Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 01:48 am GMT

PDB ID	:	4V8L
EMDB ID	:	EMD-2238
Title	:	Cryo-EM Structure of the Mycobacterial Fatty Acid Synthase
Authors	:	Boehringer, D.; Ban, N.; Leibundgut, M.
Deposited on	:	2012-12-06
Resolution	:	7.50 Å(reported)
Based on initial model	:	2UV8

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

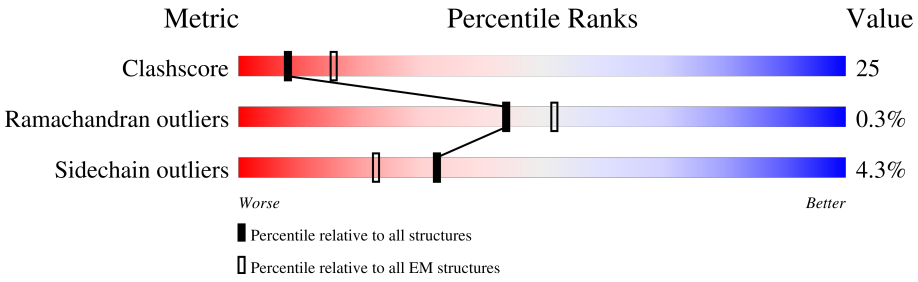
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	3089	20% 56% 33% • 9%
1	B	3089	17% 56% 33% • 9%
1	C	3089	18% 56% 33% • 9%
1	D	3089	17% 88% • 9%
1	E	3089	17% 88% • 9%
1	F	3089	15% 88% • 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 126306 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called FATTY ACID SYNTHASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	2822	Total	C	N	O	S	0	0
			21020	13294	3662	3998	66		
1	E	2822	Total	C	N	O	S	0	0
			21020	13294	3662	3998	66		
1	F	2822	Total	C	N	O	S	0	0
			21020	13294	3662	3998	66		
1	A	2822	Total	C	N	O	S	0	0
			21020	13294	3662	3998	66		
1	B	2822	Total	C	N	O	S	0	0
			21020	13294	3662	3998	66		
1	C	2822	Total	C	N	O	S	0	0
			21020	13294	3662	3998	66		

