.81	1HG1	VAL	200
H	0.085198	41.38	77.91	19.90	2HG1	VAL	200
H	0.095839	39.95	78.56	20.34	3HG1	VAL	200
C	-0.240113	40.81	80.07	22.42	CG2	VAL	200
H	0.061886	41.01	80.89	21.88	1HG2	VAL	200
H	0.057346	39.82	79.93	22.46	2HG2	VAL	200
H	0.048498	41.17	80.18	23.34	3HG2	VAL	200
C	0.403274	41.51	76.34	21.77	C	VAL	200
O	-0.528497	40.65	75.80	21.08	O	VAL	200
N	-0.401557	42.76	75.90	21.83	N	THR	201
H	0.365027	43.41	76.36	22.43	H	THR	201
C	0.331446	43.21	74.75	21.04	CA	THR	201
H	-0.020016	42.51	74.75	20.33	HA	THR	201
C	0.096580	44.65	74.93	20.51	CB	THR	201
H	-0.021314	44.92	74.16	19.92	HB	THR	201
C	-0.071834	44.79	76.24	19.74	CG2	THR	201
H	0.054873	45.73	76.34	19.41	1HG2	THR	201
H	0.022882	44.17	76.24	18.96	2HG2	THR	201
H	0.007463	44.58	77.01	20.35	3HG2	THR	201
O	-0.618021	45.58	74.90	21.61	OG1	THR	201
H	0.383201	46.51	75.01	21.27	HG1	THR	201
C	0.411915	43.18	73.41	21.78	C	THR	201
O	-0.537201	43.05	72.36	21.15	O	THR	201
N	-0.303929	43.34	73.46	23.10	N	GLY	202
H	0.306237	43.46	74.35	23.55	H	GLY	202
C	-0.233257	43.34	72.25	23.90	CA	GLY	202
H	0.157033	42.61	71.66	23.56	HA1	GLY	202
H	0.138603	43.15	72.51	24.85	HA2	GLY	202
C	0.392432	44.66	71.51	23.84	C	GLY	202
O	-0.531359	44.80	70.44	24.41	O	GLY	202
N	-0.522669	45.64	72.08	23.14	N	LYS	203
H	0.362861	45.48	72.96	22.69	H	LYS	203
C	0.238676	46.94	71.44	23.01	CA	LYS	203
H	0.029047	46.86	70.58	23.52	HA	LYS	203
C	-0.189090	47.24	71.18	21.54	CB	LYS	203
H	0.011396	48.10	70.68	21.48	HB1	LYS	203

H	0.017833	47.33	72.07	21.08	HB2	LYS	203
C	0.259070	46.17	70.39	20.83	CG	LYS	203
H	0.022488	45.28	70.84	20.95	HG1	LYS	203
H	-0.031010	46.13	69.47	21.22	HG2	LYS	203
C	0.062913	46.50	70.31	19.36	CD	LYS	203
H	-0.057173	47.45	70.02	19.26	HD1	LYS	203
H	-0.020397	46.38	71.21	18.95	HD2	LYS	203
C	-0.271669	45.61	69.32	18.63	CE	LYS	203
H	0.083346	44.65	69.62	18.69	HE1	LYS	203
H	0.092453	45.70	68.41	19.05	HE2	LYS	203
N	0.577547	46.00	69.23	17.19	NZ	LYS	203
H	-0.138033	45.41	68.58	16.72	HZ1	LYS	203
H	-0.134485	45.91	70.13	16.76	HZ2	LYS	203
H	-0.317583	46.95	68.93	17.12	HZ3	LYS	203
C	0.386088	48.05	72.28	23.62	C	LYS	203
O	-0.457820	47.82	73.39	24.10	O	LYS	203
N	-0.359318	49.27	71.74	23.59	N	GLY	204
H	0.270236	49.40	70.84	23.18	H	GLY	204
C	-0.138192	50.40	72.46	24.13	CA	GLY	204
H	0.071914	51.12	71.79	24.31	HA1	GLY	204
H	0.105544	50.11	72.88	24.99	HA2	GLY	204
C	0.438818	50.93	73.54	23.20	C	GLY	204
O	-0.614527	50.77	73.44	21.98	O	GLY	204
N	-0.163639	51.57	74.58	23.75	N	PRO	205
C	-0.173304	51.94	74.69	25.17	CD	PRO	205
H	0.066072	52.74	74.12	25.38	HD1	PRO	205
H	0.077484	51.18	74.42	25.76	HD2	PRO	205
C	0.128669	52.26	76.14	25.30	CG	PRO	205
H	-0.038428	52.86	76.31	26.09	HG1	PRO	205
H	-0.015059	51.42	76.68	25.40	HG2	PRO	205
C	0.027710	52.94	76.47	24.04	CB	PRO	205
H	0.034812	53.89	76.16	24.07	HB1	PRO	205
H	-0.001749	52.91	77.45	23.88	HB2	PRO	205
C	0.062282	52.13	75.70	22.99	CA	PRO	205
H	0.101720	51.40	76.24	22.56	HA	PRO	205
C	0.515437	53.02	75.23	21.82	C	PRO	205
O	-0.470991	52.91	75.72	20.70	O	PRO	205
N	-0.585861	53.92	74.28	22.10	N	LEU	206
H	0.294553	53.98	73.90	23.02	H	LEU	206
C	0.189923	54.80	73.78	21.05	CA	LEU	206
H	0.038287	55.13	74.62	20.62	HA	LEU	206
C	-0.188114	55.95	72.98	21.64	CB	LEU	206
H	0.052768	56.51	72.63	20.89	HB1	LEU	206
H	0.007424	55.57	72.21	22.16	HB2	LEU	206
C	0.466516	56.87	73.77	22.59	CG	LEU	206
H	-0.069626	56.37	74.02	23.42	HG	LEU	206

C	-0.389804	58.05	72.89	22.98	CD1	LEU	206
H	0.105967	58.65	73.40	23.60	1HD1	LEU	206
H	0.045883	57.71	72.07	23.44	2HD1	LEU	206
H	0.100260	58.55	72.63	22.16	3HD1	LEU	206
C	-0.657539	57.36	75.05	21.92	CD2	LEU	206
H	0.143484	57.95	75.55	22.55	1HD2	LEU	206
H	0.154725	57.87	74.83	21.09	2HD2	LEU	206
H	0.239326	56.57	75.62	21.69	3HD2	LEU	206
C	0.512211	54.07	72.96	19.98	C	LEU	206
O	-0.509234	54.44	73.01	18.80	O	LEU	206
N	-0.447991	53.04	72.20	20.36	N	GLU	207
H	0.314534	52.78	72.16	21.32	H	GLU	207
C	0.038503	52.31	71.44	19.36	CA	GLU	207
H	-0.000950	52.98	70.90	18.85	HA	GLU	207
C	0.090462	51.30	70.49	19.98	CB	GLU	207
H	0.063833	50.49	71.01	20.25	HB1	GLU	207
H	-0.011191	51.70	70.07	20.79	HB2	GLU	207
C	-0.238008	50.88	69.40	19.01	CG	GLU	207
H	0.095087	51.64	68.76	18.90	HG1	GLU	207
H	0.048028	50.68	69.82	18.12	HG2	GLU	207
C	0.624396	49.66	68.62	19.46	CD	GLU	207
O	-0.389404	49.49	68.40	20.68	OE1	GLU	207
O	-0.397066	48.87	68.20	18.57	OE2	GLU	207
C	0.513886	51.58	72.46	18.49	C	GLU	207
O	-0.601846	51.37	72.25	17.30	O	GLU	207
N	-0.540075	51.17	73.56	19.13	N	ASN	208
H	0.363801	51.33	73.65	20.11	H	ASN	208
C	0.370638	50.49	74.65	18.43	CA	ASN	208
H	-0.103311	49.63	74.27	18.07	HA	ASN	208
C	-0.521614	50.20	75.82	19.38	CB	ASN	208
H	0.157436	50.12	76.66	18.84	HB1	ASN	208
H	0.244858	50.96	75.91	20.02	HB2	ASN	208
C	0.880679	48.92	75.65	20.17	CG	ASN	208
O	-0.635108	48.66	76.42	21.09	OD1	ASN	208
N	-1.002065	48.12	74.65	19.83	ND2	ASN	208
H	0.470572	48.37	74.05	19.07	1HD2	ASN	208
H	0.384822	47.26	74.50	20.32	2HD2	ASN	208
C	0.560131	51.41	75.15	17.33	C	ASN	208
O	-0.679363	50.99	75.40	16.20	O	ASN	208
N	-0.419431	52.69	75.32	17.66	N	LEU	209
H	0.332560	52.99	75.10	18.59	H	LEU	209
C	0.100430	53.65	75.81	16.69	CA	LEU	209
H	0.038550	53.25	76.64	16.31	HA	LEU	209
C	-0.202731	54.98	76.13	17.37	CB	LEU	209
H	0.063351	55.31	75.28	17.79	HB1	LEU	209
H	0.109974	54.80	76.81	18.09	HB2	LEU	209

C	0.386462	56.08	76.67	16.47	CG	LEU	209
H	-0.073297	56.31	76.01	15.76	HG	LEU	209
C	-0.257601	55.60	77.94	15.79	CD1	LEU	209
H	0.018680	56.33	78.30	15.20	1HD1	LEU	209
H	0.022049	54.80	77.74	15.23	2HD1	LEU	209
H	0.077142	55.37	78.63	16.47	3HD1	LEU	209
C	-0.425467	57.32	76.94	17.31	CD2	LEU	209
H	0.065766	58.04	77.30	16.72	1HD2	LEU	209
H	0.131124	57.10	77.61	18.02	2HD2	LEU	209
H	0.077039	57.62	76.09	17.73	3HD2	LEU	209
C	0.536615	53.87	74.79	15.58	C	LEU	209
O	-0.622113	53.95	75.14	14.40	O	LEU	209
N	-0.548795	53.96	73.53	15.97	N	ALA	210
H	0.332893	53.89	73.31	16.94	H	ALA	210
C	0.407930	54.16	72.45	15.01	CA	ALA	210
H	-0.040087	55.01	72.66	14.52	HA	ALA	210
C	-0.330246	54.29	71.13	15.74	CB	ALA	210
H	0.038384	54.42	70.39	15.07	HB1	ALA	210
H	0.085142	55.07	71.16	16.36	HB2	ALA	210
H	0.106494	53.45	70.95	16.26	HB3	ALA	210
C	0.462027	52.99	72.40	14.02	C	ALA	210
O	-0.549290	53.19	72.27	12.81	O	ALA	210
N	-0.445091	51.77	72.52	14.54	N	ASH	211
H	0.366460	51.66	72.63	15.53	H	ASH	211
C	0.110417	50.61	72.47	13.68	CA	ASH	211
H	0.068586	50.72	71.63	13.15	HA	ASH	211
C	-0.303079	49.32	72.42	14.50	CB	ASH	211
H	0.104214	48.54	72.60	13.90	HB1	ASH	211
H	0.137272	49.36	73.12	15.21	HB2	ASH	211
C	0.693442	49.11	71.06	15.17	CG	ASH	211
O	-0.578660	49.53	70.04	14.58	OD1	ASH	211
O	-0.526131	48.51	71.01	16.27	OD2	ASH	211
H	0.417930	48.45	70.06	16.58	HD2	ASH	211
C	0.532823	50.59	73.66	12.73	C	ASH	211
O	-0.640047	50.32	73.50	11.55	O	ASH	211
N	-0.569739	50.90	74.85	13.25	N	HIS	212
H	0.358225	51.13	74.91	14.22	H	HIS	212
C	0.386145	50.91	76.05	12.43	CA	HIS	212
H	-0.010365	49.99	76.16	12.08	HA	HIS	212
C	-0.268258	51.30	77.27	13.28	CB	HIS	212
H	0.099945	52.22	77.12	13.65	HB1	HIS	212
H	0.155639	50.65	77.36	14.04	HB2	HIS	212
C	-0.068068	51.32	78.56	12.53	CG	HIS	212
N	-0.440367	50.23	79.03	11.82	ND1	HIS	212
H	0.414292	49.36	78.55	11.71	HD1	HIS	212
C	0.442048	50.52	80.21	11.29	CE1	HIS	212

H	0.026965	49.91	80.76	10.73	HE1	HIS	212
N	-0.875656	51.75	80.53	11.64	NE2	HIS	212
C	0.314038	52.28	79.51	12.41	CD2	HIS	212
H	0.062461	53.19	79.49	12.81	HD2	HIS	212
C	0.539673	51.90	75.88	11.28	C	HIS	212
O	-0.513173	51.56	76.11	10.13	O	HIS	212
N	-0.737523	53.12	75.46	11.61	N	LEU	213
H	0.409870	53.34	75.28	12.57	H	LEU	213
C	0.580960	54.14	75.26	10.58	CA	LEU	213
H	0.027294	54.21	76.14	10.11	HA	LEU	213
C	-0.742793	55.48	74.90	11.23	CB	LEU	213
H	0.190868	56.12	74.64	10.51	HB1	LEU	213
H	0.183944	55.32	74.11	11.83	HB2	LEU	213
C	0.622994	56.13	76.01	12.07	CG	LEU	213
H	-0.080769	55.45	76.38	12.71	HG	LEU	213
C	-0.324708	57.28	75.44	12.88	CD1	LEU	213
H	0.051200	57.70	76.18	13.42	1HD1	LEU	213
H	0.068455	56.94	74.73	13.49	2HD1	LEU	213
H	0.059905	57.96	75.05	12.26	3HD1	LEU	213
C	-0.480979	56.62	77.14	11.16	CD2	LEU	213
H	0.091813	57.04	77.85	11.71	1HD2	LEU	213
H	0.089619	57.29	76.77	10.51	2HD2	LEU	213
H	0.115908	55.84	77.51	10.65	3HD2	LEU	213
C	0.104404	53.74	74.19	9.56	C	LEU	213
O	-0.323866	54.17	74.23	8.42	O	LEU	213
N	-0.710201	46.14	76.23	9.55	N	ASN	219
H	0.350573	46.96	76.25	8.98	H	ASN	219
C	0.483823	46.23	76.02	10.97	CA	ASN	219
H	-0.014393	45.30	75.77	11.24	HA	ASN	219
C	-0.478155	47.22	74.90	11.28	CB	ASN	219
H	0.072502	47.19	74.71	12.27	HB1	ASN	219
H	0.126337	48.14	75.20	11.03	HB2	ASN	219
C	0.905784	46.90	73.62	10.53	CG	ASN	219
O	-0.583320	45.76	73.36	10.18	OD1	ASN	219
N	-1.064643	47.93	72.81	10.30	ND2	ASN	219
H	0.494666	48.84	73.05	10.62	1HD2	ASN	219
H	0.414350	47.78	71.95	9.81	2HD2	ASN	219
C	0.482364	46.62	77.28	11.72	C	ASN	219
O	-0.531495	47.80	77.52	11.97	O	ASN	219
N	-0.587830	45.63	78.10	12.04	N	ASN	220
H	0.341231	44.70	77.87	11.76	H	ASN	220
C	0.254115	45.86	79.31	12.81	CA	ASN	220
H	0.060214	46.61	79.13	13.44	HA	ASN	220
C	-0.326743	46.28	80.49	11.92	CB	ASN	220
H	0.076790	47.15	80.27	11.47	HB1	ASN	220
H	0.112953	46.40	81.31	12.48	HB2	ASN	220

C	0.734711	45.27	80.80	10.85	CG	ASN	220
O	-0.555688	44.11	81.08	11.14	OD1	ASN	220
N	-0.980707	45.72	80.76	9.59	ND2	ASN	220
H	0.416213	46.67	80.53	9.41	1HD2	ASN	220
H	0.413206	45.09	80.96	8.84	2HD2	ASN	220
C	0.512317	44.58	79.63	13.57	C	ASN	220
O	-0.477646	43.59	78.91	13.44	O	ASN	220
N	-0.708790	44.59	80.69	14.36	N	ALA	221
H	0.405896	45.41	81.26	14.41	H	ALA	221
C	0.590745	43.44	81.04	15.17	CA	ALA	221
H	0.016899	43.38	80.27	15.80	HA	ALA	221
C	-0.638400	43.68	82.36	15.89	CB	ALA	221
H	0.167692	42.88	82.59	16.45	HB1	ALA	221
H	0.152061	44.48	82.27	16.49	HB2	ALA	221
H	0.167614	43.85	83.08	15.22	HB3	ALA	221
C	0.101252	42.10	81.09	14.45	C	ALA	221
O	-0.361214	41.09	80.69	15.03	O	ALA	221
N	-0.517379	39.35	78.40	14.84	N	PHE	224
H	0.411689	39.97	79.19	14.84	H	PHE	224
C	0.077480	38.49	78.17	15.99	CA	PHE	224
H	0.084269	38.00	77.32	15.77	HA	PHE	224
C	-0.243187	39.31	78.01	17.27	CB	PHE	224
H	0.087913	38.73	77.66	17.99	HB1	PHE	224
H	0.090179	39.66	78.91	17.53	HB2	PHE	224
C	0.284268	40.49	77.09	17.13	CG	PHE	224
C	-0.193293	41.68	77.53	16.56	CD1	PHE	224
H	0.132498	41.76	78.48	16.25	HD1	PHE	224
C	-0.065278	42.77	76.67	16.42	CE1	PHE	224
H	0.134134	43.63	77.01	16.02	HE1	PHE	224
C	-0.190620	42.67	75.35	16.84	CZ	PHE	224
H	0.125289	43.45	74.73	16.74	HZ	PHE	224
C	-0.090476	41.48	74.90	17.40	CE2	PHE	224
H	0.134519	41.41	73.95	17.71	HE2	PHE	224
C	-0.202361	40.40	75.76	17.54	CD2	PHE	224
H	0.156496	39.55	75.43	17.95	HD2	PHE	224
C	0.803272	37.49	79.31	16.19	C	PHE	224
O	-0.487555	37.39	80.01	15.49	OC1	PHE	224
O	-0.531856	36.80	79.37	17.21	OC2	PHE	224
C	0.347900	70.83	96.64	15.61	C1	BNG	5633
C	0.095100	70.05	97.93	15.93	C2	BNG	5633
C	0.107100	71.00	98.94	16.61	C3	BNG	5633
C	0.086100	71.66	98.31	17.85	C4	BNG	5633
C	0.115100	72.36	96.99	17.45	C5	BNG	5633
C	0.125400	72.95	96.24	18.64	C6	BNG	5633
C	0.129400	69.13	94.90	15.87	C1	BNG	5633
C	-0.084400	68.20	93.99	15.10	C2	BNG	5633

C	-0.078400	67.56	92.98	16.03	C3	BNG	5633
C	-0.078400	66.12	92.71	15.66	C4	BNG	5633
C	-0.079400	65.35	92.16	16.85	C5	BNG	5633
C	-0.079400	64.85	90.75	16.57	C6	BNG	5633
C	-0.078400	63.63	90.41	17.40	C7	BNG	5633
C	-0.079400	62.48	89.96	16.50	C8	BNG	5633
C	-0.092100	62.18	88.48	16.65	C9	BNG	5633
O	-0.392600	69.99	95.68	15.02	O1	BNG	5633
O	-0.583800	69.53	98.50	14.74	O2	BNG	5633
O	-0.608800	70.27	100.10	17.00	O3	BNG	5633
O	-0.610800	72.62	99.22	18.39	O4	BNG	5633
O	-0.444600	71.42	96.09	16.81	O5	BNG	5633
O	-0.615800	74.18	96.81	19.06	O6	BNG	5633
H	0.091700	71.56	96.79	14.94	H1	BNG	5633
H	0.062700	69.24	97.75	16.50	H2	BNG	5633
H	0.064700	71.69	99.26	15.97	H3	BNG	5633
H	0.057700	71.00	98.16	18.58	H4	BNG	5633
H	0.070700	73.09	97.22	16.81	H5	BNG	5633
H	0.046200	73.13	95.29	18.40	H61	BNG	5633
H	0.046200	72.32	96.28	19.42	H62	BNG	5633
H	0.038200	69.71	94.35	16.48	1H1	BNG	5633
H	0.038200	68.59	95.54	16.42	2H1	BNG	5633
H	0.056200	68.73	93.51	14.39	1H2	BNG	5633
H	0.056200	67.49	94.54	14.66	2H2	BNG	5633
H	0.039700	67.60	93.33	16.96	1H3	BNG	5633
H	0.039700	68.08	92.12	15.97	2H3	BNG	5633
H	0.041700	66.09	92.04	14.91	1H4	BNG	5633
H	0.041700	65.70	93.56	15.36	2H4	BNG	5633
H	0.039200	64.57	92.75	17.03	1H5	BNG	5633
H	0.039200	65.95	92.14	17.65	2H5	BNG	5633
H	0.040200	65.57	90.10	16.78	1H6	BNG	5633
H	0.040200	64.61	90.68	15.60	2H6	BNG	5633
H	0.038700	63.35	91.21	17.92	1H7	BNG	5633
H	0.038700	63.86	89.67	18.03	2H7	BNG	5633
H	0.038200	62.73	90.14	15.55	1H8	BNG	5633
H	0.038200	61.67	90.48	16.74	2H8	BNG	5633
H	0.032370	61.20	88.34	16.60	1H9	BNG	5633
H	0.032370	62.63	87.97	15.92	2H9	BNG	5633
H	0.032370	62.52	88.16	17.54	3H9	BNG	5633
H	0.423000	68.91	97.84	14.30	H22	BNG	5633
H	0.428000	69.84	100.51	16.19	H32	BNG	5633
H	0.433000	72.16	100.07	18.65	H42	BNG	5633
H	0.415000	74.54	96.30	19.84	H63	BNG	5633
C	0.815510	55.95	80.37	20.78	C1	LUT	5620
C	-0.471741	54.90	79.41	20.19	C2	LUT	5620
C	0.040331	53.42	79.69	20.44	C3	LUT	5620

C	0.105178	53.12	80.60	21.63	C4	LUT	5620
C	0.602543	54.10	81.66	22.00	C5	LUT	5620
C	-0.048599	55.43	81.58	21.61	C6	LUT	5620
C	-0.535350	56.40	82.63	21.97	C7	LUT	5620
C	0.117818	56.99	82.79	23.18	C8	LUT	5620
C	0.135238	57.87	83.89	23.58	C9	LUT	5620
C	0.464246	58.44	83.82	24.80	C10	LUT	5620
C	-0.700900	59.35	84.77	25.39	C11	LUT	5620
C	0.059428	59.98	84.47	26.53	C12	LUT	5620
C	0.130150	60.96	85.25	27.28	C13	LUT	5620
C	-0.318989	61.53	84.66	28.35	C14	LUT	5620
C	0.164090	62.58	85.17	29.19	C15	LUT	5620
C	0.252948	56.83	80.85	19.60	C16	LUT	5620
C	-0.390205	56.81	79.46	21.67	C17	LUT	5620
C	0.174179	53.40	82.72	22.79	C18	LUT	5620
C	0.066555	58.10	85.01	22.59	C19	LUT	5620
C	0.108737	61.33	86.60	26.76	C20	LUT	5620
O	-0.382551	52.71	78.47	20.56	O3	LUT	5620
C	0.177063	72.83	86.66	36.72	C21	LUT	5620
C	0.293258	73.98	87.44	37.39	C22	LUT	5620
C	-0.376104	73.74	87.80	38.86	C23	LUT	5620
C	0.159635	72.31	88.27	39.11	C24	LUT	5620
C	-0.045027	71.29	88.03	38.26	C25	LUT	5620
C	0.129233	71.41	87.28	36.94	C26	LUT	5620
C	-0.409277	70.24	86.32	36.80	C27	LUT	5620
C	0.067767	69.38	86.35	35.75	C28	LUT	5620
C	0.090271	68.32	85.39	35.43	C29	LUT	5620
C	0.101005	67.58	85.61	34.33	C30	LUT	5620
C	-0.310158	66.54	84.77	33.82	C31	LUT	5620
C	0.046405	65.83	85.11	32.72	C32	LUT	5620
C	0.080772	64.73	84.39	32.08	C33	LUT	5620
C	0.055829	64.15	84.96	31.00	C34	LUT	5620
C	-0.417257	63.06	84.46	30.21	C35	LUT	5620
C	0.111255	72.87	85.20	37.26	C36	LUT	5620
C	0.117979	73.13	86.61	35.22	C37	LUT	5620
C	0.113858	69.98	88.60	38.69	C38	LUT	5620
C	-0.309136	68.13	84.21	36.36	C39	LUT	5620
C	0.077081	64.32	83.07	32.67	C40	LUT	5620
O	0.097024	74.68	88.78	39.29	O23	LUT	5620
H	0.101630	55.42	79.85	19.45	H21	LUT	5620
H	-0.320606	55.33	78.54	20.43	H22	LUT	5620
H	0.085263	53.07	80.14	19.62	H3	LUT	5620
H	0.099341	52.25	81.06	21.45	H41	LUT	5620
H	0.103581	53.02	80.02	22.44	H42	LUT	5620
H	-0.677433	56.64	83.28	21.26	H7	LUT	5620
H	0.378201	56.81	82.09	23.86	H8	LUT	5620

H	0.305849	58.22	83.02	25.36	H10	LUT	5620
H	-0.174659	59.50	85.66	24.94	H11	LUT	5620
H	0.079653	59.74	83.59	26.93	H12	LUT	5620
H	0.050933	61.18	83.75	28.59	H14	LUT	5620
H	0.502133	62.95	86.08	29.01	H15	LUT	5620
H	-0.037253	57.52	81.48	19.94	1H16	LUT	5620
H	-0.482636	57.27	80.07	19.17	2H16	LUT	5620
H	0.169329	56.25	81.32	18.93	3H16	LUT	5620
H	0.206914	57.53	80.00	22.10	1H17	LUT	5620
H	-0.331135	56.23	79.04	22.37	2H17	LUT	5620
H	0.141044	57.22	78.74	21.11	3H17	LUT	5620
H	0.221112	52.44	82.47	22.90	1H18	LUT	5620
H	0.063455	53.83	82.79	23.69	2H18	LUT	5620
H	-0.466037	53.47	83.59	22.31	3H18	LUT	5620
H	0.165420	57.57	84.84	21.77	1H19	LUT	5620
H	0.287084	57.83	85.88	23.00	2H19	LUT	5620
H	-0.334675	59.08	85.05	22.36	3H19	LUT	5620
H	0.167713	60.77	86.82	25.96	1H20	LUT	5620
H	-0.012535	61.17	87.29	27.47	2H20	LUT	5620
H	0.127030	62.30	86.61	26.51	3H20	LUT	5620
H	-0.338222	51.74	78.67	20.73	H5	LUT	5620
H	0.164369	74.13	88.29	36.88	1H22	LUT	5620
H	0.288503	74.81	86.88	37.34	2H22	LUT	5620
H	-0.363234	73.93	87.00	39.43	H23	LUT	5620
H	0.152035	72.12	88.78	39.95	H24	LUT	5620
H	-0.070268	71.31	87.93	36.19	H26	LUT	5620
H	0.136632	70.10	85.64	37.51	H27	LUT	5620
H	-0.311260	69.49	87.12	35.12	H28	LUT	5620
H	0.064038	67.78	86.44	33.81	H30	LUT	5620
H	0.088988	66.33	83.90	34.28	H31	LUT	5620
H	0.051876	66.09	85.98	32.30	H32	LUT	5620
H	-0.353107	64.52	85.85	30.72	H34	LUT	5620
H	0.090642	62.67	83.57	30.43	H35	LUT	5620
H	0.071415	72.13	84.66	36.84	1H36	LUT	5620
H	0.093345	73.75	84.78	37.02	2H36	LUT	5620
H	-0.299399	72.77	85.20	38.25	3H36	LUT	5620
H	0.100882	72.40	86.11	34.75	1H37	LUT	5620
H	0.084558	73.18	87.54	34.86	2H37	LUT	5620
H	0.061608	74.00	86.14	35.07	3H37	LUT	5620
H	-0.333872	70.10	89.06	39.58	1H38	LUT	5620
H	0.086513	69.67	89.26	38.01	2H38	LUT	5620
H	0.103858	69.31	87.87	38.78	3H38	LUT	5620
H	0.097753	68.79	84.26	37.11	1H39	LUT	5620
H	-0.337608	67.20	84.24	36.74	2H39	LUT	5620
H	0.090790	68.26	83.36	35.86	3H39	LUT	5620
H	0.109312	64.90	82.86	33.45	1H40	LUT	5620

H	0.103139	63.36	83.13	32.96	2H40	LUT	5620
H	-0.686816	64.41	82.35	31.98	3H40	LUT	5620
H	0.394721	74.51	89.00	40.25	H33	LUT	5620
C	0.815510	52.85	76.78	36.24	C1	LUT	5621
C	-0.471741	52.83	75.27	36.00	C2	LUT	5621
C	0.040331	53.91	74.60	35.15	C3	LUT	5621
C	0.105178	55.00	75.54	34.61	C4	LUT	5621
C	0.602543	55.10	76.96	35.06	C5	LUT	5621
C	-0.048599	54.12	77.59	35.82	C6	LUT	5621
C	-0.535350	54.18	79.00	36.28	C7	LUT	5621
C	0.117818	53.87	80.08	35.52	C8	LUT	5621
C	0.135238	53.93	81.51	35.87	C9	LUT	5621
C	0.464246	53.44	82.40	34.97	C10	LUT	5621
C	-0.700900	53.32	83.82	35.13	C11	LUT	5621
C	0.059428	52.72	84.61	34.21	C12	LUT	5621
C	0.130150	52.44	86.07	34.29	C13	LUT	5621
C	-0.318989	51.78	86.65	33.26	C14	LUT	5621
C	0.164090	51.35	88.02	33.16	C15	LUT	5621
C	0.252948	52.56	76.98	37.74	C16	LUT	5621
C	-0.390205	51.62	77.30	35.45	C17	LUT	5621
C	0.174179	56.38	77.53	34.57	C18	LUT	5621
C	0.066555	54.44	81.88	37.23	C19	LUT	5621
C	0.108737	52.86	86.80	35.53	C20	LUT	5621
O	-0.382551	53.33	73.85	34.09	O3	LUT	5621
C	0.177063	46.54	99.60	29.99	C21	LUT	5621
C	0.293258	46.27	101.11	30.16	C22	LUT	5621
C	-0.376104	47.22	102.04	29.39	C23	LUT	5621
C	0.159635	48.68	101.55	29.38	C24	LUT	5621
C	-0.045027	49.01	100.29	29.74	C25	LUT	5621
C	0.129233	48.03	99.20	30.20	C26	LUT	5621
C	-0.409277	48.40	97.85	29.60	C27	LUT	5621
C	0.067767	48.60	96.71	30.31	C28	LUT	5621
C	0.090271	48.75	95.35	29.77	C29	LUT	5621
C	0.101005	48.98	94.34	30.64	C30	LUT	5621
C	-0.310158	49.16	92.94	30.30	C31	LUT	5621
C	0.046405	49.57	92.02	31.20	C32	LUT	5621
C	0.080772	49.84	90.59	31.00	C33	LUT	5621
C	0.055829	50.36	89.91	32.04	C34	LUT	5621
C	-0.417257	50.75	88.52	32.07	C35	LUT	5621
C	0.111255	46.04	99.21	28.57	C36	LUT	5621
C	0.117979	45.66	98.84	31.00	C37	LUT	5621
C	0.113858	50.47	100.03	29.67	C38	LUT	5621
C	-0.309136	48.71	95.17	28.29	C39	LUT	5621
C	0.077081	49.60	90.02	29.64	C40	LUT	5621
O	0.097024	47.14	103.36	29.90	O23	LUT	5621
H	0.101630	52.80	75.19	37.00	H21	LUT	5621

H	-0.320606	51.91	75.45	35.65	H22	LUT	5621
H	0.085263	54.37	73.94	35.74	H3	LUT	5621
H	0.099341	55.88	75.13	34.83	H41	LUT	5621
H	0.103581	54.89	75.58	33.62	H42	LUT	5621
H	-0.677433	54.46	79.17	37.23	H7	LUT	5621
H	0.378201	53.56	79.88	34.59	H8	LUT	5621
H	0.305849	53.14	82.02	34.09	H10	LUT	5621
H	-0.174659	53.69	84.25	35.96	H11	LUT	5621
H	0.079653	52.43	84.15	33.36	H12	LUT	5621
H	0.050933	51.57	86.06	32.48	H14	LUT	5621
H	0.502133	51.51	88.63	33.93	H15	LUT	5621
H	-0.037253	52.56	77.95	37.96	1H16	LUT	5621
H	-0.482636	51.66	76.59	37.96	2H16	LUT	5621
H	0.169329	53.26	76.51	38.28	3H16	LUT	5621
H	0.206914	51.55	78.29	35.55	1H17	LUT	5621
H	-0.331135	51.73	77.06	34.48	2H17	LUT	5621
H	0.141044	50.79	76.87	35.81	3H17	LUT	5621
H	0.221112	56.87	76.84	34.05	1H18	LUT	5621
H	0.063455	56.19	78.32	33.98	2H18	LUT	5621
H	-0.466037	56.94	77.83	35.35	3H18	LUT	5621
H	0.165420	54.74	81.06	37.70	1H19	LUT	5621
H	0.287084	55.21	82.51	37.13	2H19	LUT	5621
H	-0.334675	53.71	82.32	37.75	3H19	LUT	5621
H	0.167713	53.32	86.17	36.15	1H20	LUT	5621
H	-0.012535	53.48	87.54	35.28	2H20	LUT	5621
H	0.127030	52.05	87.18	35.99	3H20	LUT	5621
H	-0.338222	54.05	73.43	33.55	H5	LUT	5621
H	0.164369	46.35	101.34	31.13	1H22	LUT	5621
H	0.288503	45.34	101.30	29.85	2H22	LUT	5621
H	-0.363234	46.90	102.10	28.44	H23	LUT	5621
H	0.152035	49.40	102.18	29.10	H24	LUT	5621
H	-0.070268	48.15	99.10	31.18	H26	LUT	5621
H	0.136632	48.51	97.79	28.61	H27	LUT	5621
H	-0.311260	48.64	96.80	31.30	H28	LUT	5621
H	0.064038	49.04	94.57	31.61	H30	LUT	5621
H	0.088988	48.97	92.65	29.36	H31	LUT	5621
H	0.051876	49.71	92.36	32.13	H32	LUT	5621
H	-0.353107	50.48	90.42	32.89	H34	LUT	5621
H	0.090642	50.58	87.94	31.28	H35	LUT	5621
H	0.071415	46.20	98.23	28.42	1H36	LUT	5621
H	0.093345	45.07	99.41	28.49	2H36	LUT	5621
H	-0.299399	46.55	99.74	27.89	3H36	LUT	5621
H	0.100882	45.82	97.86	30.91	1H37	LUT	5621
H	0.084558	45.89	99.13	31.93	2H37	LUT	5621
H	0.061608	44.70	99.04	30.83	3H37	LUT	5621
H	-0.333872	50.94	100.85	29.35	1H38	LUT	5621

H	0.086513	50.81	99.78	30.58	2H38	LUT	5621
H	0.103858	50.65	99.28	29.03	3H38	LUT	5621
H	0.097753	48.53	96.06	27.85	1H39	LUT	5621
H	-0.337608	49.60	94.82	27.97	2H39	LUT	5621
H	0.090790	47.99	94.53	28.05	3H39	LUT	5621
H	0.109312	49.22	90.72	29.04	1H40	LUT	5621
H	0.103139	50.47	89.69	29.25	2H40	LUT	5621
H	-0.686816	48.96	89.25	29.70	3H40	LUT	5621
H	0.394721	47.76	103.95	29.39	H33	LUT	5621
C	0.000200	68.39	81.10	61.70	C1	NEX	5623
C	-0.105400	67.66	82.05	62.67	C2	NEX	5623
C	0.137100	68.20	83.47	62.88	C3	NEX	5623
C	-0.138400	68.51	84.15	61.53	C4	NEX	5623
C	0.210000	69.33	83.34	60.51	C5	NEX	5623
C	-0.160500	68.69	81.91	60.38	C6	NEX	5623
C	-0.147100	67.84	80.94	57.92	C8	NEX	5623
C	-0.059200	66.45	81.01	57.42	C9	NEX	5623
C	-0.133000	66.21	80.55	56.18	C10	NEX	5623
C	-0.129000	65.03	80.75	55.39	C11	NEX	5623
C	-0.121000	64.92	80.26	54.14	C12	NEX	5623
C	-0.068200	63.82	80.41	53.22	C13	NEX	5623
C	-0.126000	63.98	79.87	51.99	C14	NEX	5623
C	-0.125000	63.08	79.96	50.88	C15	NEX	5623
C	-0.088600	67.48	79.88	61.47	C16	NEX	5623
C	-0.088600	69.70	80.60	62.32	C17	NEX	5623
C	-0.086100	69.36	84.11	59.18	C18	NEX	5623
C	-0.063900	65.47	81.85	58.20	C19	NEX	5623
C	-0.061900	62.63	81.20	53.66	C20	NEX	5623
O	-0.591800	67.23	84.25	63.57	O3	NEX	5623
O	-0.590800	70.67	83.23	60.98	O4	NEX	5623
C	-0.025000	62.87	76.47	39.41	C21	NEX	5623
C	-0.071400	62.88	75.37	38.33	C22	NEX	5623
C	0.141100	62.49	73.96	38.75	C23	NEX	5623
C	-0.101400	61.16	73.83	39.49	C24	NEX	5623
C	0.096800	60.90	74.94	40.48	C25	NEX	5623
C	0.123000	61.70	76.24	40.47	C26	NEX	5623
C	-0.158200	61.07	77.48	41.04	C27	NEX	5623
C	-0.108000	61.20	78.02	42.26	C28	NEX	5623
C	-0.075200	60.46	79.18	42.83	C29	NEX	5623
C	-0.123000	60.73	79.57	44.10	C30	NEX	5623
C	-0.127000	61.71	79.03	45.00	C31	NEX	5623
C	-0.124000	61.77	79.45	46.28	C32	NEX	5623
C	-0.064200	62.74	79.08	47.32	C33	NEX	5623
C	-0.131000	62.56	79.59	48.56	C34	NEX	5623
C	-0.120000	63.39	79.39	49.71	C35	NEX	5623
C	-0.087100	62.72	77.82	38.69	C36	NEX	5623

C	-0.087100	64.21	76.44	40.14	C37	NEX	5623
C	-0.086100	59.51	74.86	41.06	C38	NEX	5623
C	-0.062900	59.43	79.84	41.98	C39	NEX	5623
C	-0.063900	63.86	78.16	46.94	C40	NEX	5623
O	-0.599800	62.49	73.08	37.63	O23	NEX	5623
O	-0.403600	61.95	75.18	41.42	O24	NEX	5623
H	0.052700	66.72	82.14	62.34	H21	NEX	5623
H	0.052700	67.65	81.61	63.57	H22	NEX	5623
H	0.074700	69.01	83.45	63.46	H3	NEX	5623
H	0.062200	67.63	84.38	61.09	H41	NEX	5623
H	0.062200	69.01	85.00	61.72	H42	NEX	5623
H	0.143000	68.51	80.52	57.32	H8	NEX	5623
H	0.124000	66.93	80.00	55.76	H10	NEX	5623
H	0.127000	64.26	81.27	55.78	H11	NEX	5623
H	0.123000	65.70	79.73	53.81	H12	NEX	5623
H	0.122000	64.81	79.35	51.84	H14	NEX	5623
H	0.125000	62.21	80.44	50.98	H15	NEX	5623
H	0.040030	67.93	79.25	60.84	1H16	NEX	5623
H	0.040030	67.31	79.43	62.34	2H16	NEX	5623
H	0.040030	66.61	80.19	61.08	3H16	NEX	5623
H	0.040030	70.16	79.99	61.68	1H17	NEX	5623
H	0.040030	70.29	81.38	62.53	2H17	NEX	5623
H	0.040030	69.50	80.10	63.17	3H17	NEX	5623
H	0.049030	69.78	85.01	59.32	1H18	NEX	5623
H	0.049030	69.89	83.60	58.51	2H18	NEX	5623
H	0.049030	68.42	84.23	58.84	3H18	NEX	5623
H	0.046370	65.87	82.08	59.09	1H19	NEX	5623
H	0.046370	65.28	82.70	57.70	2H19	NEX	5623
H	0.046370	64.62	81.34	58.33	3H19	NEX	5623
H	0.045030	62.75	81.49	54.61	1H20	NEX	5623
H	0.045030	62.52	82.00	53.08	2H20	NEX	5623
H	0.045030	61.81	80.62	53.60	3H20	NEX	5623
H	0.397000	67.02	83.81	64.45	H5	NEX	5623
H	0.401000	71.07	84.14	61.06	H4	NEX	5623
H	0.058700	63.80	75.33	37.95	1H22	NEX	5623
H	0.058700	62.24	75.65	37.61	2H22	NEX	5623
H	0.050700	63.21	73.64	39.36	H23	NEX	5623
H	0.060200	61.16	72.97	40.00	1H24	NEX	5623
H	0.060200	60.42	73.83	38.82	2H24	NEX	5623
H	0.135000	60.46	77.98	40.42	H27	NEX	5623
H	0.141000	61.88	77.59	42.86	H28	NEX	5623
H	0.123000	60.17	80.32	44.45	H30	NEX	5623
H	0.131000	62.36	78.35	44.68	H31	NEX	5623
H	0.122000	61.06	80.10	46.56	H32	NEX	5623
H	0.121000	61.76	80.17	48.69	H34	NEX	5623
H	0.126000	64.21	78.82	49.63	H35	NEX	5623

H	0.041530	62.71	78.56	39.37	1H36	NEX	5623
H	0.041530	63.49	77.95	38.07	2H36	NEX	5623
H	0.041530	61.87	77.84	38.18	3H36	NEX	5623
H	0.041530	64.23	77.14	40.85	1H37	NEX	5623
H	0.041530	64.35	75.54	40.56	2H37	NEX	5623
H	0.041530	64.95	76.61	39.48	3H37	NEX	5623
H	0.051370	59.16	73.92	40.96	1H38	NEX	5623
H	0.051370	59.54	75.10	42.03	2H38	NEX	5623
H	0.051370	58.91	75.49	40.58	3H38	NEX	5623
H	0.044030	59.40	79.39	41.09	1H39	NEX	5623
H	0.044030	58.54	79.76	42.42	2H39	NEX	5623
H	0.044030	59.67	80.80	41.87	3H39	NEX	5623
H	0.046700	63.78	77.92	45.97	1H40	NEX	5623
H	0.046700	64.73	78.62	47.10	2H40	NEX	5623
H	0.046700	63.82	77.33	47.50	3H40	NEX	5623
H	0.400000	62.24	72.16	37.93	H6	NEX	5623
C	0.004200	68.27	81.42	59.14	C7	NEX	5623
O	-0.870600	62.35	100.48	15.26	O1	LHG	5630
C	0.291800	63.27	99.71	16.02	C1	LHG	5630
C	0.191200	63.53	100.39	17.36	C2	LHG	5630
O	-0.876600	64.79	101.02	17.33	O2	LHG	5630
C	0.281800	63.48	99.38	18.50	C3	LHG	5630
O	-0.396400	62.26	98.70	18.43	O3	LHG	5630
P	0.657000	61.88	97.93	19.78	P	LHG	5630
O	-0.552600	61.74	98.91	20.90	O5	LHG	5630
O	-0.402400	60.52	97.11	19.53	O6	LHG	5630
C	0.337800	59.87	96.81	20.71	C4	LHG	5630
C	0.244200	58.91	95.66	20.42	C5	LHG	5630
C	0.257800	58.87	94.65	21.56	C6	LHG	5630
O	-0.593800	57.55	96.15	20.25	O7	LHG	5630
C	0.965200	56.76	95.52	19.19	C7	LHG	5630
O	-0.740000	57.08	94.46	18.66	O9	LHG	5630
C	-0.099800	55.48	96.19	18.69	C8	LHG	5630
C	-0.006800	54.24	95.55	19.29	C9	LHG	5630
C	0.002200	53.01	95.74	18.40	C10	LHG	5630
O	-0.593800	59.63	94.88	22.78	O8	LHG	5630
C	0.961200	58.87	95.08	23.99	C23	LHG	5630
O	-0.678000	58.94	96.13	24.63	O10	LHG	5630
C	-0.137800	57.98	94.03	24.65	C24	LHG	5630
C	0.000200	52.21	94.44	18.27	C11	LHG	5630
C	-0.003800	50.86	94.54	18.97	C12	LHG	5630
C	-0.001800	49.89	93.47	18.50	C13	LHG	5630
C	-0.000800	48.72	93.34	19.47	C14	LHG	5630
C	-0.000800	47.53	92.65	18.83	C15	LHG	5630
C	0.001200	46.96	91.55	19.73	C16	LHG	5630
C	0.000200	45.54	91.85	20.22	C17	LHG	5630

C	-0.000800	44.49	91.10	19.40	C18	LHG	5630
C	-0.000800	43.32	90.65	20.26	C19	LHG	5630
C	0.000200	42.45	89.65	19.51	C20	LHG	5630
C	-0.000800	41.55	88.83	20.44	C21	LHG	5630
C	0.025800	41.77	87.33	20.28	C22	LHG	5630
C	0.000200	54.79	92.92	22.46	C27	LHG	5630
C	-0.002800	55.02	92.56	21.00	C28	LHG	5630
C	0.001200	55.23	91.08	20.80	C29	LHG	5630
C	-0.002800	54.53	90.57	19.56	C30	LHG	5630
C	-0.004800	55.41	90.69	18.32	C31	LHG	5630
C	0.002200	54.65	91.40	17.21	C32	LHG	5630
C	-0.008800	55.55	92.35	16.44	C33	LHG	5630
C	0.002200	54.95	92.71	15.10	C34	LHG	5630
C	0.000200	55.45	91.79	14.00	C35	LHG	5630
C	-0.000800	56.53	92.45	13.16	C36	LHG	5630
C	-0.001800	57.67	91.48	12.89	C37	LHG	5630
C	0.025800	58.97	92.22	12.67	C38	LHG	5630
H	0.613000	62.19	100.03	14.38	H1	LHG	5630
H	0.021400	62.88	98.80	16.14	H11	LHG	5630
H	0.021400	64.12	99.64	15.49	H12	LHG	5630
H	0.019400	62.86	101.11	17.51	H2	LHG	5630
H	0.611000	64.96	101.46	18.21	H4	LHG	5630
H	0.029900	64.22	98.71	18.43	H31	LHG	5630
H	0.029900	63.54	99.84	19.39	H32	LHG	5630
H	0.039900	60.03	96.06	21.36	H41	LHG	5630
H	0.039900	58.93	97.13	20.79	H42	LHG	5630
H	0.060400	59.21	95.24	19.57	H5	LHG	5630
H	0.023900	57.92	94.56	21.85	H61	LHG	5630
H	0.023900	59.20	93.78	21.21	H62	LHG	5630
H	0.044400	55.49	97.16	18.95	H81	LHG	5630
H	0.044400	55.43	96.11	17.70	H82	LHG	5630
H	0.020400	54.41	94.57	19.41	H91	LHG	5630
H	0.020400	54.06	95.96	20.18	H92	LHG	5630
H	0.002400	52.43	96.44	18.81	1H10	LHG	5630
H	0.002400	53.31	96.03	17.50	2H10	LHG	5630
H	0.036400	58.38	93.13	24.51	1H24	LHG	5630
H	0.036400	57.92	94.22	25.63	2H24	LHG	5630
H	0.004400	52.73	93.69	18.68	1H11	LHG	5630
H	0.004400	52.06	94.25	17.30	2H11	LHG	5630
H	0.001400	51.00	94.44	19.95	1H12	LHG	5630
H	0.001400	50.47	95.44	18.78	2H12	LHG	5630
H	0.001400	49.54	93.71	17.60	1H13	LHG	5630
H	0.001400	50.37	92.59	18.45	2H13	LHG	5630
H	-0.000100	49.01	92.81	20.27	1H14	LHG	5630
H	-0.000100	48.44	94.26	19.76	2H14	LHG	5630
H	0.001400	46.81	93.33	18.67	1H15	LHG	5630

H	0.001400	47.81	92.25	17.96	2H15	LHG	5630
H	-0.000600	46.95	90.69	19.22	1H16	LHG	5630
H	-0.000600	47.56	91.45	20.53	2H16	LHG	5630
H	0.000400	45.46	91.58	21.17	1H17	LHG	5630
H	0.000400	45.37	92.83	20.13	2H17	LHG	5630
H	-0.000100	44.15	91.71	18.68	1H18	LHG	5630
H	-0.000100	44.91	90.30	18.99	2H18	LHG	5630
H	0.000400	43.67	90.23	21.10	1H19	LHG	5630
H	0.000400	42.76	91.45	20.50	2H19	LHG	5630
H	-0.000600	41.88	90.14	18.86	1H20	LHG	5630
H	-0.000600	43.05	89.02	19.01	2H20	LHG	5630
H	-0.001100	41.74	89.09	21.38	1H21	LHG	5630
H	-0.001100	40.59	89.04	20.22	2H21	LHG	5630
H	-0.006900	41.16	86.84	20.90	1H22	LHG	5630
H	-0.006900	41.57	87.06	19.34	2H22	LHG	5630
H	-0.006900	42.72	87.11	20.50	3H22	LHG	5630
H	0.003900	54.26	92.19	22.89	1H27	LHG	5630
H	0.003900	54.29	93.78	22.51	2H27	LHG	5630
H	0.001400	54.22	92.85	20.47	1H28	LHG	5630
H	0.001400	55.83	93.05	20.67	2H28	LHG	5630
H	-0.000100	56.22	90.90	20.72	1H29	LHG	5630
H	-0.000100	54.88	90.59	21.60	2H29	LHG	5630
H	0.000400	54.29	89.61	19.69	1H30	LHG	5630
H	0.000400	53.70	91.11	19.42	2H30	LHG	5630
H	0.005400	56.23	91.21	18.55	1H31	LHG	5630
H	0.005400	55.67	89.78	18.02	2H31	LHG	5630
H	-0.004100	54.28	90.71	16.59	1H32	LHG	5630
H	-0.004100	53.90	91.92	17.62	2H32	LHG	5630
H	0.011400	55.69	93.18	16.97	1H33	LHG	5630
H	0.011400	56.44	91.90	16.29	2H33	LHG	5630
H	-0.002100	53.95	92.64	15.16	1H34	LHG	5630
H	-0.002100	55.20	93.65	14.87	2H34	LHG	5630
H	-0.001600	55.81	90.96	14.41	1H35	LHG	5630
H	-0.001600	54.68	91.56	13.40	2H35	LHG	5630
H	0.001900	56.14	92.75	12.29	1H36	LHG	5630
H	0.001900	56.89	93.25	13.65	2H36	LHG	5630
H	-0.002100	57.77	90.87	13.67	1H37	LHG	5630
H	-0.002100	57.46	90.94	12.07	2H37	LHG	5630
H	-0.007600	59.71	91.57	12.49	1H38	LHG	5630
H	-0.007600	58.88	92.84	11.88	2H38	LHG	5630
H	-0.007600	59.19	92.76	13.49	3H38	LHG	5630
O	-0.738800	62.88	96.89	20.15	O4	LHG	5630
H	0.689000	63.76	97.33	20.32	H6	LHG	5630
C	0.000200	56.14	93.07	23.19	C26	LHG	5630
H	0.004900	56.86	93.09	22.50	1H26	LHG	5630
H	0.004900	56.26	92.27	23.78	2H26	LHG	5630

C	0.002200	56.55	94.07	24.03	C25	LHG	5630
H	0.014900	55.87	94.07	24.76	1H25	LHG	5630
H	0.014900	56.45	94.90	23.48	2H25	LHG	5630
Mg	1.169200	53.81	100.31	18.62	MG	CHL	601
C	-0.004739	49.45	99.76	21.53	CAA	CHL	601
C	-0.112834	53.05	102.64	13.46	CAB	CHL	601
C	0.160477	59.54	101.01	18.51	CAC	CHL	601
C	0.627291	53.68	97.75	23.26	CAD	CHL	601
N	-0.489633	51.83	99.60	19.16	NA	CHL	601
C	-0.219908	47.99	100.10	21.83	CBA	CHL	601
C	-0.367704	54.20	103.13	12.91	CBB	CHL	601
C	-0.168957	59.87	102.20	19.38	CBC	CHL	601
C	-0.692237	52.24	97.84	22.66	CBD	CHL	601
N	-0.549527	53.09	101.08	16.88	NB	CHL	601
O	-0.531678	53.87	97.29	24.38	OBD	CHL	601
C	0.826782	46.97	99.01	21.58	CGA	CHL	601
C	0.975656	51.63	96.42	22.52	CGD	CHL	601
N	-0.548096	55.75	100.78	18.08	NC	CHL	601
N	-0.486413	54.56	99.40	20.26	ND	CHL	601
C	0.040004	49.30	95.59	22.60	CED	CHL	601
C	0.087495	52.44	98.53	21.31	CHA	CHL	601
C	-0.519448	50.70	100.45	17.14	CHB	CHL	601
C	-0.373104	55.24	101.72	15.86	CHC	CHL	601
C	-0.358246	56.94	99.86	20.03	CHD	CHL	601
C	-0.410730	48.95	97.92	18.34	CMA	CHL	601
C	-0.236326	50.32	101.82	14.42	CMB	CHL	601
C	0.440869	58.28	102.14	15.77	CMC	CHL	601
C	-0.266591	57.14	98.41	22.89	CMD	CHL	601
O	-0.537107	57.99	102.61	14.67	OMC	CHL	601
C	0.018007	51.49	98.94	20.33	C1A	CHL	601
C	0.290707	51.77	101.04	16.46	C1B	CHL	601
C	0.332773	56.14	101.35	16.89	C1C	CHL	601
C	0.191076	55.85	99.32	20.73	C1D	CHL	601
O	-0.589721	46.93	97.92	22.16	O1A	CHL	601
O	-0.623224	52.19	95.49	21.94	O1D	CHL	601
C	0.037093	49.98	98.82	20.43	C2A	CHL	601
C	0.078577	51.68	101.64	15.15	C2B	CHL	601
C	-0.147964	57.59	101.55	16.91	C2C	CHL	601
C	0.084438	55.89	98.63	22.01	C2D	CHL	601
O	-0.485288	46.01	99.33	20.58	O2A	CHL	601
O	-0.399841	50.36	96.33	23.10	O2D	CHL	601
C	0.179052	49.50	99.17	19.04	C3A	CHL	601
C	-0.054715	52.95	101.99	14.76	C3B	CHL	601
C	-0.234405	58.04	101.05	18.08	C3C	CHL	601
C	-0.158062	54.59	98.30	22.28	C3D	CHL	601
C	0.345332	50.71	99.78	18.37	C4A	CHL	601

C	0.233194	53.85	101.60	15.85	C4B	CHL	601
C	0.342833	56.90	100.53	18.80	C4C	CHL	601
C	0.130108	53.80	98.77	21.19	C4D	CHL	601
C	0.345381	44.75	98.59	20.59	C1	CHL	601
C	-0.477083	44.54	98.09	19.25	C2	CHL	601
C	0.260847	44.97	96.88	18.73	C3	CHL	601
C	-0.269607	45.77	95.82	19.53	C4	CHL	601
C	-0.336279	44.76	96.48	17.27	C5	CHL	601
C	0.119257	43.46	95.83	16.86	C6	CHL	601
C	-0.175039	43.75	94.82	15.75	C7	CHL	601
C	0.331362	42.55	94.14	15.10	C8	CHL	601
C	-0.313835	42.83	93.65	13.69	C9	CHL	601
C	-0.284648	41.55	93.41	16.02	C10	CHL	601
C	0.041634	40.94	92.08	15.67	C11	CHL	601
C	-0.154439	39.98	91.76	16.81	C12	CHL	601
C	0.196709	39.33	90.39	16.96	C13	CHL	601
C	-0.232704	39.06	89.60	15.70	C14	CHL	601
C	-0.201414	38.12	90.45	17.89	C15	CHL	601
C	0.209589	38.00	89.44	19.00	C16	CHL	601
C	-0.269983	36.64	88.81	19.27	C17	CHL	601
C	0.432452	36.26	88.39	20.70	C18	CHL	601
C	-0.315373	35.00	87.55	20.73	C19	CHL	601
C	-0.315373	37.29	87.58	21.51	C20	CHL	601
H	0.003832	49.88	100.64	21.36	1HAA	CHL	601
H	0.003832	49.79	99.38	22.39	2HAA	CHL	601
H	0.140703	52.21	102.73	12.92	HAB	CHL	601
H	-0.000428	59.72	100.18	19.02	1HAC	CHL	601
H	-0.000428	60.12	101.05	17.70	2HAC	CHL	601
H	0.057072	47.93	100.35	22.80	1HBA	CHL	601
H	0.057072	47.74	100.88	21.26	2HBA	CHL	601
H	0.167066	55.06	103.05	13.41	1HBB	CHL	601
H	0.167066	54.18	103.56	12.01	2HBB	CHL	601
H	0.046995	60.84	102.15	19.65	1HBC	CHL	601
H	0.046995	59.70	103.04	18.88	2HBC	CHL	601
H	0.046995	59.30	102.18	20.21	3HBC	CHL	601
H	0.218234	51.60	98.35	23.23	HBD	CHL	601
H	0.063428	48.51	95.69	23.20	1HED	CHL	601
H	0.063428	49.07	95.92	21.69	2HED	CHL	601
H	0.063428	49.56	94.62	22.55	3HED	CHL	601
H	0.175319	49.81	100.50	16.69	HHB	CHL	601
H	0.209400	55.66	102.12	15.04	HHC	CHL	601
H	0.200579	57.84	99.75	20.45	HHD	CHL	601
H	0.104969	48.63	98.17	17.42	1HMA	CHL	601
H	0.104969	49.67	97.24	18.27	2HMA	CHL	601
H	0.104969	48.18	97.56	18.87	3HMA	CHL	601
H	0.077125	50.48	102.25	13.53	1HMB	CHL	601

H	0.077125	49.90	100.93	14.28	2HMB	CHL	601
H	0.077125	49.72	102.40	14.97	3HMB	CHL	601
H	0.021209	59.27	102.16	15.93	HMC	CHL	601
H	0.090203	56.88	97.91	23.71	1HMD	CHL	601
H	0.090203	57.82	97.88	22.37	2HMD	CHL	601
H	0.090203	57.53	99.29	23.14	3HMD	CHL	601
H	0.205820	44.02	98.68	18.64	H2	CHL	601
H	-0.019695	41.89	94.86	14.89	H8	CHL	601
H	0.016242	44.00	99.18	20.85	H11	CHL	601
H	0.016242	44.81	97.82	21.23	H12	CHL	601
H	-0.010572	40.05	89.84	17.39	H13	CHL	601
H	-0.061651	36.17	89.28	21.14	H18	CHL	601
H	0.059830	49.66	97.90	20.68	H2A	CHL	601
H	0.085694	45.96	95.03	18.94	H41	CHL	601
H	0.085694	46.63	96.22	19.85	H42	CHL	601
H	0.085694	45.23	95.52	20.32	H43	CHL	601
H	0.032055	48.74	99.82	19.03	H3A	CHL	601
H	0.096900	45.49	95.84	17.02	H51	CHL	601
H	0.096900	44.85	97.31	16.72	H52	CHL	601
H	-0.002304	42.82	96.53	16.53	H61	CHL	601
H	-0.002304	43.06	95.36	17.65	H62	CHL	601
H	0.027697	44.32	94.11	16.14	H71	CHL	601
H	0.027697	44.25	95.30	15.03	H72	CHL	601
H	0.069285	42.01	93.21	13.32	H91	CHL	601
H	0.069285	43.08	94.42	13.11	H92	CHL	601
H	0.069285	43.58	92.98	13.71	H93	CHL	601
H	0.073653	40.79	94.04	16.15	1H10	CHL	601
H	0.073653	42.03	93.27	16.89	2H10	CHL	601
H	0.015417	41.64	91.37	15.60	1H11	CHL	601
H	0.015417	40.44	92.14	14.80	2H11	CHL	601
H	0.036623	39.23	92.42	16.74	1H12	CHL	601
H	0.036623	40.49	91.93	17.65	2H12	CHL	601
H	0.048461	38.64	88.73	15.93	1H14	CHL	601
H	0.048461	38.45	90.12	15.10	2H14	CHL	601
H	0.048461	39.92	89.43	15.22	3H14	CHL	601
H	0.037455	37.31	90.36	17.32	1H15	CHL	601
H	0.037455	38.13	91.36	18.31	2H15	CHL	601
H	-0.021542	38.28	89.90	19.84	1H16	CHL	601
H	-0.021542	38.64	88.70	18.79	2H16	CHL	601
H	0.043717	36.59	88.00	18.69	1H17	CHL	601
H	0.043717	35.96	89.48	18.97	2H17	CHL	601
H	0.058595	34.79	87.29	21.67	1H19	CHL	601
H	0.058595	34.24	88.08	20.35	2H19	CHL	601
H	0.058595	35.13	86.72	20.18	3H19	CHL	601
H	0.058595	36.91	87.38	22.42	1H20	CHL	601
H	0.058595	37.50	86.73	21.04	2H20	CHL	601

H	0.058595	38.13	88.12	21.61	3H20	CHL	601
Mg	1.440381	53.20	98.09	31.22	MG	CLA	602
C	0.296003	53.93	101.47	30.70	CHA	CLA	602
C	-0.860850	52.34	98.84	34.49	CHB	CLA	602
C	-0.490961	52.16	94.86	31.61	CHC	CLA	602
C	-0.646114	53.94	97.50	27.90	CHD	CLA	602
N	-0.718243	53.16	99.89	32.43	NA	CLA	602
C	0.064196	53.45	101.18	31.99	C1A	CLA	602
C	-0.224146	53.21	102.17	33.12	C2A	CLA	602
C	0.397216	53.12	101.29	34.34	C3A	CLA	602
C	0.699142	52.83	99.91	33.77	C4A	CLA	602
C	-0.476446	54.44	101.35	35.15	CMA	CLA	602
C	-0.257131	52.02	103.10	32.91	CAA	CLA	602
C	-0.017336	50.61	102.62	32.56	CBA	CLA	602
C	0.557726	49.81	102.01	33.72	CGA	CLA	602
O	-0.479966	49.65	102.61	34.79	O1A	CLA	602
O	-0.471399	49.27	100.70	33.57	O2A	CLA	602
N	-0.869051	52.32	97.06	32.76	NB	CLA	602
C	0.656418	52.09	97.54	34.03	C1B	CLA	602
C	0.049634	51.54	96.47	34.84	C2B	CLA	602
C	-0.300216	51.51	95.34	34.07	C3B	CLA	602
C	0.570735	52.01	95.71	32.74	C4B	CLA	602
C	-0.351576	51.06	96.67	36.31	CMB	CLA	602
C	0.105971	50.92	94.18	34.72	CAB	CLA	602
C	-0.510597	51.01	92.91	34.27	CBB	CLA	602
N	-0.832036	53.08	96.47	29.96	NC	CLA	602
C	0.418922	52.64	95.21	30.32	C1C	CLA	602
C	0.149989	52.76	94.32	29.18	C2C	CLA	602
C	-0.511810	53.23	95.07	28.13	C3C	CLA	602
C	0.637582	53.45	96.41	28.63	C4C	CLA	602
C	-0.398501	52.45	92.81	29.04	CMC	CLA	602
C	0.305775	53.50	94.64	26.67	CAC	CLA	602
C	-0.189740	52.22	94.66	25.84	CBC	CLA	602
N	-0.472588	53.93	99.16	29.68	ND	CLA	602
C	0.322404	54.17	98.80	28.38	C1D	CLA	602
C	0.093768	54.66	99.94	27.60	C2D	CLA	602
C	-0.274124	54.63	100.99	28.47	C3D	CLA	602
C	-0.094145	54.12	100.51	29.72	C4D	CLA	602
C	-0.334352	55.10	99.94	26.13	CMD	CLA	602
C	0.701706	54.86	102.41	28.64	CAD	CLA	602
O	-0.635898	55.27	103.27	27.86	OBD	CLA	602
C	-0.624694	54.46	102.78	30.11	CBD	CLA	602
C	0.657412	55.72	103.32	30.88	CGD	CLA	602
O	-0.483436	55.94	104.53	30.93	O1D	CLA	602
O	-0.390338	56.58	102.34	31.49	O2D	CLA	602
C	-0.000618	57.57	102.70	32.42	CED	CLA	602

C	0.406198	48.98	99.96	34.80	C1	CLA	602
C	-0.221030	48.48	98.70	34.42	C2	CLA	602
C	0.008522	47.53	97.84	34.93	C3	CLA	602
C	-0.450819	46.70	98.12	36.21	C4	CLA	602
C	0.090695	47.29	96.62	34.03	C5	CLA	602
C	0.130068	46.16	95.65	34.24	C6	CLA	602
C	-0.291517	44.90	95.97	33.49	C7	CLA	602
C	0.279668	44.30	94.65	33.03	C8	CLA	602
C	-0.400727	43.29	93.89	33.88	C9	CLA	602
C	-0.055499	43.79	94.67	31.63	C10	CLA	602
C	0.178256	44.79	93.89	30.84	C11	CLA	602
C	-0.170621	44.03	93.78	29.57	C12	CLA	602
C	0.384011	45.03	93.79	28.47	C13	CLA	602
C	-0.383632	45.00	95.14	27.74	C14	CLA	602
C	-0.181140	44.89	92.47	27.73	C15	CLA	602
C	0.036961	45.52	92.34	26.37	C16	CLA	602
C	-0.154197	46.98	92.00	26.37	C17	CLA	602
C	0.445466	47.41	91.35	25.07	C18	CLA	602
C	-0.266674	47.68	92.31	23.90	C19	CLA	602
C	-0.556965	48.66	90.62	25.51	C20	CLA	602
H	0.241453	52.13	99.01	35.45	HHB	CLA	602
H	0.201825	51.89	93.91	31.74	HHC	CLA	602
H	0.295085	54.16	97.33	26.94	HHD	CLA	602
H	0.137917	53.96	102.83	33.21	H2A	CLA	602
H	-0.061345	52.41	101.58	34.98	H3A	CLA	602
H	0.100686	54.36	100.76	35.95	1HMA	CLA	602
H	0.170683	55.19	101.03	34.58	2HMA	CLA	602
H	0.063146	54.61	102.29	35.44	3HMA	CLA	602
H	0.117223	52.28	103.72	32.17	1HAA	CLA	602
H	0.034370	51.92	103.61	33.76	2HAA	CLA	602
H	0.068168	50.09	103.40	32.21	1HBA	CLA	602
H	0.028034	50.68	101.92	31.85	2HBA	CLA	602
H	0.110837	50.72	95.80	36.67	1HMB	CLA	602
H	0.115373	51.82	96.99	36.87	2HMB	CLA	602
H	0.136992	50.33	97.35	36.33	3HMB	CLA	602
H	0.118306	50.41	94.33	35.56	HAB	CLA	602
H	0.225187	51.51	92.71	33.42	1HBB	CLA	602
H	0.182188	50.57	92.17	34.78	2HBB	CLA	602
H	0.151763	52.65	92.50	28.11	1HMC	CLA	602
H	0.105949	53.01	92.29	29.69	2HMC	CLA	602
H	0.131387	51.48	92.65	29.25	3HMC	CLA	602
H	-0.062770	54.15	95.27	26.25	1HAC	CLA	602
H	-0.028620	53.87	93.72	26.65	2HAC	CLA	602
H	0.049872	52.42	94.38	24.90	1HBC	CLA	602
H	0.054496	51.55	94.03	26.24	2HBC	CLA	602
H	0.066739	51.84	95.58	25.84	3HBC	CLA	602

H	0.084121	55.39	100.86	25.87	1HMD	CLA	602
H	0.088401	55.87	99.30	26.01	2HMD	CLA	602
H	0.120861	54.34	99.65	25.55	3HMD	CLA	602
H	0.245531	53.76	103.49	30.17	HBD	CLA	602
H	0.102687	58.05	101.88	32.72	1HED	CLA	602
H	0.053431	58.22	103.33	31.99	2HED	CLA	602
H	0.049996	57.15	103.15	33.21	3HED	CLA	602
H	0.042307	48.30	100.44	35.34	H11	CLA	602
H	-0.059898	49.82	99.84	35.34	H12	CLA	602
H	0.021758	48.92	98.34	33.59	H2	CLA	602
H	0.160937	46.08	97.36	36.38	H41	CLA	602
H	0.143119	47.33	98.22	36.99	H42	CLA	602
H	0.155595	46.18	98.96	36.10	H43	CLA	602
H	-0.047222	48.13	96.08	34.08	H51	CLA	602
H	0.024573	47.18	96.98	33.10	H52	CLA	602
H	-0.011469	45.94	95.63	35.21	H61	CLA	602
H	-0.058810	46.47	94.74	33.94	H62	CLA	602
H	0.051788	45.11	96.55	32.70	H71	CLA	602
H	0.076666	44.26	96.45	34.09	H72	CLA	602
H	-0.013635	45.15	94.12	33.13	H8	CLA	602
H	0.107741	43.03	93.05	33.41	H91	CLA	602
H	0.072814	43.70	93.66	34.77	H92	CLA	602
H	0.091969	42.48	94.46	34.03	H93	CLA	602
H	-0.000402	43.73	95.61	31.29	1H10	CLA	602
H	0.013073	42.89	94.24	31.58	2H10	CLA	602
H	-0.062624	44.98	92.99	31.24	1H11	CLA	602
H	-0.044644	45.65	94.38	30.72	2H11	CLA	602
H	0.028763	43.40	94.55	29.47	1H12	CLA	602
H	0.029073	43.50	92.93	29.55	2H12	CLA	602
H	-0.080740	45.99	93.79	28.75	H13	CLA	602
H	0.086693	45.67	95.14	27.01	1H14	CLA	602
H	0.067667	44.09	95.28	27.36	2H14	CLA	602
H	0.086486	45.21	95.87	28.39	3H14	CLA	602
H	0.033992	43.92	92.29	27.62	1H15	CLA	602
H	0.036765	45.30	91.77	28.31	2H15	CLA	602
H	-0.016467	45.40	93.21	25.89	1H16	CLA	602
H	0.008068	45.03	91.62	25.88	2H16	CLA	602
H	0.040028	47.17	91.37	27.12	1H17	CLA	602
H	0.025223	47.51	92.84	26.50	2H17	CLA	602
H	-0.057629	46.68	90.78	24.69	H18	CLA	602
H	0.067430	47.95	91.78	23.09	1H19	CLA	602
H	0.041552	46.84	92.82	23.69	2H19	CLA	602
H	0.027859	48.41	92.94	24.15	3H19	CLA	602
H	0.131969	49.06	90.13	24.73	1H20	CLA	602
H	0.112314	49.33	91.27	25.86	2H20	CLA	602
H	0.131652	48.43	89.96	26.23	3H20	CLA	602

Mg	0.743847	48.45	89.80	37.97	MG	CLA	603
C	0.063221	47.78	92.09	40.54	CHA	CLA	603
C	-0.408136	46.69	91.85	35.79	CHB	CLA	603
C	-0.106655	48.48	87.30	35.60	CHC	CLA	603
C	-0.345683	49.54	87.52	40.34	CHD	CLA	603
N	-0.228028	47.48	91.77	38.11	NA	CLA	603
C	-0.223899	47.35	92.54	39.26	C1A	CLA	603
C	0.399316	46.63	93.85	38.95	C2A	CLA	603
C	-0.103658	46.24	93.72	37.50	C3A	CLA	603
C	0.121905	46.83	92.39	37.06	C4A	CLA	603
C	0.002402	44.71	93.79	37.42	CMA	CLA	603
C	-0.203143	47.40	95.17	39.05	CAA	CLA	603
C	-0.160571	46.80	96.47	39.57	CBA	CLA	603
C	0.575464	45.31	96.64	39.81	CGA	CLA	603
O	-0.480478	44.64	97.39	39.10	O1A	CLA	603
O	-0.409901	44.65	95.91	40.87	O2A	CLA	603
N	-0.434425	47.83	89.65	36.02	NB	CLA	603
C	0.266792	47.14	90.61	35.31	C1B	CLA	603
C	-0.010896	46.99	90.16	33.95	C2B	CLA	603
C	0.007647	47.36	88.85	33.91	C3B	CLA	603
C	0.096810	47.94	88.53	35.21	C4B	CLA	603
C	-0.304909	46.46	91.10	32.85	CMB	CLA	603
C	-0.087299	47.08	88.16	32.65	CAB	CLA	603
C	-0.438534	47.43	86.88	32.37	CBB	CLA	603
N	-0.334732	49.02	87.78	37.96	NC	CLA	603
C	-0.085389	48.98	86.94	36.86	C1C	CLA	603
C	0.284218	49.50	85.64	37.24	C2C	CLA	603
C	-0.402467	49.89	85.73	38.55	C3C	CLA	603
C	0.323845	49.45	87.03	39.03	C4C	CLA	603
C	-0.443867	49.60	84.38	36.37	CMC	CLA	603
C	0.308141	50.72	84.66	39.32	CAC	CLA	603
C	-0.272914	52.22	84.60	38.93	CBC	CLA	603
N	-0.378455	48.68	89.78	39.94	ND	CLA	603
C	0.045825	49.18	88.80	40.79	C1D	CLA	603
C	0.302180	49.22	89.29	42.16	C2D	CLA	603
C	-0.416707	48.75	90.58	42.11	C3D	CLA	603
C	0.174329	48.36	90.83	40.75	C4D	CLA	603
C	-0.404104	49.66	88.50	43.38	CMD	CLA	603
C	0.734691	48.55	91.81	42.83	CAD	CLA	603
O	-0.499868	48.89	92.15	43.96	OBD	CLA	603
C	-0.643192	47.78	92.79	41.90	CBD	CLA	603
C	0.750547	46.30	93.03	42.47	CGD	CLA	603
O	-0.476713	46.14	93.89	43.33	O1D	CLA	603
O	-0.310194	45.26	92.19	41.99	O2D	CLA	603
C	-0.119380	44.02	92.15	42.57	CED	CLA	603
C	0.225015	43.26	96.24	41.14	C1	CLA	603

C	-0.433741	42.39	95.31	40.35	C2	CLA	603
C	0.235271	41.36	95.60	39.45	C3	CLA	603
C	-0.342309	40.89	97.02	39.08	C4	CLA	603
C	-0.298864	40.47	94.54	38.78	C5	CLA	603
C	0.409166	40.95	93.79	37.55	C6	CLA	603
C	-0.425196	41.10	92.31	37.88	C7	CLA	603
C	0.456929	40.17	91.42	37.07	C8	CLA	603
C	-0.482191	40.84	90.76	35.89	C9	CLA	603
C	-0.210603	39.22	90.48	37.82	C10	CLA	603
C	0.343651	39.86	89.48	38.77	C11	CLA	603
C	-0.189752	39.00	88.23	38.67	C12	CLA	603
C	0.234328	38.54	87.53	39.93	C13	CLA	603
C	-0.434898	37.37	88.30	40.54	C14	CLA	603
C	0.100744	39.62	87.07	40.91	C15	CLA	603
C	-0.078463	40.57	85.94	40.53	C16	CLA	603
C	-0.027000	41.41	85.50	41.73	C17	CLA	603
C	0.416339	41.39	84.08	42.30	C18	CLA	603
C	-0.456567	41.76	84.19	43.78	C19	CLA	603
C	-0.352546	40.16	83.18	42.07	C20	CLA	603
H	0.184640	46.20	92.41	35.13	HHB	CLA	603
H	0.140439	48.50	86.58	34.90	HHC	CLA	603
H	0.201516	49.89	86.88	41.04	HHD	CLA	603
H	-0.043357	45.91	93.92	39.64	H2A	CLA	603
H	0.065014	46.59	94.45	36.91	H3A	CLA	603
H	0.005234	44.43	93.71	36.46	1HMA	CLA	603
H	0.089112	44.32	93.04	37.95	2HMA	CLA	603
H	0.020008	44.40	94.67	37.79	3HMA	CLA	603
H	0.064014	47.72	95.38	38.12	1HAA	CLA	603
H	0.077293	48.19	94.99	39.64	2HAA	CLA	603
H	0.093335	47.24	96.66	40.44	1HBA	CLA	603
H	0.089951	47.05	97.18	38.91	2HBA	CLA	603
H	0.099362	46.43	90.61	31.98	1HMB	CLA	603
H	0.105973	45.54	91.41	33.09	2HMB	CLA	603
H	0.104336	47.07	91.89	32.76	3HMB	CLA	603
H	0.153008	46.59	88.68	31.94	HAB	CLA	603
H	0.187718	47.92	86.33	33.04	1HBB	CLA	603
H	0.168595	47.20	86.48	31.48	2HBB	CLA	603
H	0.161094	50.00	83.64	36.90	1HMC	CLA	603
H	0.132040	48.68	84.12	36.06	2HMC	CLA	603
H	0.121375	50.17	84.57	35.57	3HMC	CLA	603
H	-0.046354	50.67	84.86	40.30	1HAC	CLA	603
H	-0.029316	50.33	83.76	39.14	2HAC	CLA	603
H	0.060828	52.68	83.90	39.47	1HBC	CLA	603
H	0.068693	52.30	84.39	37.96	2HBC	CLA	603
H	0.065890	52.64	85.49	39.12	3HBC	CLA	603
H	0.137885	49.58	89.08	44.20	1HMD	CLA	603

H	0.129136	49.07	87.70	43.49	2HMD	CLA	603
H	0.115590	50.60	88.21	43.27	3HMD	CLA	603
H	0.261295	48.21	93.69	41.82	HBD	CLA	603
H	0.110322	43.44	91.50	42.08	1HED	CLA	603
H	0.098739	44.12	91.86	43.52	2HED	CLA	603
H	0.103841	43.61	93.06	42.54	3HED	CLA	603
H	0.061011	43.09	97.19	40.86	H11	CLA	603
H	0.073337	43.07	96.13	42.11	H12	CLA	603
H	0.155971	42.57	94.34	40.48	H2	CLA	603
H	0.091297	40.14	96.96	38.42	H41	CLA	603
H	0.100022	40.58	97.50	39.90	H42	CLA	603
H	0.120289	41.65	97.52	38.67	H43	CLA	603
H	0.090458	39.62	95.00	38.51	H51	CLA	603
H	0.065156	40.27	93.84	39.47	H52	CLA	603
H	-0.118172	41.84	94.16	37.27	H61	CLA	603
H	-0.059502	40.29	93.91	36.81	H62	CLA	603
H	0.078098	40.91	92.18	38.85	H71	CLA	603
H	0.043844	42.04	92.04	37.69	H72	CLA	603
H	-0.075786	39.53	92.11	36.73	H8	CLA	603
H	0.105136	40.18	90.19	35.40	H91	CLA	603
H	0.103280	41.20	91.46	35.27	H92	CLA	603
H	0.121638	41.60	90.19	36.22	H93	CLA	603
H	0.028191	38.72	89.96	37.14	1H10	CLA	603
H	0.025495	38.59	91.04	38.35	2H10	CLA	603
H	-0.072943	39.86	89.84	39.71	1H11	CLA	603
H	-0.084717	40.80	89.28	38.50	2H11	CLA	603
H	-0.000268	39.52	87.56	38.14	1H12	CLA	603
H	0.038771	38.17	88.49	38.16	2H12	CLA	603
H	-0.028629	38.20	86.63	39.65	H13	CLA	603
H	0.098103	37.06	87.84	41.37	1H14	CLA	603
H	0.093721	37.66	89.23	40.76	2H14	CLA	603
H	0.110343	36.61	88.33	39.88	3H14	CLA	603
H	-0.010028	39.16	86.79	41.75	1H15	CLA	603
H	-0.071484	40.20	87.87	41.10	2H15	CLA	603
H	0.028270	41.18	86.25	39.80	1H16	CLA	603
H	-0.015100	40.03	85.16	40.21	2H16	CLA	603
H	-0.023337	41.14	86.10	42.48	1H17	CLA	603
H	-0.002081	42.36	85.69	41.48	2H17	CLA	603
H	-0.073296	42.07	83.58	41.76	H18	CLA	603
H	0.110551	41.76	83.28	44.19	1H19	CLA	603
H	0.082713	42.67	84.60	43.87	2H19	CLA	603
H	0.112931	41.09	84.77	44.25	3H19	CLA	603
H	0.088292	40.31	82.30	42.50	1H20	CLA	603
H	0.067161	39.36	83.62	42.46	2H20	CLA	603
H	0.087724	40.03	83.05	41.09	3H20	CLA	603
Mg	1.156918	59.55	73.78	36.00	MG	CLA	604

C	0.039600	59.01	70.36	36.46	CHA	CLA	604
C	-0.504259	56.97	74.48	38.17	CHB	CLA	604
C	-0.225889	60.44	77.06	35.89	CHC	CLA	604
C	-0.481308	62.42	72.99	34.20	CHD	CLA	604
N	-0.559822	58.14	72.58	37.11	NA	CLA	604
C	0.102817	58.11	71.19	37.16	C1A	CLA	604
C	-0.055721	57.02	70.75	38.14	C2A	CLA	604
C	0.106719	56.20	72.00	38.34	C3A	CLA	604
C	0.362759	57.12	73.12	37.88	C4A	CLA	604
C	-0.353386	54.96	71.84	37.46	CMA	CLA	604
C	0.186996	57.40	70.35	39.58	CAA	CLA	604
C	-0.211581	58.65	69.61	39.95	CBA	CLA	604
C	0.608738	59.45	69.90	41.19	CGA	CLA	604
O	-0.467971	59.58	68.91	41.90	O1A	CLA	604
O	-0.467951	60.03	71.13	41.62	O2A	CLA	604
N	-0.516195	58.87	75.45	36.91	NB	CLA	604
C	0.193679	57.78	75.55	37.74	C1B	CLA	604
C	0.173880	57.70	76.93	38.23	C2B	CLA	604
C	-0.210684	58.63	77.67	37.51	C3B	CLA	604
C	0.225697	59.36	76.73	36.71	C4B	CLA	604
C	-0.319638	56.71	77.21	39.36	CMB	CLA	604
C	-0.014517	58.74	79.13	37.59	CAB	CLA	604
C	-0.499658	57.96	80.04	38.30	CBB	CLA	604
N	-0.590212	61.09	74.85	35.09	NC	CLA	604
C	0.046806	61.25	76.21	35.15	C1C	CLA	604
C	0.284194	62.44	76.60	34.43	C2C	CLA	604
C	-0.426448	63.02	75.46	33.99	C3C	CLA	604
C	0.499686	62.18	74.35	34.40	C4C	CLA	604
C	-0.496809	63.00	78.03	34.33	CMC	CLA	604
C	0.275835	64.37	75.33	33.25	CAC	CLA	604
C	-0.221540	65.50	75.23	34.27	CBC	CLA	604
N	-0.589037	60.48	72.10	35.37	ND	CLA	604
C	0.366086	61.64	71.92	34.65	C1D	CLA	604
C	0.087739	61.91	70.50	34.44	C2D	CLA	604
C	-0.218553	60.90	69.85	35.10	C3D	CLA	604
C	0.141330	60.06	70.84	35.69	C4D	CLA	604
C	-0.342399	63.10	69.88	33.67	CMD	CLA	604
C	0.620434	60.35	68.57	35.48	CAD	CLA	604
O	-0.496289	60.74	67.42	35.24	OBD	CLA	604
C	-0.519101	59.07	68.84	36.34	CBD	CLA	604
C	0.808302	57.81	68.25	35.63	CGD	CLA	604
O	-0.557587	57.01	67.59	36.30	O1D	CLA	604
O	-0.438718	57.61	68.56	34.27	O2D	CLA	604
C	0.146616	56.44	68.24	33.63	CED	CLA	604
C	0.287818	61.04	71.05	42.67	C1	CLA	604
C	-0.347112	62.35	70.88	42.05	C2	CLA	604

C	0.157380	63.61	71.37	42.39	C3	CLA	604
C	-0.380582	63.89	72.28	43.62	C4	CLA	604
C	-0.353443	64.87	71.12	41.51	C5	CLA	604
C	-0.019519	65.32	69.68	41.22	C6	CLA	604
C	-0.153953	65.70	68.78	42.42	C7	CLA	604
C	0.299395	66.72	67.64	42.36	C8	CLA	604
C	-0.454194	67.75	67.71	43.49	C9	CLA	604
C	0.078132	67.12	67.03	41.00	C10	CLA	604
C	-0.051254	68.36	67.51	40.22	C11	CLA	604
C	-0.055620	68.08	67.23	38.75	C12	CLA	604
C	0.368747	69.17	67.43	37.70	C13	CLA	604
C	-0.455481	68.93	68.75	36.98	C14	CLA	604
C	-0.340808	69.20	66.25	36.73	C15	CLA	604
C	0.329211	70.53	65.76	36.14	C16	CLA	604
C	-0.149143	70.85	66.05	34.67	C17	CLA	604
H	0.186287	56.19	74.72	38.76	HHB	CLA	604
H	0.153074	60.67	78.03	35.84	HHC	CLA	604
H	0.215201	63.25	72.75	33.68	HHD	CLA	604
H	0.068959	56.62	69.94	37.72	H2A	CLA	604
H	0.028488	55.90	72.18	39.28	H3A	CLA	604
H	0.089230	54.38	72.65	37.56	1HMA	CLA	604
H	0.112549	55.24	71.74	36.51	2HMA	CLA	604
H	0.104176	54.45	71.03	37.75	3HMA	CLA	604
H	-0.007634	56.65	69.78	39.91	1HAA	CLA	604
H	-0.046977	57.43	71.20	40.10	2HAA	CLA	604
H	0.092228	58.40	68.64	40.01	1HBA	CLA	604
H	0.037350	59.29	69.74	39.18	2HBA	CLA	604
H	0.080864	56.75	78.19	39.60	1HMB	CLA	604
H	0.114102	55.79	76.98	39.07	2HMB	CLA	604
H	0.106792	56.96	76.67	40.16	3HMB	CLA	604
H	0.109363	59.48	79.53	37.05	HAB	CLA	604
H	0.196350	57.20	79.72	38.86	1HBB	CLA	604
H	0.163158	58.16	81.02	38.25	2HBB	CLA	604
H	0.156123	63.83	78.03	33.77	1HMC	CLA	604
H	0.129785	62.32	78.63	33.91	2HMC	CLA	604
H	0.126095	63.22	78.37	35.25	3HMC	CLA	604
H	-0.027453	64.36	74.51	32.67	1HAC	CLA	604
H	-0.022139	64.51	76.14	32.67	2HAC	CLA	604
H	0.031239	66.38	75.14	33.79	1HBC	CLA	604
H	0.056540	65.52	76.05	34.84	2HBC	CLA	604
H	0.080442	65.36	74.42	34.84	3HBC	CLA	604
H	0.142125	63.02	68.88	33.70	1HMD	CLA	604
H	0.110606	63.07	70.19	32.72	2HMD	CLA	604
H	0.103726	63.95	70.16	34.10	3HMD	CLA	604
H	0.184957	59.10	68.42	37.25	HBD	CLA	604
H	0.091058	56.49	68.54	32.67	1HED	CLA	604

H	0.067393	56.29	67.25	33.66	2HED	CLA	604
H	0.009283	55.68	68.71	34.08	3HED	CLA	604
H	0.037913	60.85	70.26	43.26	H11	CLA	604
H	0.054571	61.04	71.89	43.21	H12	CLA	604
H	0.165303	62.35	70.31	41.23	H2	CLA	604
H	0.119918	64.86	72.50	43.66	H41	CLA	604
H	0.139869	63.35	73.12	43.55	H42	CLA	604
H	0.105104	63.63	71.79	44.46	H43	CLA	604
H	0.132423	65.64	71.57	41.97	H51	CLA	604
H	0.113227	64.71	71.56	40.63	H52	CLA	604
H	0.043256	66.12	69.74	40.62	H61	CLA	604
H	0.056877	64.57	69.23	40.73	H62	CLA	604
H	0.030616	64.84	68.36	42.72	H71	CLA	604
H	0.061421	66.03	69.40	43.13	H72	CLA	604
H	-0.042613	66.16	66.83	42.58	H8	CLA	604
H	0.100763	68.39	66.94	43.41	H91	CLA	604
H	0.088852	68.25	68.57	43.43	H92	CLA	604
H	0.110393	67.28	67.66	44.37	H93	CLA	604
H	-0.054902	66.34	67.17	40.39	1H10	CLA	604
H	-0.001867	67.26	66.05	41.16	2H10	CLA	604
H	-0.004056	69.17	67.00	40.51	1H11	CLA	604
H	-0.014678	68.51	68.49	40.36	2H11	CLA	604
H	0.003732	67.31	67.82	38.48	1H12	CLA	604
H	-0.001818	67.80	66.27	38.68	2H12	CLA	604
H	-0.049197	70.06	67.47	38.14	H13	CLA	604
H	0.109875	69.64	68.89	36.29	1H14	CLA	604
H	0.095733	68.03	68.73	36.53	2H14	CLA	604
H	0.097587	68.95	69.50	37.64	3H14	CLA	604
H	0.050497	68.62	66.51	35.95	1H15	CLA	604
H	0.078662	68.80	65.48	37.21	2H15	CLA	604
H	-0.063101	70.55	64.77	36.26	1H16	CLA	604
H	-0.094377	71.26	66.18	36.69	2H16	CLA	604
H	0.020290	71.74	65.67	34.44	1H17	CLA	604
H	0.031939	70.15	65.63	34.09	2H17	CLA	604
H	0.025312	70.86	67.04	34.52	3H17	CLA	604
Mg	1.169200	56.29	74.11	43.53	MG	CHL	606
C	-0.004739	61.36	74.99	45.90	CAA	CHL	606
C	-0.112834	53.65	78.54	41.21	CAB	CHL	606
C	0.160477	52.98	70.37	40.68	CAC	CHL	606
C	0.627291	59.27	70.37	45.82	CAD	CHL	606
N	-0.489633	57.93	74.93	44.74	NA	CHL	606
C	-0.219908	61.93	74.56	47.26	CBA	CHL	606
C	-0.367704	54.04	79.62	40.43	CBB	CHL	606
C	-0.168957	51.69	70.16	41.43	CBC	CHL	606
C	-0.692237	59.74	71.76	46.29	CBD	CHL	606
N	-0.549527	55.67	75.98	43.04	NB	CHL	606

O	-0.531678	59.81	69.34	46.22	OBD	CHL	606
C	0.826782	63.42	74.47	47.61	CGA	CHL	606
C	0.975656	59.51	71.90	47.81	CGD	CHL	606
N	-0.548096	54.95	73.24	42.21	NC	CHL	606
N	-0.486413	57.00	72.25	43.88	ND	CHL	606
C	0.040004	60.45	71.07	49.91	CED	CHL	606
C	0.087495	58.89	72.75	45.47	CHA	CHL	606
C	-0.519448	57.39	77.30	44.28	CHB	CHL	606
C	-0.373104	53.92	75.33	41.41	CHC	CHL	606
C	-0.358246	55.44	70.87	42.60	CHD	CHL	606
C	-0.410730	58.81	77.12	47.19	CMA	CHL	606
C	-0.236326	55.71	79.74	43.38	CMB	CHL	606
C	0.440869	52.32	73.45	39.67	CMC	CHL	606
C	-0.266591	57.07	68.45	43.88	CMD	CHL	606
O	-0.537107	51.49	72.77	39.08	OMC	CHL	606
C	0.018007	58.86	74.20	45.45	C1A	CHL	606
C	0.290707	56.26	77.17	43.43	C1B	CHL	606
C	0.332773	54.05	73.93	41.43	C1C	CHL	606
C	0.191076	56.52	71.02	43.49	C1D	CHL	606
O	-0.589721	64.19	74.79	46.69	O1A	CHL	606
O	-0.623224	58.40	72.22	48.27	O1D	CHL	606
C	0.037093	59.84	75.14	46.16	C2A	CHL	606
C	0.078577	55.47	78.27	42.88	C2B	CHL	606
C	-0.147964	53.26	72.97	40.66	C2C	CHL	606
C	0.084438	57.26	69.94	44.11	C2D	CHL	606
O	-0.485288	64.03	74.05	48.93	O2A	CHL	606
O	-0.399841	60.63	71.60	48.62	O2D	CHL	606
C	0.179052	59.29	76.52	45.87	C3A	CHL	606
C	-0.054715	54.51	77.71	42.05	C3B	CHL	606
C	-0.234405	53.61	71.73	41.09	C3C	CHL	606
C	-0.158062	58.18	70.56	44.90	C3D	CHL	606
C	0.345332	58.15	76.29	44.89	C4A	CHL	606
C	0.233194	54.66	76.27	42.15	C4B	CHL	606
C	0.342833	54.72	71.89	42.00	C4C	CHL	606
C	0.130108	58.02	71.97	44.74	C4D	CHL	606
C	0.345381	63.80	74.93	50.06	C1	CHL	606
C	-0.477083	65.08	75.09	50.82	C2	CHL	606
C	0.260847	65.39	75.38	52.16	C3	CHL	606
C	-0.269607	64.41	75.62	53.34	C4	CHL	606
C	-0.336279	66.84	75.54	52.73	C5	CHL	606
H	0.003832	61.76	75.86	45.61	1HAA	CHL	606
H	0.003832	61.54	74.29	45.21	2HAA	CHL	606
H	0.140703	52.67	78.31	41.19	HAB	CHL	606
H	-0.000428	52.79	70.37	39.70	1HAC	CHL	606
H	-0.000428	53.61	69.63	40.90	2HAC	CHL	606
H	0.057072	61.55	75.21	47.93	1HBA	CHL	606

H	0.057072	61.56	73.65	47.43	2HBA	CHL	606
H	0.167066	55.00	79.89	40.41	1HBB	CHL	606
H	0.167066	53.37	80.12	39.89	2HBB	CHL	606
H	0.046995	51.29	69.29	41.17	1HBC	CHL	606
H	0.046995	51.87	70.16	42.42	2HBC	CHL	606
H	0.046995	51.05	70.90	41.22	3HBC	CHL	606
H	0.218234	60.72	71.93	46.14	HBD	CHL	606
H	0.063428	61.35	70.92	50.34	1HED	CHL	606
H	0.063428	59.92	71.71	50.46	2HED	CHL	606
H	0.063428	59.96	70.20	49.85	3HED	CHL	606
H	0.175319	57.68	78.24	44.46	HHB	CHL	606
H	0.209400	53.23	75.70	40.80	HHC	CHL	606
H	0.200579	55.17	69.94	42.38	HHD	CHL	606
H	0.104969	58.45	78.04	47.02	1HMA	CHL	606
H	0.104969	58.10	76.54	47.58	2HMA	CHL	606
H	0.104969	59.58	77.18	47.82	3HMA	CHL	606
H	0.077125	55.09	80.36	42.90	1HMB	CHL	606
H	0.077125	55.55	79.80	44.36	2HMB	CHL	606
H	0.077125	56.66	80.00	43.18	3HMB	CHL	606
H	0.021209	52.34	74.43	39.46	HMC	CHL	606
H	0.090203	57.72	67.94	44.44	1HMD	CHL	606
H	0.090203	56.13	68.19	44.13	2HMD	CHL	606
H	0.090203	57.22	68.24	42.92	3HMD	CHL	606
H	0.205820	65.89	74.97	50.25	H2	CHL	606
H	0.016242	63.10	74.53	50.65	H11	CHL	606
H	0.016242	63.48	75.82	49.73	H12	CHL	606
H	0.059830	59.83	74.90	47.13	H2A	CHL	606
H	0.085694	64.94	75.80	54.18	H41	CHL	606
H	0.085694	63.83	76.40	53.14	H42	CHL	606
H	0.085694	63.85	74.80	53.48	H43	CHL	606
H	0.032055	59.95	77.16	45.48	H3A	CHL	606
H	0.058595	67.50	75.40	52.00	H51	CHL	606
H	0.058595	66.95	76.46	53.10	H52	CHL	606
H	0.058595	66.99	74.87	53.45	H53	CHL	606
Mg	1.169200	48.13	74.84	38.79	MG	CHL	607
C	-0.004739	43.85	73.53	35.19	CAA	CHL	607
C	-0.112834	49.94	80.18	38.95	CAB	CHL	607
C	0.160477	50.81	73.71	43.80	CAC	CHL	607
C	0.627291	45.83	70.07	38.38	CAD	CHL	607
N	-0.489633	46.80	74.69	37.06	NA	CHL	607
C	-0.219908	43.03	73.77	33.89	CBA	CHL	607
C	-0.367704	50.91	80.80	38.16	CBB	CHL	607
C	-0.168957	50.03	73.94	45.08	CBC	CHL	607
C	-0.692237	45.44	70.95	37.13	CBD	CHL	607
N	-0.549527	48.40	76.82	38.45	NB	CHL	607
O	-0.531678	45.43	68.92	38.50	OBD	CHL	607

C	0.826782	42.34	75.15	33.81	CGA	CHL	607
C	0.975656	45.97	70.26	35.83	CGD	CHL	607
N	-0.548096	49.20	74.97	40.59	NC	CHL	607
N	-0.486413	47.66	72.95	39.31	ND	CHL	607
C	0.040004	45.29	68.80	33.91	CED	CHL	607
C	0.087495	46.12	72.31	37.40	CHA	CHL	607
C	-0.519448	47.12	77.04	36.34	CHB	CHL	607
C	-0.373104	49.79	77.34	40.43	CHC	CHL	607
C	-0.358246	48.80	72.72	41.47	CHD	CHL	607
C	-0.410730	46.23	75.57	33.68	CMA	CHL	607
C	-0.236326	48.24	79.93	36.28	CMB	CHL	607
C	0.440869	51.01	76.88	43.18	CMC	CHL	607
C	-0.266591	47.69	69.74	41.36	CMD	CHL	607
O	-0.537107	51.18	78.10	43.10	OMC	CHL	607
C	0.018007	46.09	73.56	36.64	C1A	CHL	607
C	0.290707	47.95	77.52	37.35	C1B	CHL	607
C	0.332773	49.81	76.11	41.08	C1C	CHL	607
C	0.191076	48.00	72.21	40.43	C1D	CHL	607
O	-0.589721	42.19	75.76	34.86	O1A	CHL	607
O	-0.623224	47.19	70.22	35.57	O1D	CHL	607
C	0.037093	45.36	73.85	35.33	C2A	CHL	607
C	0.078577	48.52	78.86	37.41	C2B	CHL	607
C	-0.147964	50.40	75.82	42.39	C2C	CHL	607
C	0.084438	47.44	70.88	40.36	C2D	CHL	607
O	-0.485288	41.87	75.80	32.61	O2A	CHL	607
O	-0.399841	44.98	69.49	35.09	O2D	CHL	607
C	0.179052	45.65	75.33	35.06	C3A	CHL	607
C	-0.054715	49.24	78.96	38.58	C3B	CHL	607
C	-0.234405	50.21	74.50	42.62	C3C	CHL	607
C	-0.158062	46.68	70.87	39.22	C3D	CHL	607
C	0.345332	46.58	75.75	36.19	C4A	CHL	607
C	0.233194	49.15	77.67	39.23	C4B	CHL	607
C	0.342833	49.36	73.99	41.55	C4C	CHL	607
C	0.130108	46.83	72.14	38.59	C4D	CHL	607
C	0.345381	42.85	76.53	31.83	C1	CHL	607
C	-0.477083	43.12	77.88	32.47	C2	CHL	607
C	0.260847	44.14	78.72	32.05	C3	CHL	607
C	-0.269607	45.11	78.39	30.89	C4	CHL	607
C	-0.336279	44.52	80.09	32.60	C5	CHL	607
C	0.119257	44.90	80.24	34.05	C6	CHL	607
C	-0.175039	44.07	81.43	34.56	C7	CHL	607
C	0.331362	44.77	82.61	35.23	C8	CHL	607
C	-0.313835	45.88	83.26	34.43	C9	CHL	607
C	-0.284648	44.97	82.62	36.73	C10	CHL	607
C	0.041634	45.77	83.70	37.43	C11	CHL	607
C	-0.154439	46.39	82.93	38.59	C12	CHL	607

C	0.196709	45.91	83.18	40.02	C13	CHL	607
C	-0.232704	44.46	82.87	40.38	C14	CHL	607
C	-0.201414	46.33	84.49	40.64	C15	CHL	607
C	0.209589	47.60	84.44	41.44	C16	CHL	607
C	-0.269983	47.61	83.70	42.76	C17	CHL	607
C	0.432452	47.98	84.70	43.84	C18	CHL	607
C	-0.315373	46.96	84.50	44.96	C19	CHL	607
C	-0.315373	49.45	84.67	44.27	C20	CHL	607
H	0.003832	43.40	74.07	35.91	1HAA	CHL	607
H	0.003832	43.77	72.56	35.40	2HAA	CHL	607
H	0.140703	49.72	80.60	39.83	HAB	CHL	607
H	-0.000428	50.78	72.73	43.58	1HAC	CHL	607
H	-0.000428	51.76	73.99	43.94	2HAC	CHL	607
H	0.057072	43.64	73.68	33.10	1HBA	CHL	607
H	0.057072	42.31	73.07	33.84	2HBA	CHL	607
H	0.167066	51.16	80.41	37.27	1HBB	CHL	607
H	0.167066	51.35	81.64	38.48	2HBB	CHL	607
H	0.046995	50.44	73.42	45.83	1HBC	CHL	607
H	0.046995	50.05	74.92	45.31	2HBC	CHL	607
H	0.046995	49.08	73.65	44.96	3HBC	CHL	607
H	0.218234	44.46	71.08	37.00	HBD	CHL	607
H	0.063428	44.47	68.34	33.56	1HED	CHL	607
H	0.063428	45.62	69.44	33.22	2HED	CHL	607
H	0.063428	45.99	68.11	34.10	3HED	CHL	607
H	0.175319	46.89	77.69	35.62	HHB	CHL	607
H	0.209400	50.29	78.08	40.88	HHC	CHL	607
H	0.200579	48.98	72.10	42.23	HHD	CHL	607
H	0.104969	46.39	76.55	33.55	1HMA	CHL	607
H	0.104969	47.09	75.07	33.58	2HMA	CHL	607
H	0.104969	45.58	75.25	32.98	3HMA	CHL	607
H	0.077125	48.72	80.78	36.49	1HMB	CHL	607
H	0.077125	48.57	79.57	35.40	2HMB	CHL	607
H	0.077125	47.26	80.10	36.22	3HMB	CHL	607
H	0.021209	51.40	76.51	44.02	HMC	CHL	607
H	0.090203	47.18	68.93	41.07	1HMD	CHL	607
H	0.090203	48.67	69.53	41.38	2HMD	CHL	607
H	0.090203	47.39	70.03	42.26	3HMD	CHL	607
H	0.205820	42.53	78.17	33.23	H2	CHL	607
H	-0.019695	44.00	83.25	35.20	H8	CHL	607
H	0.016242	42.49	76.66	30.90	H11	CHL	607
H	0.016242	43.69	76.00	31.79	H12	CHL	607
H	-0.010572	46.44	82.45	40.46	H13	CHL	607
H	-0.061651	47.90	85.63	43.49	H18	CHL	607
H	0.059830	45.73	73.21	34.66	H2A	CHL	607
H	0.085694	45.76	79.14	30.77	H41	CHL	607
H	0.085694	45.60	77.54	31.10	H42	CHL	607

H	0.085694	44.58	78.26	30.05	H43	CHL	607
H	0.032055	44.81	75.88	35.06	H3A	CHL	607
H	0.096900	43.74	80.69	32.45	H51	CHL	607
H	0.096900	45.31	80.41	32.07	H52	CHL	607
H	-0.002304	45.88	80.43	34.14	H61	CHL	607
H	-0.002304	44.68	79.41	34.56	H62	CHL	607
H	0.027697	43.42	81.07	35.22	H71	CHL	607
H	0.027697	43.58	81.80	33.77	H72	CHL	607
H	0.069285	46.27	84.02	34.95	H91	CHL	607
H	0.069285	46.59	82.59	34.23	H92	CHL	607
H	0.069285	45.50	83.61	33.57	H93	CHL	607
H	0.073653	45.41	81.75	36.95	1H10	CHL	607
H	0.073653	44.05	82.65	37.13	2H10	CHL	607
H	0.015417	45.18	84.44	37.76	1H11	CHL	607
H	0.015417	46.48	84.08	36.83	2H11	CHL	607
H	0.036623	47.37	83.13	38.57	1H12	CHL	607
H	0.036623	46.24	81.96	38.39	2H12	CHL	607
H	0.048461	44.31	83.08	41.34	1H14	CHL	607
H	0.048461	43.86	83.43	39.82	2H14	CHL	607
H	0.048461	44.28	81.90	40.21	3H14	CHL	607
H	0.037455	45.60	84.80	41.24	1H15	CHL	607
H	0.037455	46.47	85.15	39.90	2H15	CHL	607
H	-0.021542	47.86	85.38	41.64	1H16	CHL	607
H	-0.021542	48.29	84.01	40.87	2H16	CHL	607
H	0.043717	48.29	82.96	42.73	1H17	CHL	607
H	0.043717	46.71	83.32	42.94	2H17	CHL	607
H	0.058595	47.16	85.14	45.71	1H19	CHL	607
H	0.058595	46.04	84.67	44.61	2H19	CHL	607
H	0.058595	47.02	83.56	45.30	3H19	CHL	607
H	0.058595	49.61	85.35	44.99	1H20	CHL	607
H	0.058595	49.68	83.76	44.63	2H20	CHL	607
H	0.058595	50.03	84.87	43.48	3H20	CHL	607
Mg	1.169200	64.10	87.28	47.36	MG	CHL	608
C	-0.004739	64.07	84.71	42.49	CAA	CHL	608
C	-0.112834	66.08	84.01	51.62	CAB	CHL	608
C	0.160477	65.45	92.21	50.00	CAC	CHL	608
C	0.627291	62.46	89.56	42.88	CAD	CHL	608
N	-0.489633	63.70	85.85	45.78	NA	CHL	608
C	-0.219908	65.52	84.29	42.65	CBA	CHL	608
C	-0.367704	66.58	84.74	52.68	CBB	CHL	608
C	-0.168957	66.88	92.57	49.65	CBC	CHL	608
C	-0.692237	62.51	88.01	42.70	CBD	CHL	608
N	-0.549527	64.74	85.77	48.58	NB	CHL	608
O	-0.531678	62.09	90.29	41.97	OBD	CHL	608
C	0.826782	66.53	85.33	42.39	CGA	CHL	608
C	0.975656	61.08	87.46	42.38	CGD	CHL	608

N	-0.548096	64.67	88.70	48.77	NC	CHL	608
N	-0.486413	63.63	88.78	46.13	ND	CHL	608
C	0.040004	59.77	86.54	40.51	CED	CHL	608
C	0.087495	63.05	87.48	44.04	CHA	CHL	608
C	-0.519448	64.34	83.85	47.06	CHB	CHL	608
C	-0.373104	65.43	87.14	50.52	CHC	CHL	608
C	-0.358246	64.15	90.73	47.49	CHD	CHL	608
C	-0.410730	61.91	83.13	44.98	CMA	CHL	608
C	-0.236326	65.77	82.20	49.26	CMB	CHL	608
C	0.440869	66.18	89.74	51.98	CMC	CHL	608
C	-0.266591	63.21	92.37	44.92	CMD	CHL	608
O	-0.537107	66.62	88.93	52.79	OMC	CHL	608
C	0.018007	63.29	86.15	44.48	C1A	CHL	608
C	0.290707	64.77	84.43	48.26	C1B	CHL	608
C	0.332773	65.18	88.44	50.03	C1C	CHL	608
C	0.191076	63.69	90.15	46.31	C1D	CHL	608
O	-0.589721	66.59	86.30	43.14	O1A	CHL	608
O	-0.623224	60.20	87.34	43.23	O1D	CHL	608
C	0.037093	63.13	84.87	43.68	C2A	CHL	608
C	0.078577	65.40	83.71	49.35	C2B	CHL	608
C	-0.147964	65.53	89.71	50.67	C2C	CHL	608
C	0.084438	63.26	90.85	45.11	C2D	CHL	608
O	-0.485288	67.46	85.21	41.28	O2A	CHL	608
O	-0.399841	60.90	87.15	41.01	O2D	CHL	608
C	0.179052	63.28	83.77	44.71	C3A	CHL	608
C	-0.054715	65.60	84.60	50.37	C3B	CHL	608
C	-0.234405	65.19	90.70	49.81	C3C	CHL	608
C	-0.158062	62.92	89.86	44.22	C3D	CHL	608
C	0.345332	63.84	84.48	45.93	C4A	CHL	608
C	0.233194	65.23	85.92	49.86	C4B	CHL	608
C	0.342833	64.61	90.07	48.64	C4C	CHL	608
C	0.130108	63.22	88.60	44.84	C4D	CHL	608
C	0.345381	68.30	86.37	40.99	C1	CHL	608
C	-0.477083	69.60	86.16	41.60	C2	CHL	608
C	0.260847	70.55	85.15	41.45	C3	CHL	608
C	-0.269607	70.49	83.91	40.52	C4	CHL	608
C	-0.336279	71.79	85.07	42.35	C5	CHL	608
C	0.119257	71.69	85.09	43.89	C6	CHL	608
C	-0.175039	70.47	84.65	44.72	C7	CHL	608
C	0.331362	70.49	83.42	45.61	C8	CHL	608
C	-0.313835	71.21	83.73	46.93	C9	CHL	608
C	-0.284648	69.01	83.09	45.79	C10	CHL	608
C	0.041634	68.54	81.64	45.77	C11	CHL	608
C	-0.154439	67.86	81.36	44.43	C12	CHL	608
C	0.196709	66.85	80.21	44.34	C13	CHL	608
C	-0.232704	67.46	78.82	44.11	C14	CHL	608

C	-0.201414	65.56	80.61	43.61	C15	CHL	608
C	0.209589	65.10	80.03	42.27	C16	CHL	608
C	-0.269983	64.77	80.96	41.10	C17	CHL	608
C	0.432452	65.71	81.11	39.89	C18	CHL	608
C	-0.315373	66.99	81.90	40.11	C19	CHL	608
C	-0.315373	66.22	79.84	39.25	C20	CHL	608
H	0.003832	64.09	85.60	42.03	1HAA	CHL	608
H	0.003832	63.64	84.04	41.88	2HAA	CHL	608
H	0.140703	66.04	83.02	51.71	HAB	CHL	608
H	-0.000428	64.83	92.73	49.40	1HAC	CHL	608
H	-0.000428	65.27	92.46	50.95	2HAC	CHL	608
H	0.057072	65.65	83.97	43.59	1HBA	CHL	608
H	0.057072	65.70	83.53	42.02	2HBA	CHL	608
H	0.167066	66.63	85.73	52.62	1HBB	CHL	608
H	0.167066	66.89	84.26	53.50	2HBB	CHL	608
H	0.046995	67.02	93.56	49.79	1HBC	CHL	608
H	0.046995	67.51	92.07	50.25	2HBC	CHL	608
H	0.046995	67.07	92.34	48.70	3HBC	CHL	608
H	0.218234	63.10	87.71	41.95	HBD	CHL	608
H	0.063428	59.87	86.42	39.52	1HED	CHL	608
H	0.063428	59.66	85.65	40.94	2HED	CHL	608
H	0.063428	58.97	87.11	40.70	3HED	CHL	608
H	0.175319	64.41	82.85	47.01	HHB	CHL	608
H	0.209400	65.79	87.09	51.45	HHC	CHL	608
H	0.200579	64.15	91.73	47.52	HHD	CHL	608
H	0.104969	62.01	82.40	45.66	1HMA	CHL	608
H	0.104969	61.28	83.82	45.33	2HMA	CHL	608
H	0.104969	61.55	82.74	44.13	3HMA	CHL	608
H	0.077125	66.19	81.92	50.12	1HMB	CHL	608
H	0.077125	64.95	81.66	49.09	2HMB	CHL	608
H	0.077125	66.42	82.07	48.51	3HMB	CHL	608
H	0.021209	66.29	90.68	52.30	HMC	CHL	608
H	0.090203	62.87	92.58	44.00	1HMD	CHL	608
H	0.090203	62.60	92.77	45.60	2HMD	CHL	608
H	0.090203	64.13	92.74	45.03	3HMD	CHL	608
H	0.205820	69.87	86.87	42.25	H2	CHL	608
H	-0.019695	70.99	82.64	45.23	H8	CHL	608
H	0.016242	67.88	87.20	41.38	H11	CHL	608
H	0.016242	68.40	86.48	40.00	H12	CHL	608
H	-0.010572	66.51	80.03	45.26	H13	CHL	608
H	-0.061651	65.07	81.60	39.29	H18	CHL	608
H	0.059830	62.24	84.84	43.22	H2A	CHL	608
H	0.085694	71.32	83.37	40.64	H41	CHL	608
H	0.085694	69.69	83.36	40.76	H42	CHL	608
H	0.085694	70.42	84.22	39.57	H43	CHL	608
H	0.032055	63.88	83.03	44.41	H3A	CHL	608

H	0.096900	72.36	85.85	42.09	H51	CHL	608
H	0.096900	72.26	84.23	42.10	H52	CHL	608
H	-0.002304	71.86	86.04	44.15	H61	CHL	608
H	-0.002304	72.45	84.51	44.21	H62	CHL	608
H	0.027697	69.72	84.50	44.07	H71	CHL	608
H	0.027697	70.24	85.41	45.32	H72	CHL	608
H	0.069285	71.22	82.91	47.51	H91	CHL	608
H	0.069285	72.15	84.01	46.73	H92	CHL	608
H	0.069285	70.74	84.47	47.40	H93	CHL	608
H	0.073653	68.51	83.57	45.07	1H10	CHL	608
H	0.073653	68.73	83.47	46.68	2H10	CHL	608
H	0.015417	67.90	81.48	46.51	1H11	CHL	608
H	0.015417	69.34	81.04	45.87	2H11	CHL	608
H	0.036623	68.58	81.17	43.77	1H12	CHL	608
H	0.036623	67.37	82.19	44.17	2H12	CHL	608
H	0.048461	66.73	78.14	44.06	1H14	CHL	608
H	0.048461	67.97	78.82	43.25	2H14	CHL	608
H	0.048461	68.07	78.59	44.86	3H14	CHL	608
H	0.037455	65.62	81.60	43.47	1H15	CHL	608
H	0.037455	64.81	80.42	44.26	2H15	CHL	608
H	-0.021542	64.27	79.50	42.46	1H16	CHL	608
H	-0.021542	65.83	79.42	41.96	2H16	CHL	608
H	0.043717	64.67	81.88	41.49	1H17	CHL	608
H	0.043717	63.89	80.65	40.74	2H17	CHL	608
H	0.058595	67.51	81.93	39.26	1H19	CHL	608
H	0.058595	66.76	82.83	40.39	2H19	CHL	608
H	0.058595	67.53	81.46	40.82	3H19	CHL	608
H	0.058595	66.81	80.06	38.48	1H20	CHL	608
H	0.058595	66.73	79.31	39.93	2H20	CHL	608
H	0.058595	65.44	79.30	38.93	3H20	CHL	608
Mg	1.169200	53.47	87.38	46.16	MG	CHL	609
C	-0.004739	51.02	92.11	47.18	CAA	CHL	609
C	-0.112834	52.54	84.00	50.70	CAB	CHL	609
C	0.160477	53.40	83.00	42.42	CAC	CHL	609
C	0.627291	53.02	91.17	42.45	CAD	CHL	609
N	-0.489633	53.06	89.35	46.97	NA	CHL	609
C	-0.219908	49.96	91.08	46.76	CBA	CHL	609
C	-0.367704	52.65	82.67	50.45	CBB	CHL	609
C	-0.168957	52.00	82.47	42.09	CBC	CHL	609
C	-0.692237	52.82	91.79	43.88	CBD	CHL	609
N	-0.549527	53.09	86.55	48.00	NB	CHL	609
O	-0.531678	53.00	91.88	41.44	OBD	CHL	609
C	0.826782	48.50	91.28	46.88	CGA	CHL	609
C	0.975656	53.91	92.88	44.14	CGD	CHL	609
N	-0.548096	53.44	85.49	45.29	NC	CHL	609
N	-0.486413	53.46	88.17	44.28	ND	CHL	609

C	0.040004	54.35	95.18	43.48	CED	CHL	609
C	0.087495	52.97	90.59	44.83	CHA	CHL	609
C	-0.519448	52.83	88.64	49.31	CHB	CHL	609
C	-0.373104	53.12	84.17	47.36	CHC	CHL	609
C	-0.358246	53.38	86.16	42.91	CHD	CHL	609
C	-0.410730	54.06	91.70	49.12	CMA	CHL	609
C	-0.236326	52.90	86.80	51.74	CMB	CHL	609
C	0.440869	53.34	81.81	45.43	CMC	CHL	609
C	-0.266591	53.21	88.26	40.45	CMD	CHL	609
O	-0.537107	53.19	81.20	46.49	OMC	CHL	609
C	0.018007	52.88	90.52	46.24	C1A	CHL	609
C	0.290707	52.91	87.25	49.17	C1B	CHL	609
C	0.332773	53.32	84.29	45.96	C1C	CHL	609
C	0.191076	53.39	87.55	43.05	C1D	CHL	609
O	-0.589721	48.02	92.33	47.30	O1A	CHL	609
O	-0.623224	55.01	92.59	44.60	O1D	CHL	609
C	0.037093	52.49	91.66	47.18	C2A	CHL	609
C	0.078577	52.87	86.32	50.27	C2B	CHL	609
C	-0.147964	53.37	83.20	44.99	C2C	CHL	609
C	0.084438	53.27	88.53	41.97	C2D	CHL	609
O	-0.485288	47.63	90.17	46.51	O2A	CHL	609
O	-0.399841	53.49	94.19	43.91	O2D	CHL	609
C	0.179052	52.77	91.11	48.55	C3A	CHL	609
C	-0.054715	52.83	85.06	49.73	C3B	CHL	609
C	-0.234405	53.41	83.76	43.76	C3C	CHL	609
C	-0.158062	53.19	89.74	42.61	C3D	CHL	609
C	0.345332	52.90	89.61	48.32	C4A	CHL	609
C	0.233194	53.01	85.21	48.29	C4B	CHL	609
C	0.342833	53.42	85.20	43.93	C4C	CHL	609
C	0.130108	53.21	89.48	44.02	C4D	CHL	609
C	0.345381	46.35	90.51	45.91	C1	CHL	609
C	-0.477083	46.12	89.63	44.80	C2	CHL	609
C	0.260847	45.45	88.42	44.72	C3	CHL	609
C	-0.269607	44.74	87.68	45.89	C4	CHL	609
C	-0.336279	45.37	87.69	43.37	C5	CHL	609
C	0.119257	44.46	88.25	42.27	C6	CHL	609
C	-0.175039	45.13	88.09	40.91	C7	CHL	609
C	0.331362	44.39	88.49	39.64	C8	CHL	609
C	-0.313835	44.57	89.97	39.33	C9	CHL	609
C	-0.284648	44.84	87.71	38.42	C10	CHL	609
C	0.041634	43.70	87.30	37.51	C11	CHL	609
C	-0.154439	44.29	87.38	36.12	C12	CHL	609
C	0.196709	43.31	87.39	34.96	C13	CHL	609
C	-0.232704	43.43	88.68	34.16	C14	CHL	609
C	-0.201414	43.18	86.04	34.26	C15	CHL	609
C	0.209589	43.59	85.81	32.80	C16	CHL	609

C	-0.269983	42.80	84.68	32.14	C17	CHL	609
C	0.432452	42.99	84.40	30.66	C18	CHL	609
C	-0.315373	42.00	83.33	30.26	C19	CHL	609
C	-0.315373	42.57	85.56	29.77	C20	CHL	609
H	0.003832	50.94	92.89	46.55	1HAA	CHL	609
H	0.003832	50.79	92.41	48.11	2HAA	CHL	609
H	0.140703	52.24	84.28	51.61	HAB	CHL	609
H	-0.000428	53.70	83.61	41.69	1HAC	CHL	609
H	-0.000428	54.04	82.22	42.48	2HAC	CHL	609
H	0.057072	50.11	90.89	45.79	1HBA	CHL	609
H	0.057072	50.14	90.25	47.29	2HBA	CHL	609
H	0.167066	52.94	82.35	49.55	1HBB	CHL	609
H	0.167066	52.43	82.01	51.17	2HBB	CHL	609
H	0.046995	52.03	81.98	41.22	1HBC	CHL	609
H	0.046995	51.70	81.85	42.82	2HBC	CHL	609
H	0.046995	51.37	83.24	42.03	3HBC	CHL	609
H	0.218234	51.94	92.23	44.02	HBD	CHL	609
H	0.063428	53.84	96.04	43.38	1HED	CHL	609
H	0.063428	55.09	95.30	44.14	2HED	CHL	609
H	0.063428	54.74	94.92	42.59	3HED	CHL	609
H	0.175319	52.70	88.98	50.24	HHB	CHL	609
H	0.209400	53.04	83.24	47.72	HHC	CHL	609
H	0.200579	53.35	85.81	41.97	HHD	CHL	609
H	0.104969	54.23	91.33	50.03	1HMA	CHL	609
H	0.104969	54.83	91.47	48.51	2HMA	CHL	609
H	0.104969	53.98	92.70	49.18	3HMA	CHL	609
H	0.077125	52.87	86.01	52.35	1HMB	CHL	609
H	0.077125	53.73	87.32	51.91	2HMB	CHL	609
H	0.077125	52.10	87.39	51.91	3HMB	CHL	609
H	0.021209	53.47	81.18	44.67	HMC	CHL	609
H	0.090203	53.12	89.13	39.96	1HMD	CHL	609
H	0.090203	54.04	87.79	40.15	2HMD	CHL	609
H	0.090203	52.41	87.69	40.24	3HMD	CHL	609
H	0.205820	46.51	89.95	43.94	H2	CHL	609
H	-0.019695	43.43	88.29	39.83	H8	CHL	609
H	0.016242	46.36	91.45	45.58	H11	CHL	609
H	0.016242	45.61	90.40	46.58	H12	CHL	609
H	-0.010572	42.37	87.45	35.30	H13	CHL	609
H	-0.061651	43.96	84.18	30.54	H18	CHL	609
H	0.059830	53.02	92.47	46.90	H2A	CHL	609
H	0.085694	44.34	86.83	45.55	H41	CHL	609
H	0.085694	45.41	87.47	46.60	H42	CHL	609
H	0.085694	44.02	88.26	46.27	H43	CHL	609
H	0.032055	52.04	91.33	49.20	H3A	CHL	609
H	0.096900	45.06	86.76	43.55	H51	CHL	609
H	0.096900	46.29	87.67	42.99	H52	CHL	609

H	-0.002304	44.28	89.22	42.44	H61	CHL	609
H	-0.002304	43.59	87.75	42.27	H62	CHL	609
H	0.027697	45.37	87.12	40.82	H71	CHL	609
H	0.027697	45.97	88.64	40.94	H72	CHL	609
H	0.069285	44.08	90.20	38.49	H91	CHL	609
H	0.069285	44.22	90.52	40.09	H92	CHL	609
H	0.069285	45.55	90.16	39.20	H93	CHL	609
H	0.073653	45.31	86.88	38.73	1H10	CHL	609
H	0.073653	45.48	88.27	37.89	2H10	CHL	609
H	0.015417	42.92	87.92	37.61	1H11	CHL	609
H	0.015417	43.40	86.36	37.71	2H11	CHL	609
H	0.036623	44.89	86.59	36.01	1H12	CHL	609
H	0.036623	44.82	88.22	36.08	2H12	CHL	609
H	0.048461	42.78	88.66	33.40	1H14	CHL	609
H	0.048461	43.24	89.46	34.75	2H14	CHL	609
H	0.048461	44.36	88.76	33.80	3H14	CHL	609
H	0.037455	42.21	85.80	34.31	1H15	CHL	609
H	0.037455	43.72	85.40	34.80	2H15	CHL	609
H	-0.021542	44.56	85.58	32.77	1H16	CHL	609
H	-0.021542	43.43	86.65	32.29	2H16	CHL	609
H	0.043717	41.84	84.88	32.28	1H17	CHL	609
H	0.043717	43.04	83.84	32.63	2H17	CHL	609
H	0.058595	42.10	83.13	29.29	1H19	CHL	609
H	0.058595	42.17	82.50	30.79	2H19	CHL	609
H	0.058595	41.07	83.66	30.44	3H19	CHL	609
H	0.058595	42.71	85.31	28.81	1H20	CHL	609
H	0.058595	41.60	85.75	29.92	2H20	CHL	609
H	0.058595	43.11	86.37	29.99	3H20	CHL	609
Mg	0.988885	66.88	90.75	36.64	MG	CLA	610
C	-0.248758	68.88	92.37	39.03	CHA	CLA	610
C	-0.093585	68.55	92.48	34.16	CHB	CLA	610
C	-0.014122	65.56	88.58	34.33	CHC	CLA	610
C	-0.320450	65.49	88.90	39.22	CHD	CLA	610
N	-0.471184	68.41	92.29	36.60	NA	CLA	610
C	0.284481	69.17	92.73	37.69	C1A	CLA	610
C	-0.124913	70.29	93.61	37.18	C2A	CLA	610
C	0.095258	69.81	94.02	35.81	C3A	CLA	610
C	0.037815	68.84	92.91	35.45	C4A	CLA	610
C	-0.328981	69.06	95.38	35.81	CMA	CLA	610
C	0.317603	71.65	92.88	37.14	CAA	CLA	610
C	-0.161281	71.89	91.44	36.59	CBA	CLA	610
C	0.687537	71.93	91.24	35.05	CGA	CLA	610
O	-0.542233	72.25	92.22	34.36	O1A	CLA	610
O	-0.661682	71.60	89.97	34.38	O2A	CLA	610
N	-0.250663	67.09	90.52	34.62	NB	CLA	610
C	-0.107131	67.77	91.39	33.78	C1B	CLA	610

C	0.072858	67.49	91.02	32.41	C2B	CLA	610
C	0.117795	66.73	89.88	32.43	C3B	CLA	610
C	-0.155342	66.41	89.60	33.84	C4B	CLA	610
C	-0.282443	68.01	91.86	31.22	CMB	CLA	610
C	-0.254125	66.50	89.29	31.11	CAB	CLA	610
C	-0.328350	65.79	88.20	30.87	CBB	CLA	610
N	-0.365548	65.68	89.06	36.77	NC	CLA	610
C	-0.059640	65.23	88.33	35.69	C1C	CLA	610
C	0.201507	64.36	87.26	36.19	C2C	CLA	610
C	-0.316570	64.41	87.31	37.55	C3C	CLA	610
C	0.186797	65.20	88.46	37.92	C4C	CLA	610
C	-0.453747	63.57	86.21	35.41	CMC	CLA	610
C	0.324955	63.74	86.34	38.57	CAC	CLA	610
C	0.015876	64.63	85.12	38.86	CBC	CLA	610
N	-0.833487	66.92	90.80	38.66	ND	CLA	610
C	0.321441	66.30	89.99	39.59	C1D	CLA	610
C	0.037327	66.67	90.39	40.95	C2D	CLA	610
C	-0.266963	67.64	91.34	40.79	C3D	CLA	610
C	0.492494	67.83	91.53	39.38	C4D	CLA	610
C	-0.291118	66.09	89.86	42.26	CMD	CLA	610
C	0.601942	68.57	92.23	41.45	CAD	CLA	610
O	-0.445079	68.66	92.57	42.63	OBD	CLA	610
C	-0.579060	69.53	92.79	40.35	CBD	CLA	610
C	0.766237	69.67	94.33	40.49	CGD	CLA	610
O	-0.516295	68.72	95.10	40.32	O1D	CLA	610
O	-0.402165	71.01	94.75	40.78	O2D	CLA	610
C	0.036010	71.31	95.99	41.35	CED	CLA	610
C	1.199790	71.23	90.05	32.97	C1	CLA	610
C	-0.878268	70.63	88.78	32.56	C2	CLA	610
C	0.309015	71.23	87.74	31.84	C3	CLA	610
C	-0.405165	72.71	87.73	31.35	C4	CLA	610
C	-0.324908	70.42	86.50	31.43	C5	CLA	610
C	0.274037	70.67	85.23	32.23	C6	CLA	610
C	-0.101500	70.10	83.96	31.59	C7	CLA	610
C	0.417045	70.05	82.76	32.54	C8	CLA	610
C	-0.389623	71.39	82.04	32.71	C9	CLA	610
C	-0.365008	68.94	81.75	32.26	C10	CLA	610
C	0.506051	68.29	81.32	33.57	C11	CLA	610
C	-0.389841	67.53	80.00	33.40	C12	CLA	610
C	0.381461	67.08	79.18	34.61	C13	CLA	610
C	-0.086919	66.27	79.92	35.67	C14	CLA	610
C	-0.231164	68.15	78.16	35.00	C15	CLA	610
C	0.194682	68.05	77.35	36.28	C16	CLA	610
C	-0.204822	69.27	76.54	36.71	C17	CLA	610
C	0.444563	69.05	75.59	37.89	C18	CLA	610
C	-0.424301	70.22	74.61	37.96	C19	CLA	610

C	-0.349598	68.85	76.24	39.26	C20	CLA	610
H	0.128998	68.95	93.02	33.42	HHB	CLA	610
H	0.147395	65.14	87.98	33.65	HHC	CLA	610
H	0.162465	65.08	88.38	39.97	HHD	CLA	610
H	0.091350	70.44	94.41	37.76	H2A	CLA	610
H	0.080596	70.58	94.12	35.18	H3A	CLA	610
H	0.078073	68.77	95.59	34.87	1HMA	CLA	610
H	0.084566	68.27	95.32	36.40	2HMA	CLA	610
H	0.106282	69.68	96.09	36.13	3HMA	CLA	610
H	-0.076675	71.97	92.85	38.09	1HAA	CLA	610
H	-0.068696	72.26	93.46	36.60	2HAA	CLA	610
H	0.084108	72.76	91.12	36.95	1HBA	CLA	610
H	0.063653	71.15	90.86	36.94	2HBA	CLA	610
H	0.066027	67.71	91.44	30.36	1HMB	CLA	610
H	0.088663	67.65	92.79	31.29	2HMB	CLA	610
H	0.126583	69.01	91.89	31.25	3HMB	CLA	610
H	0.199497	66.92	89.76	30.33	HAB	CLA	610
H	0.168135	65.36	87.71	31.62	1HBB	CLA	610
H	0.167559	65.69	87.87	29.93	2HBB	CLA	610
H	0.156307	63.07	85.62	36.05	1HMC	CLA	610
H	0.094565	62.92	86.66	34.80	2HMC	CLA	610
H	0.181014	64.20	85.65	34.87	3HMC	CLA	610
H	-0.086504	63.56	86.82	39.42	1HAC	CLA	610
H	-0.058919	62.87	86.01	38.19	2HAC	CLA	610
H	-0.033765	64.17	84.52	39.51	1HBC	CLA	610
H	0.004739	64.80	84.63	38.01	2HBC	CLA	610
H	0.030974	65.50	85.44	39.24	3HBC	CLA	610
H	0.129643	66.54	90.32	43.03	1HMD	CLA	610
H	0.067407	65.11	90.04	42.29	2HMD	CLA	610
H	0.146968	66.26	88.87	42.32	3HMD	CLA	610
H	0.252505	70.47	92.45	40.40	HBD	CLA	610
H	0.093995	72.30	96.07	41.47	1HED	CLA	610
H	0.051124	70.99	96.72	40.74	2HED	CLA	610
H	0.071934	70.86	96.07	42.24	3HED	CLA	610
H	-0.162848	72.05	90.22	32.42	H11	CLA	610
H	-0.292171	70.58	90.79	32.83	H12	CLA	610
H	0.331312	69.68	88.64	32.82	H2	CLA	610
H	0.136201	72.89	86.88	30.86	H41	CLA	610
H	0.119462	72.86	88.51	30.73	H42	CLA	610
H	0.135922	73.32	87.81	32.13	H43	CLA	610
H	0.091426	70.63	86.30	30.47	H51	CLA	610
H	0.081966	69.44	86.72	31.51	H52	CLA	610
H	-0.042398	70.24	85.33	33.13	H61	CLA	610
H	-0.050036	71.65	85.11	32.34	H62	CLA	610
H	-0.004755	70.68	83.72	30.81	H71	CLA	610
H	-0.001033	69.17	84.15	31.28	H72	CLA	610

H	-0.115353	69.82	83.19	33.41	H8	CLA	610
H	0.100111	71.28	81.27	33.34	H91	CLA	610
H	0.092151	71.70	81.70	31.82	H92	CLA	610
H	0.068924	72.07	82.67	33.08	H93	CLA	610
H	0.069029	69.32	80.95	31.80	1H10	CLA	610
H	0.061629	68.25	82.18	31.67	2H10	CLA	610
H	-0.111606	67.65	82.03	33.86	1H11	CLA	610
H	-0.112571	69.00	81.20	34.26	2H11	CLA	610
H	0.066443	68.12	79.40	32.86	1H12	CLA	610
H	0.053647	66.70	80.21	32.88	2H12	CLA	610
H	-0.064459	66.31	78.60	34.35	H13	CLA	610
H	0.001093	66.03	79.28	36.41	1H14	CLA	610
H	-0.043936	66.81	80.67	36.04	2H14	CLA	610
H	0.010206	65.43	80.28	35.26	3H14	CLA	610
H	0.024125	69.01	78.66	35.05	1H15	CLA	610
H	0.050903	68.19	77.50	34.25	2H15	CLA	610
H	-0.039279	67.29	76.70	36.17	1H16	CLA	610
H	-0.027613	67.84	77.99	37.02	2H16	CLA	610
H	0.020039	69.99	77.19	36.96	1H17	CLA	610
H	0.038779	69.57	76.00	35.92	2H17	CLA	610
H	-0.074994	68.19	75.13	37.69	H18	CLA	610
H	0.099281	70.09	73.98	38.73	1H19	CLA	610
H	0.091432	70.27	74.09	37.11	2H19	CLA	610
H	0.094621	71.07	75.12	38.09	3H19	CLA	610
H	0.087563	68.72	75.52	39.95	1H20	CLA	610
H	0.075366	69.66	76.78	39.49	2H20	CLA	610
H	0.053427	68.05	76.83	39.24	3H20	CLA	610
Mg	1.342619	63.85	94.97	19.32	MG	CLA	611
C	0.087461	66.26	95.15	21.87	CHA	CLA	611
C	-0.575487	66.01	96.69	17.24	CHB	CLA	611
C	-0.318916	61.85	94.17	16.66	CHC	CLA	611
C	-0.502407	62.09	92.67	21.28	CHD	CLA	611
N	-0.737527	65.83	95.86	19.55	NA	CLA	611
C	0.066774	66.64	95.81	20.67	C1A	CLA	611
C	0.317943	67.99	96.45	20.37	C2A	CLA	611
C	-0.017837	67.74	97.20	19.10	C3A	CLA	611
C	0.468831	66.47	96.57	18.55	C4A	CLA	611
C	-0.403505	67.58	98.70	19.41	CMA	CLA	611
C	-0.100557	69.17	95.62	19.87	CAA	CLA	611
C	0.014388	69.48	94.18	20.21	CBA	CLA	611
C	0.618203	70.09	93.17	19.26	CGA	CLA	611
O	-0.511748	71.09	93.47	18.60	O1A	CLA	611
O	-0.451026	69.53	91.85	19.08	O2A	CLA	611
N	-0.716056	63.87	95.44	17.34	NB	CLA	611
C	0.281630	64.84	96.17	16.68	C1B	CLA	611
C	0.141051	64.51	96.25	15.28	C2B	CLA	611

C	-0.252949	63.35	95.54	15.09	C3B	CLA	611
C	0.412461	62.94	95.02	16.40	C4B	CLA	611
C	-0.344417	65.40	96.99	14.25	CMB	CLA	611
C	-0.011389	62.85	95.51	13.72	CAB	CLA	611
C	-0.454523	61.88	94.66	13.27	CBB	CLA	611
N	-0.707764	62.19	93.72	19.06	NC	CLA	611
C	0.213139	61.50	93.57	17.88	C1C	CLA	611
C	0.200428	60.38	92.68	18.09	C2C	CLA	611
C	-0.353579	60.46	92.23	19.38	C3C	CLA	611
C	0.489722	61.62	92.86	19.97	C4C	CLA	611
C	-0.452389	59.34	92.24	17.05	CMC	CLA	611
C	0.157503	59.45	91.30	20.09	CAC	CLA	611
C	-0.220205	59.77	89.81	19.96	CBC	CLA	611
N	-0.640163	64.00	94.21	21.19	ND	CLA	611
C	0.347504	63.20	93.30	21.87	C1D	CLA	611
C	0.129357	63.74	93.04	23.20	C2D	CLA	611
C	-0.286759	64.90	93.77	23.27	C3D	CLA	611
C	0.207445	65.07	94.44	22.01	C4D	CLA	611
C	-0.347760	63.15	92.10	24.25	CMD	CLA	611
C	0.666102	66.07	94.11	24.07	CAD	CLA	611
O	-0.514954	66.42	93.73	25.19	OBD	CLA	611
C	-0.545725	66.97	95.07	23.22	CBD	CLA	611
C	0.776027	67.07	96.45	23.93	CGD	CLA	611
O	-0.506632	66.15	97.27	23.87	O1D	CLA	611
O	-0.432965	68.25	96.65	24.71	O2D	CLA	611
C	0.117631	68.45	97.83	25.44	CED	CLA	611
C	0.375242	70.37	90.74	19.49	C1	CLA	611
C	-0.489743	69.53	89.67	19.97	C2	CLA	611
C	0.222476	68.73	88.72	19.33	C3	CLA	611
C	-0.347416	68.54	88.58	17.81	C4	CLA	611
C	-0.289548	67.89	87.69	20.10	C5	CLA	611
C	0.243217	68.71	86.62	20.81	C6	CLA	611
C	-0.482513	68.52	86.72	22.32	C7	CLA	611
C	0.408378	68.09	85.50	23.15	C8	CLA	611
C	-0.445179	69.18	85.07	24.12	C9	CLA	611
C	0.015317	67.24	84.43	22.45	C10	CLA	611
C	0.072899	66.74	83.20	23.17	C11	CLA	611
C	-0.259841	66.80	82.01	22.22	C12	CLA	611
C	0.357243	65.58	81.11	22.01	C13	CLA	611
C	-0.524289	64.75	81.61	20.83	C14	CLA	611
C	-0.104346	64.75	80.65	23.23	C15	CLA	611
C	0.075153	65.33	79.69	24.27	C16	CLA	611
C	-0.129706	64.84	78.24	24.20	C17	CLA	611
C	0.389800	64.74	77.50	25.53	C18	CLA	611
C	-0.407579	63.47	76.67	25.57	C19	CLA	611
C	-0.408977	65.90	76.54	25.72	C20	CLA	611

H	0.189702	66.60	97.22	16.62	HHB	CLA	611
H	0.164262	61.25	93.97	15.88	HHC	CLA	611
H	0.239495	61.59	92.03	21.85	HHD	CLA	611
H	-0.023921	68.23	96.88	21.24	H2A	CLA	611
H	0.052651	68.49	97.13	18.45	H3A	CLA	611
H	0.111257	67.41	99.20	18.56	1HMA	CLA	611
H	0.081420	66.81	98.83	20.03	2HMA	CLA	611
H	0.114998	68.41	99.04	19.84	3HMA	CLA	611
H	0.003768	69.99	96.12	20.14	1HAA	CLA	611
H	0.013821	69.10	95.62	18.87	2HAA	CLA	611
H	0.061180	70.10	94.22	21.00	1HBA	CLA	611
H	-0.019213	68.60	93.79	20.50	2HBA	CLA	611
H	0.104809	64.99	96.93	13.34	1HMB	CLA	611
H	0.090777	65.48	97.95	14.51	2HMB	CLA	611
H	0.104150	66.31	96.57	14.24	3HMB	CLA	611
H	0.121208	63.24	96.16	13.07	HAB	CLA	611
H	0.196789	61.46	94.00	13.89	1HBB	CLA	611
H	0.164693	61.58	94.70	12.31	2HBB	CLA	611
H	0.175218	58.68	91.62	17.48	1HMC	CLA	611
H	0.140939	58.86	93.05	16.70	2HMC	CLA	611
H	0.110110	59.80	91.77	16.30	3HMC	CLA	611
H	-0.014721	59.44	91.52	21.07	1HAC	CLA	611
H	0.029755	58.54	91.45	19.70	2HAC	CLA	611
H	0.064761	59.08	89.27	20.44	1HBC	CLA	611
H	0.067532	59.77	89.56	18.99	2HBC	CLA	611
H	0.051630	60.67	89.63	20.35	3HBC	CLA	611
H	0.139725	63.71	92.11	25.07	1HMD	CLA	611
H	0.130465	62.22	92.40	24.48	2HMD	CLA	611
H	0.106866	63.12	91.17	23.88	3HMD	CLA	611
H	0.174838	67.91	94.75	23.10	HBD	CLA	611
H	0.070035	69.32	97.78	25.92	1HED	CLA	611
H	0.023578	68.45	98.61	24.81	2HED	CLA	611
H	0.027910	67.71	97.93	26.10	3HED	CLA	611
H	0.007440	71.00	91.03	20.21	H11	CLA	611
H	0.003476	70.91	90.41	18.70	H12	CLA	611
H	0.190987	69.51	89.59	20.97	H2	CLA	611
H	0.090291	67.92	87.82	17.63	H41	CLA	611
H	0.121102	68.16	89.42	17.44	H42	CLA	611
H	0.112963	69.43	88.39	17.39	H43	CLA	611
H	0.106873	67.28	87.23	19.45	H51	CLA	611
H	0.083896	67.35	88.17	20.79	H52	CLA	611
H	-0.038091	69.68	86.75	20.59	H61	CLA	611
H	-0.040967	68.41	85.72	20.50	H62	CLA	611
H	0.129647	67.82	87.42	22.47	H71	CLA	611
H	0.114607	69.39	87.02	22.70	H72	CLA	611
H	-0.087041	67.35	85.82	23.75	H8	CLA	611

H	0.112295	68.87	84.27	24.64	H91	CLA	611
H	0.076715	70.01	84.83	23.60	H92	CLA	611
H	0.102338	69.39	85.82	24.74	H93	CLA	611
H	-0.025597	67.78	84.09	21.68	1H10	CLA	611
H	0.014503	66.42	84.89	22.10	2H10	CLA	611
H	-0.003178	65.80	83.35	23.47	1H11	CLA	611
H	-0.023552	67.32	83.03	23.97	2H11	CLA	611
H	0.058316	67.54	81.42	22.54	1H12	CLA	611
H	0.043866	67.05	82.38	21.32	2H12	CLA	611
H	-0.056546	65.98	80.23	21.78	H13	CLA	611
H	0.121422	63.95	81.02	20.71	1H14	CLA	611
H	0.120582	64.44	82.54	21.02	2H14	CLA	611
H	0.130739	65.30	81.60	20.00	3H14	CLA	611
H	0.015972	63.93	80.21	22.86	1H15	CLA	611
H	0.008955	64.49	81.48	23.72	2H15	CLA	611
H	-0.013331	65.09	80.04	25.18	1H16	CLA	611
H	-0.010767	66.32	79.68	24.16	2H16	CLA	611
H	0.020869	65.48	77.73	23.62	1H17	CLA	611
H	0.020201	63.94	78.24	23.78	2H17	CLA	611
H	-0.050739	64.74	78.19	26.26	H18	CLA	611
H	0.097982	63.41	76.19	26.45	1H19	CLA	611
H	0.083816	62.68	77.27	25.46	2H19	CLA	611
H	0.100471	63.48	76.00	24.83	3H19	CLA	611
H	0.095762	65.81	76.07	26.60	1H20	CLA	611
H	0.107142	65.90	75.87	24.98	2H20	CLA	611
H	0.066524	66.76	77.05	25.70	3H20	CLA	611
Mg	1.343183	65.88	87.59	25.37	MG	CLA	612
C	-0.093872	68.37	90.05	25.04	CHA	CLA	612
C	-0.540529	67.80	86.13	27.90	CHB	CLA	612
C	-0.329536	64.01	84.70	25.16	CHC	CLA	612
C	-0.449269	64.60	88.59	22.31	CHD	CLA	612
N	-0.540340	67.76	88.11	26.44	NA	CLA	612
C	-0.067258	68.59	89.19	26.16	C1A	CLA	612
C	0.412566	69.73	89.25	27.16	C2A	CLA	612
C	-0.064845	69.64	87.94	27.90	C3A	CLA	612
C	0.330603	68.32	87.34	27.44	C4A	CLA	612
C	-0.245494	70.87	87.09	27.56	CMA	CLA	612
C	-0.019159	69.77	90.42	28.14	CAA	CLA	612
C	-0.313079	70.98	90.64	29.06	CBA	CLA	612
C	0.711499	72.32	90.85	28.38	CGA	CLA	612
O	-0.512712	72.56	91.93	27.85	O1A	CLA	612
O	-0.571616	73.35	89.84	28.36	O2A	CLA	612
N	-0.720294	65.78	85.82	26.48	NB	CLA	612
C	0.443415	66.66	85.43	27.47	C1B	CLA	612
C	0.000977	66.31	84.10	27.90	C2B	CLA	612
C	-0.004004	65.25	83.68	27.15	C3B	CLA	612

C	0.274585	64.94	84.76	26.22	C4B	CLA	612
C	-0.279911	67.09	83.38	29.04	CMB	CLA	612
C	-0.130003	64.74	82.35	27.47	CAB	CLA	612
C	-0.416041	63.58	81.83	26.99	CBB	CLA	612
N	-0.681351	64.43	86.88	24.06	NC	CLA	612
C	0.212990	63.77	85.67	24.17	C1C	CLA	612
C	0.167467	62.86	85.52	23.05	C2C	CLA	612
C	-0.312054	63.04	86.59	22.23	C3C	CLA	612
C	0.414235	64.05	87.43	22.85	C4C	CLA	612
C	-0.464362	61.97	84.30	22.71	CMC	CLA	612
C	0.203082	62.34	86.91	20.90	CAC	CLA	612
C	-0.223703	63.12	86.39	19.70	CBC	CLA	612
N	-0.637089	66.22	89.09	24.08	ND	CLA	612
C	0.265568	65.62	89.37	22.86	C1D	CLA	612
C	0.156923	66.33	90.44	22.18	C2D	CLA	612
C	-0.300772	67.36	90.78	23.01	C3D	CLA	612
C	0.239774	67.32	89.90	24.14	C4D	CLA	612
C	-0.383548	66.00	91.02	20.81	CMD	CLA	612
C	0.648522	68.48	91.66	23.22	CAD	CLA	612
O	-0.533693	68.90	92.58	22.54	OBD	CLA	612
C	-0.492649	69.17	91.27	24.54	CBD	CLA	612
C	0.685942	70.66	90.93	24.27	CGD	CLA	612
O	-0.485170	71.52	91.52	24.93	O1D	CLA	612
O	-0.402315	70.96	90.05	23.18	O2D	CLA	612
C	0.117167	71.91	89.06	23.23	CED	CLA	612
C	0.758091	73.91	89.50	27.05	C1	CLA	612
C	-0.579598	74.79	88.35	27.21	C2	CLA	612
C	0.212309	75.21	87.33	26.35	C3	CLA	612
C	-0.339460	74.83	87.13	24.86	C4	CLA	612
C	-0.156926	76.14	86.19	26.84	C5	CLA	612
C	0.136251	75.61	85.34	28.00	C6	CLA	612
C	-0.229782	74.74	84.17	27.53	C7	CLA	612
C	0.453669	73.47	83.81	28.31	C8	CLA	612
C	-0.365079	73.73	83.40	29.75	C9	CLA	612
C	-0.228426	72.69	82.66	27.67	C10	CLA	612
C	-0.047505	71.81	82.91	26.45	C11	CLA	612
C	-0.075127	70.41	82.45	26.87	C12	CLA	612
C	0.371202	69.86	81.06	26.54	C13	CLA	612
C	-0.294104	68.75	81.18	25.51	C14	CLA	612
C	-0.123006	69.54	80.27	27.82	C15	CLA	612
C	0.258295	68.57	79.09	27.97	C16	CLA	612
C	-0.188068	68.89	78.31	29.24	C17	CLA	612
C	0.494189	68.18	76.98	29.47	C18	CLA	612
C	-0.458069	68.79	75.84	28.66	C19	CLA	612
C	-0.417946	68.21	76.61	30.95	C20	CLA	612
H	0.206689	68.31	85.70	28.64	HHB	CLA	612

H	0.158986	63.45	83.87	25.12	HHC	CLA	612
H	0.221184	64.23	88.90	21.43	HHD	CLA	612
H	0.005830	70.59	89.38	26.65	H2A	CLA	612
H	0.067697	69.64	88.03	28.90	H3A	CLA	612
H	0.069477	70.82	86.22	28.05	1HMA	CLA	612
H	0.101359	70.90	86.92	26.57	2HMA	CLA	612
H	0.045775	71.70	87.57	27.84	3HMA	CLA	612
H	0.032093	68.97	90.31	28.73	1HAA	CLA	612
H	-0.014187	69.67	91.25	27.59	2HAA	CLA	612
H	0.138895	70.80	91.44	29.62	1HBA	CLA	612
H	0.074914	71.07	89.83	29.64	2HBA	CLA	612
H	0.127319	66.69	82.47	29.19	1HMB	CLA	612
H	0.035260	68.05	83.29	28.78	2HMB	CLA	612
H	0.141606	67.01	83.91	29.88	3HMB	CLA	612
H	0.204367	65.29	81.79	28.09	HAB	CLA	612
H	0.169492	63.00	82.36	26.37	1HBB	CLA	612
H	0.173222	63.30	80.91	27.26	2HBB	CLA	612
H	0.183690	61.46	84.49	21.87	1HMC	CLA	612
H	0.126563	62.55	83.50	22.58	2HMC	CLA	612
H	0.136698	61.34	84.14	23.46	3HMC	CLA	612
H	0.009074	61.44	86.47	20.89	1HAC	CLA	612
H	-0.024413	62.23	87.90	20.81	2HAC	CLA	612
H	0.052560	62.63	86.62	18.86	1HBC	CLA	612
H	0.044387	64.02	86.83	19.68	2HBC	CLA	612
H	0.073047	63.23	85.40	19.77	3HBC	CLA	612
H	0.142395	66.65	91.75	20.58	1HMD	CLA	612
H	0.115236	66.06	90.30	20.12	2HMD	CLA	612
H	0.117093	65.07	91.40	20.82	3HMD	CLA	612
H	0.223180	69.18	91.99	25.24	HBD	CLA	612
H	0.069038	71.93	88.58	22.35	1HED	CLA	612
H	0.040612	72.80	89.47	23.41	2HED	CLA	612
H	0.014757	71.68	88.41	23.96	3HED	CLA	612
H	-0.053690	74.42	90.28	26.70	H11	CLA	612
H	-0.144784	73.17	89.28	26.42	H12	CLA	612
H	0.188069	75.18	88.27	28.13	H2	CLA	612
H	0.106586	75.28	86.31	24.51	H41	CLA	612
H	0.094147	73.83	87.02	24.78	H42	CLA	612
H	0.094957	75.11	87.92	24.33	H43	CLA	612
H	0.038652	77.00	86.60	27.14	H51	CLA	612
H	0.059370	76.31	85.58	26.07	H52	CLA	612
H	-0.042159	75.06	85.92	28.60	H61	CLA	612
H	-0.005755	76.39	84.97	28.51	H62	CLA	612
H	0.032207	75.32	83.36	27.53	H71	CLA	612
H	0.054059	74.46	84.38	26.59	H72	CLA	612
H	-0.085571	72.94	84.66	28.28	H8	CLA	612
H	0.089407	72.87	83.18	30.20	H91	CLA	612

H	0.074006	74.33	82.59	29.77	H92	CLA	612
H	0.046120	74.18	84.15	30.24	H93	CLA	612
H	0.033554	72.10	82.29	28.38	1H10	CLA	612
H	0.045435	73.37	81.98	27.40	2H10	CLA	612
H	0.023664	72.13	82.38	25.67	1H11	CLA	612
H	0.003254	71.80	83.88	26.22	2H11	CLA	612
H	0.002800	69.77	83.10	26.46	1H12	CLA	612
H	0.044901	70.38	82.53	27.87	2H12	CLA	612
H	-0.075649	70.55	80.49	26.09	H13	CLA	612
H	0.051867	68.39	80.27	25.29	1H14	CLA	612
H	0.026211	68.02	81.75	25.88	2H14	CLA	612
H	0.064042	69.12	81.60	24.68	3H14	CLA	612
H	-0.008907	69.21	80.95	28.47	1H15	CLA	612
H	-0.010182	70.42	79.91	28.13	2H15	CLA	612
H	-0.070785	68.66	78.49	27.18	1H16	CLA	612
H	-0.078319	67.64	79.44	28.02	2H16	CLA	612
H	0.026083	68.66	78.90	30.01	1H17	CLA	612
H	0.008441	69.87	78.12	29.23	2H17	CLA	612
H	-0.081209	67.24	77.10	29.17	H18	CLA	612
H	0.106891	68.30	74.99	28.85	1H19	CLA	612
H	0.093401	68.73	76.05	27.69	2H19	CLA	612
H	0.097985	69.75	75.72	28.91	3H19	CLA	612
H	0.101967	67.75	75.73	31.09	1H20	CLA	612
H	0.077257	69.16	76.53	31.26	2H20	CLA	612
H	0.093043	67.75	77.32	31.48	3H20	CLA	612
Mg	1.213279	49.28	83.11	19.77	MG	CLA	613
C	-0.177595	47.83	80.64	17.76	CHA	CLA	613
C	-0.479921	52.33	82.61	18.20	CHB	CLA	613
C	-0.333252	50.50	85.86	21.38	CHC	CLA	613
C	-0.466832	46.10	83.86	20.98	CHD	CLA	613
N	-0.572095	50.00	81.77	18.22	NA	CLA	613
C	0.264236	49.23	80.83	17.53	C1A	CLA	613
C	-0.113606	50.07	80.19	16.42	C2A	CLA	613
C	0.222243	51.47	80.74	16.64	C3A	CLA	613
C	0.301205	51.31	81.75	17.76	C4A	CLA	613
C	-0.310648	52.42	79.56	16.90	CMA	CLA	613
C	0.139152	49.61	80.40	14.96	CAA	CLA	613
C	-0.219597	49.34	81.77	14.33	CBA	CLA	613
C	0.619661	48.11	82.50	14.85	CGA	CLA	613
O	-0.512999	46.97	82.04	14.69	O1A	CLA	613
O	-0.548839	48.28	83.68	15.66	O2A	CLA	613
N	-0.586561	51.11	84.01	19.86	NB	CLA	613
C	0.251452	52.24	83.65	19.15	C1B	CLA	613
C	0.147120	53.32	84.58	19.49	C2B	CLA	613
C	-0.267082	52.80	85.49	20.40	C3B	CLA	613
C	0.316384	51.40	85.14	20.58	C4B	CLA	613

C	-0.305951	54.69	84.37	18.79	CMB	CLA	613
C	0.073286	53.59	86.55	21.03	CAB	CLA	613
C	-0.500289	54.95	86.78	20.98	CBB	CLA	613
N	-0.593622	48.45	84.55	21.03	NC	CLA	613
C	0.085592	49.15	85.60	21.59	C1C	CLA	613
C	0.268474	48.26	86.39	22.43	C2C	CLA	613
C	-0.451947	47.02	85.84	22.30	C3C	CLA	613
C	0.455664	47.14	84.69	21.42	C4C	CLA	613
C	-0.457782	48.68	87.64	23.23	CMC	CLA	613
C	0.293164	45.73	86.33	23.02	CAC	CLA	613
C	-0.247522	45.06	87.46	22.27	CBC	CLA	613
N	-0.768997	47.40	82.41	19.52	ND	CLA	613
C	0.368372	46.21	82.79	20.09	C1D	CLA	613
C	0.098325	45.13	81.92	19.64	C2D	CLA	613
C	-0.308054	45.70	81.06	18.75	C3D	CLA	613
C	0.485045	47.09	81.38	18.67	C4D	CLA	613
C	-0.312568	43.66	82.00	20.11	CMD	CLA	613
C	0.717536	45.49	79.95	17.84	CAD	CLA	613
O	-0.480341	44.49	79.26	17.63	OBD	CLA	613
C	-0.733916	46.82	79.71	17.06	CBD	CLA	613
C	0.798979	47.23	78.20	17.14	CGD	CLA	613
O	-0.439467	47.64	77.65	18.16	O1D	CLA	613
O	-0.423946	47.11	77.53	15.85	O2D	CLA	613
C	0.059234	47.55	76.24	15.57	CED	CLA	613
C	0.763545	47.06	84.35	16.08	C1	CLA	613
C	-0.609112	47.40	85.43	16.94	C2	CLA	613
C	0.221404	46.61	86.14	17.85	C3	CLA	613
C	-0.291093	45.11	85.85	18.12	C4	CLA	613
C	-0.282276	47.08	87.32	18.71	C5	CLA	613
C	0.265558	48.52	87.78	18.65	C6	CLA	613
C	-0.342427	48.73	88.86	17.61	C7	CLA	613
C	0.384024	50.15	88.90	17.10	C8	CLA	613
C	-0.243224	51.18	89.35	18.15	C9	CLA	613
C	-0.120790	50.23	89.53	15.71	C10	CLA	613
C	0.278345	51.59	89.60	15.04	C11	CLA	613
C	-0.326301	51.31	89.67	13.57	C12	CLA	613
C	0.437179	52.54	89.76	12.70	C13	CLA	613
C	-0.344903	52.33	90.84	11.65	C14	CLA	613
C	-0.127926	52.76	88.39	12.08	C15	CLA	613
C	0.051226	53.94	87.58	12.56	C16	CLA	613
C	-0.122781	54.60	86.90	11.37	C17	CLA	613
C	0.382315	55.33	85.58	11.57	C18	CLA	613
C	-0.385565	55.50	84.93	10.20	C19	CLA	613
C	-0.292434	56.67	85.75	12.29	C20	CLA	613
H	0.180036	53.22	82.48	17.78	HHB	CLA	613
H	0.169495	50.88	86.66	21.85	HHC	CLA	613

H	0.207815	45.19	84.05	21.35	HHD	CLA	613
H	0.111409	49.98	79.20	16.52	H2A	CLA	613
H	-0.013278	51.89	81.21	15.86	H3A	CLA	613
H	0.076858	53.35	79.91	17.04	1HMA	CLA	613
H	0.130947	52.12	79.06	17.71	2HMA	CLA	613
H	0.084142	52.41	78.95	16.11	3HMA	CLA	613
H	-0.032786	48.76	79.88	14.86	1HAA	CLA	613
H	0.008394	50.32	79.98	14.39	2HAA	CLA	613
H	0.050135	50.13	82.35	14.49	1HBA	CLA	613
H	0.102801	49.21	81.64	13.34	2HBA	CLA	613
H	0.073494	55.33	85.07	19.11	1HMB	CLA	613
H	0.120476	55.05	83.46	19.02	2HMB	CLA	613
H	0.096460	54.58	84.45	17.80	3HMB	CLA	613
H	0.073632	53.07	87.20	21.58	HAB	CLA	613
H	0.201174	55.54	86.17	20.45	1HBB	CLA	613
H	0.166073	55.35	87.55	21.48	2HBB	CLA	613
H	0.127800	47.89	88.00	23.72	1HMC	CLA	613
H	0.144638	49.39	87.39	23.89	2HMC	CLA	613
H	0.119988	49.03	88.34	22.60	3HMC	CLA	613
H	-0.029215	45.09	85.57	23.08	1HAC	CLA	613
H	-0.023783	45.96	86.64	23.94	2HAC	CLA	613
H	0.039264	44.24	87.75	22.76	1HBC	CLA	613
H	0.050613	45.70	88.24	22.20	2HBC	CLA	613
H	0.072927	44.82	87.16	21.35	3HBC	CLA	613
H	0.124690	43.12	81.29	19.65	1HMD	CLA	613
H	0.116571	43.61	81.86	21.10	2HMD	CLA	613
H	0.079629	43.28	82.90	19.88	3HMD	CLA	613
H	0.280742	46.76	79.92	16.09	HBD	CLA	613
H	0.072136	47.35	76.02	14.62	1HED	CLA	613
H	0.046763	48.54	76.18	15.73	2HED	CLA	613
H	0.065345	47.08	75.59	16.17	3HED	CLA	613
H	-0.084329	46.47	83.72	16.57	H11	CLA	613
H	-0.059404	46.57	84.71	15.28	H12	CLA	613
H	0.189414	48.35	85.74	16.88	H2	CLA	613
H	0.083332	44.77	86.49	18.81	H41	CLA	613
H	0.079654	44.59	85.97	17.27	H42	CLA	613
H	0.095946	45.00	84.92	18.45	H43	CLA	613
H	0.063640	46.90	87.08	19.67	H51	CLA	613
H	0.083993	46.52	88.11	18.46	H52	CLA	613
H	-0.049014	49.10	87.00	18.43	H61	CLA	613
H	-0.002067	48.78	88.14	19.55	H62	CLA	613
H	0.043358	48.50	89.75	18.01	H71	CLA	613
H	0.062791	48.12	88.68	16.84	H72	CLA	613
H	-0.044726	50.45	87.96	16.95	H8	CLA	613
H	0.033539	52.10	89.36	17.74	H91	CLA	613
H	0.021789	50.96	90.28	18.46	H92	CLA	613

H	0.033086	51.17	88.72	18.93	H93	CLA	613
H	-0.017268	49.88	90.46	15.78	1H10	CLA	613
H	0.010629	49.63	88.99	15.11	2H10	CLA	613
H	-0.089752	52.14	88.79	15.25	1H11	CLA	613
H	-0.062160	52.09	90.42	15.33	2H11	CLA	613
H	0.051269	50.75	90.48	13.39	1H12	CLA	613
H	0.072820	50.81	88.85	13.31	2H12	CLA	613
H	-0.095083	53.36	90.00	13.23	H13	CLA	613
H	0.067007	53.14	90.91	11.07	1H14	CLA	613
H	0.065591	51.53	90.61	11.09	2H14	CLA	613
H	0.065917	52.17	91.72	12.11	3H14	CLA	613
H	0.007858	52.87	88.53	11.09	1H15	CLA	613
H	0.027353	51.93	87.86	12.25	2H15	CLA	613
H	0.002917	53.62	86.88	13.21	1H16	CLA	613
H	-0.015088	54.60	88.18	13.01	2H16	CLA	613
H	0.024234	55.26	87.55	11.00	1H17	CLA	613
H	0.010839	53.88	86.74	10.69	2H17	CLA	613
H	-0.060905	54.78	84.99	12.16	H18	CLA	613
H	0.091646	55.98	84.06	10.30	1H19	CLA	613
H	0.084068	54.60	84.77	9.79	2H19	CLA	613
H	0.078707	56.04	85.53	9.61	3H19	CLA	613
H	0.071070	57.11	84.86	12.40	1H20	CLA	613
H	0.059264	57.26	86.35	11.75	2H20	CLA	613
H	0.042943	56.51	86.16	13.19	3H20	CLA	613
Mg	1.140797	52.89	82.46	11.22	MG	CLA	614
C	0.073563	50.27	84.79	11.44	CHA	CLA	614
C	-0.530666	52.49	82.46	7.76	CHB	CLA	614
C	-0.293706	55.93	80.88	10.88	CHC	CLA	614
C	-0.381654	53.68	83.19	14.53	CHD	CLA	614
N	-0.401782	51.46	83.33	9.82	NA	CLA	614
C	-0.027935	50.48	84.27	10.13	C1A	CLA	614
C	-0.100818	49.74	84.67	8.85	C2A	CLA	614
C	0.259931	50.22	83.67	7.83	C3A	CLA	614
C	0.273045	51.48	83.10	8.46	C4A	CLA	614
C	-0.347802	49.15	82.61	7.57	CMA	CLA	614
C	-0.066561	49.98	86.13	8.37	CAA	CLA	614
C	-0.370595	51.35	86.65	7.89	CBA	CLA	614
C	0.722546	51.77	88.09	8.08	CGA	CLA	614
O	-0.577588	50.94	89.00	8.08	O1A	CLA	614
O	-0.390978	53.16	88.42	8.30	O2A	CLA	614
N	-0.522883	54.01	81.79	9.62	NB	CLA	614
C	0.290613	53.66	81.88	8.28	C1B	CLA	614
C	0.056235	54.69	81.25	7.49	C2B	CLA	614
C	-0.059508	55.62	80.74	8.34	C3B	CLA	614
C	0.201631	55.21	81.11	9.70	C4B	CLA	614
C	-0.196671	54.59	81.19	5.94	CMB	CLA	614

C	-0.082924	56.70	79.97	7.70	CAB	CLA	614
C	-0.377552	57.70	79.32	8.35	CBB	CLA	614
N	-0.500171	54.45	81.99	12.53	NC	CLA	614
C	0.173876	55.59	81.28	12.19	C1C	CLA	614
C	0.126254	56.43	81.14	13.37	C2C	CLA	614
C	-0.311689	55.80	81.77	14.39	C3C	CLA	614
C	0.313793	54.59	82.37	13.85	C4C	CLA	614
C	-0.242247	57.84	80.53	13.42	CMC	CLA	614
C	0.190617	56.28	81.84	15.87	CAC	CLA	614
C	-0.128605	57.11	83.07	16.24	CBC	CLA	614
N	-0.496512	52.05	83.51	12.74	ND	CLA	614
C	0.199807	52.50	83.75	14.02	C1D	CLA	614
C	0.067465	51.70	84.80	14.65	C2D	CLA	614
C	-0.256041	50.76	85.15	13.74	C3D	CLA	614
C	0.145335	51.04	84.42	12.54	C4D	CLA	614
C	-0.257732	51.93	85.44	16.02	CMD	CLA	614
C	0.711103	49.60	85.97	13.47	CAD	CLA	614
O	-0.574720	48.89	86.66	14.21	OBD	CLA	614
C	-0.635795	49.30	85.87	11.95	CBD	CLA	614
C	0.907866	47.80	85.48	11.72	CGD	CLA	614
O	-0.603021	47.24	86.15	10.85	O1D	CLA	614
O	-0.381813	47.15	84.46	12.49	O2D	CLA	614
C	0.011315	45.75	84.39	12.55	CED	CLA	614
C	0.183261	53.72	89.50	7.50	C1	CLA	614
C	-0.404524	54.94	89.98	8.16	C2	CLA	614
C	0.231494	56.09	90.61	7.67	C3	CLA	614
C	-0.171786	56.34	90.97	6.18	C4	CLA	614
H	0.181940	52.38	82.41	6.77	HHB	CLA	614
H	0.147981	56.78	80.36	10.79	HHC	CLA	614
H	0.220211	53.91	83.41	15.48	HHD	CLA	614
H	0.118910	48.75	84.63	9.01	H2A	CLA	614
H	0.009865	50.41	84.08	6.94	H3A	CLA	614
H	0.088879	49.48	81.96	6.89	1HMA	CLA	614
H	0.088879	48.94	82.13	8.42	2HMA	CLA	614
H	0.088879	48.32	83.05	7.22	3HMA	CLA	614
H	0.074129	49.72	86.72	9.13	1HAA	CLA	614
H	0.074129	49.35	86.28	7.60	2HAA	CLA	614
H	0.123685	52.04	86.09	8.35	1HBA	CLA	614
H	0.123685	51.39	86.48	6.90	2HBA	CLA	614
H	0.069103	55.40	80.72	5.58	1HMB	CLA	614
H	0.069103	53.77	80.69	5.68	2HMB	CLA	614
H	0.069103	54.55	82.12	5.57	3HMB	CLA	614
H	0.130228	56.69	79.92	6.70	HAB	CLA	614
H	0.160920	57.75	79.34	9.35	1HBB	CLA	614
H	0.160920	58.40	78.82	7.83	2HBB	CLA	614
H	0.079840	58.18	80.56	14.36	1HMC	CLA	614

H	0.079840	57.81	79.57	13.12	2HMC	CLA	614
H	0.079840	58.46	81.04	12.83	3HMC	CLA	614
H	-0.010598	55.48	81.82	16.46	1HAC	CLA	614
H	-0.010598	56.85	81.03	16.04	2HAC	CLA	614
H	0.029396	57.37	83.01	17.21	1HBC	CLA	614
H	0.029396	57.94	83.10	15.68	2HBC	CLA	614
H	0.029396	56.57	83.89	16.09	3HBC	CLA	614
H	0.084447	51.23	86.13	16.19	1HMD	CLA	614
H	0.084447	51.89	84.73	16.73	2HMD	CLA	614
H	0.084447	52.83	85.87	16.04	3HMD	CLA	614
H	0.195581	49.44	86.72	11.45	HBD	CLA	614
H	0.069208	45.48	83.62	13.13	1HED	CLA	614
H	0.069208	45.39	85.24	12.93	2HED	CLA	614
H	0.069208	45.39	84.26	11.63	3HED	CLA	614
H	0.067685	53.05	90.24	7.43	H11	CLA	614
H	0.067685	53.94	89.16	6.59	H12	CLA	614
H	0.189077	54.95	89.83	9.15	H2	CLA	614
H	0.059658	57.23	91.41	6.09	H41	CLA	614
H	0.059658	56.32	90.13	5.63	H42	CLA	614
H	0.059658	55.62	91.59	5.87	H43	CLA	614
H	0.067685	56.12	91.45	8.21	H31	CLA	614
H	0.067685	56.81	89.99	7.97	H32	CLA	614
C	-0.022500	40.36	74.66	40.84	C1	XAT	6622
C	0.009700	40.08	74.64	39.32	C2	XAT	6622
C	0.255200	41.19	75.02	38.33	C3	XAT	6622
C	-0.020800	42.53	74.32	38.62	C4	XAT	6622
C	0.167100	42.94	74.44	40.06	C5	XAT	6622
C	0.204000	41.91	74.61	41.18	C6	XAT	6622
C	-0.162900	42.27	74.28	42.60	C7	XAT	6622
C	-0.112500	42.89	75.15	43.41	C8	XAT	6622
C	-0.076400	43.26	75.01	44.81	C9	XAT	6622
C	-0.125000	43.86	76.07	45.41	C10	XAT	6622
C	-0.127000	44.22	76.15	46.80	C11	XAT	6622
C	-0.122500	44.85	77.17	47.41	C12	XAT	6622
C	-0.070900	45.08	77.25	48.87	C13	XAT	6622
C	-0.128500	45.77	78.31	49.35	C14	XAT	6622
C	-0.123000	46.08	78.58	50.73	C15	XAT	6622
C	0.031300	39.62	73.48	41.47	C16	XAT	6622
C	0.031300	39.76	75.96	41.38	C17	XAT	6622
C	0.031800	44.33	73.94	40.34	C18	XAT	6622
C	0.059700	42.93	73.72	45.50	C19	XAT	6622
C	0.059200	44.52	76.15	49.73	C20	XAT	6622
O	-0.870600	40.78	74.73	37.00	O3	XAT	6622
O	-0.548200	42.65	75.73	40.63	O4	XAT	6622
C	-0.022500	47.28	84.94	61.68	C21	XAT	6622
C	0.009700	47.27	85.05	63.22	C22	XAT	6622

C	0.255200	48.57	85.46	63.91	C23	XAT	6622
C	-0.020800	49.92	84.95	63.39	C24	XAT	6622
C	0.167100	49.90	84.39	61.98	C25	XAT	6622
C	0.204000	48.64	84.37	61.12	C26	XAT	6622
C	-0.162900	48.79	84.34	59.62	C27	XAT	6622
C	-0.112500	48.43	83.33	58.78	C28	XAT	6622
C	-0.076400	48.64	83.32	57.32	C29	XAT	6622
C	-0.125000	48.19	82.28	56.59	C30	XAT	6622
C	-0.127000	48.28	82.15	55.15	C31	XAT	6622
C	-0.122500	47.73	81.13	54.48	C32	XAT	6622
C	-0.070900	47.72	80.96	53.02	C33	XAT	6622
C	-0.128500	47.02	79.92	52.51	C34	XAT	6622
C	-0.123000	46.80	79.63	51.12	C35	XAT	6622
C	0.031300	47.00	86.32	61.09	C36	XAT	6622
C	0.031300	46.13	83.98	61.37	C37	XAT	6622
C	0.031800	51.28	84.35	61.38	C38	XAT	6622
C	0.059700	49.32	84.51	56.72	C39	XAT	6622
C	0.059200	48.42	82.00	52.19	C40	XAT	6622
O	-0.870600	48.63	86.87	64.03	O23	XAT	6622
O	-0.548200	49.11	83.18	61.81	O24	XAT	6622
H	0.019650	39.80	73.71	39.09	H21	XAT	6622
H	0.019650	39.32	75.27	39.15	H22	XAT	6622
H	0.000900	41.32	76.01	38.37	H3	XAT	6622
H	0.020400	42.44	73.35	38.40	H41	XAT	6622
H	0.020400	43.24	74.73	38.06	H42	XAT	6622
H	0.136000	42.03	73.38	42.95	H7	XAT	6622
H	0.140000	43.14	76.02	42.99	H8	XAT	6622
H	0.124500	44.07	76.86	44.84	H10	XAT	6622
H	0.127000	43.96	75.37	47.37	H11	XAT	6622
H	0.123000	45.19	77.92	46.84	H12	XAT	6622
H	0.122000	46.10	78.97	48.67	H14	XAT	6622
H	0.125000	45.73	77.96	51.43	H15	XAT	6622
H	0.002317	39.78	73.47	42.45	1H16	XAT	6622
H	0.002317	38.64	73.57	41.29	2H16	XAT	6622
H	0.002317	39.96	72.63	41.07	3H16	XAT	6622
H	0.002317	38.87	76.36	41.59	1H17	XAT	6622
H	0.002317	40.43	76.28	42.06	2H17	XAT	6622
H	0.002317	40.05	76.25	40.47	3H17	XAT	6622
H	0.011900	44.54	74.05	41.31	1H18	XAT	6622
H	0.011900	44.40	72.98	40.09	2H18	XAT	6622
H	0.011900	44.99	74.48	39.80	3H18	XAT	6622
H	0.005233	42.49	73.10	44.85	1H19	XAT	6622
H	0.005233	43.76	73.30	45.85	2H19	XAT	6622
H	0.005233	42.30	73.90	46.26	3H19	XAT	6622
H	0.006067	44.06	75.48	49.15	1H20	XAT	6622
H	0.006067	45.27	75.70	50.22	2H20	XAT	6622

H	0.006067	43.88	76.53	50.38	3H20	XAT	6622
H	0.599000	41.51	74.99	36.37	HO3	XAT	6622
H	0.019650	47.01	84.16	63.58	1H22	XAT	6622
H	0.019650	46.58	85.73	63.47	2H22	XAT	6622
H	0.000900	48.48	85.05	64.82	H23	XAT	6622
H	0.020400	50.24	84.22	64.00	1H24	XAT	6622
H	0.020400	50.57	85.71	63.40	2H24	XAT	6622
H	0.136000	49.20	85.14	59.20	H27	XAT	6622
H	0.140000	47.98	82.53	59.18	H28	XAT	6622
H	0.124500	47.75	81.53	57.08	H30	XAT	6622
H	0.127000	48.78	82.85	54.64	H31	XAT	6622
H	0.123000	47.28	80.42	55.02	H32	XAT	6622
H	0.122000	46.62	79.28	53.17	H34	XAT	6622
H	0.125000	47.20	80.14	50.36	H35	XAT	6622
H	0.002317	47.00	86.27	60.09	1H36	XAT	6622
H	0.002317	46.10	86.64	61.41	2H36	XAT	6622
H	0.002317	47.70	86.96	61.39	3H36	XAT	6622
H	0.002317	45.88	83.83	62.32	1H37	XAT	6622
H	0.002317	45.33	83.85	60.79	2H37	XAT	6622
H	0.002317	46.85	83.33	61.11	3H37	XAT	6622
H	0.011900	51.23	83.98	60.46	1H38	XAT	6622
H	0.011900	51.66	85.28	61.35	2H38	XAT	6622
H	0.011900	51.87	83.77	61.95	3H38	XAT	6622
H	0.005233	49.40	84.38	55.73	1H39	XAT	6622
H	0.005233	48.77	85.33	56.91	2H39	XAT	6622
H	0.005233	50.23	84.61	57.13	3H39	XAT	6622
H	0.006067	48.86	82.67	52.79	1H40	XAT	6622
H	0.006067	49.11	81.56	51.61	2H40	XAT	6622
H	0.006067	47.75	82.47	51.61	3H40	XAT	6622
H	0.599000	49.48	87.13	64.48	2H23	XAT	6622