There are 1086 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	929	UNK	GLU	conflict	UNP A0R1H7
D	930	UNK	PRO	conflict	UNP A0R1H7
D	931	UNK	VAL	conflict	UNP A0R1H7
D	932	UNK	GLU	conflict	UNP A0R1H7
D	933	UNK	VAL	conflict	UNP A0R1H7
D	934	UNK	LEU	conflict	UNP A0R1H7
D	935	UNK	SER	conflict	UNP A0R1H7
D	936	UNK	ARG	conflict	UNP A0R1H7
D	937	UNK	ARG	conflict	UNP A0R1H7
D	938	UNK	GLN	conflict	UNP A0R1H7
D	939	UNK	ALA	conflict	UNP A0R1H7
D	940	UNK	ARG	conflict	UNP A0R1H7
D	941	UNK	ARG	conflict	UNP A0R1H7
D	942	UNK	ASP	conflict	UNP A0R1H7
D	943	UNK	ALA	conflict	UNP A0R1H7
D	944	UNK	SER	conflict	UNP A0R1H7
D	974	UNK	THR	conflict	UNP A0R1H7
D	975	UNK	GLU	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	976	UNK	TRP	conflict	UNP A0R1H7
D	977	UNK	GLN	conflict	UNP A0R1H7
D	978	UNK	VAL	conflict	UNP A0R1H7
D	979	UNK	ARG	conflict	UNP A0R1H7
D	980	UNK	GLU	conflict	UNP A0R1H7
D	981	UNK	GLY	conflict	UNP A0R1H7
D	982	UNK	SER	conflict	UNP A0R1H7
D	983	UNK	ASP	conflict	UNP A0R1H7
D	984	UNK	ASN	conflict	UNP A0R1H7
D	985	UNK	ARG	conflict	UNP A0R1H7
D	986	UNK	SER	conflict	UNP A0R1H7
D	987	UNK	ALA	conflict	UNP A0R1H7
D	988	UNK	SER	conflict	UNP A0R1H7
D	989	UNK	HIS	conflict	UNP A0R1H7
D	990	UNK	PRO	conflict	UNP A0R1H7
D	991	UNK	SER	conflict	UNP A0R1H7
D	992	UNK	THR	conflict	UNP A0R1H7
D	993	UNK	GLY	conflict	UNP A0R1H7
D	994	UNK	ALA	conflict	UNP A0R1H7
D	995	UNK	ARG	conflict	UNP A0R1H7
D	996	UNK	LEU	conflict	UNP A0R1H7
D	997	UNK	GLU	conflict	UNP A0R1H7
D	998	UNK	VAL	conflict	UNP A0R1H7
D	999	UNK	ALA	conflict	UNP A0R1H7
D	1000	UNK	ASP	conflict	UNP A0R1H7
D	1001	UNK	ASP	conflict	UNP A0R1H7
D	1002	UNK	GLN	conflict	UNP A0R1H7
D	1003	UNK	HIS	conflict	UNP A0R1H7
D	1004	UNK	VAL	conflict	UNP A0R1H7
D	1005	UNK	VAL	conflict	UNP A0R1H7
D	1006	UNK	LEU	conflict	UNP A0R1H7
D	1007	UNK	SER	conflict	UNP A0R1H7
D	1008	UNK	VAL	conflict	UNP A0R1H7
D	1009	UNK	PRO	conflict	UNP A0R1H7
D	1010	UNK	LEU	conflict	UNP A0R1H7
D	1011	UNK	SER	conflict	UNP A0R1H7
D	1012	UNK	GLY	conflict	UNP A0R1H7
D	1013	UNK	THR	conflict	UNP A0R1H7
D	1014	UNK	TRP	conflict	UNP A0R1H7
D	1196	UNK	GLY	conflict	UNP A0R1H7
D	1197	UNK	ARG	conflict	UNP A0R1H7
D	1198	UNK	THR	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1199	UNK	GLY	conflict	UNP A0R1H7
D	1200	UNK	ALA	conflict	UNP A0R1H7
D	1201	UNK	ALA	conflict	UNP A0R1H7
D	1202	UNK	GLU	conflict	UNP A0R1H7
D	1203	UNK	LEU	conflict	UNP A0R1H7
D	1204	UNK	THR	conflict	UNP A0R1H7
D	1205	UNK	ASP	conflict	UNP A0R1H7
D	1206	UNK	PRO	conflict	UNP A0R1H7
D	1207	UNK	VAL	conflict	UNP A0R1H7
D	1208	UNK	ARG	conflict	UNP A0R1H7
D	1209	UNK	ALA	conflict	UNP A0R1H7
D	1210	UNK	GLY	conflict	UNP A0R1H7
D	1211	UNK	GLY	conflict	UNP A0R1H7
D	1212	UNK	ALA	conflict	UNP A0R1H7
D	1213	UNK	ILE	conflict	UNP A0R1H7
D	1214	UNK	SER	conflict	UNP A0R1H7
D	1215	UNK	ASP	conflict	UNP A0R1H7
D	1216	UNK	ASN	conflict	UNP A0R1H7
D	1217	UNK	ALA	conflict	UNP A0R1H7
D	1218	UNK	THR	conflict	UNP A0R1H7
D	1219	UNK	ASP	conflict	UNP A0R1H7
D	1220	UNK	THR	conflict	UNP A0R1H7
D	1221	UNK	PRO	conflict	UNP A0R1H7
D	1222	UNK	ARG	conflict	UNP A0R1H7
D	1223	UNK	ARG	conflict	UNP A0R1H7
D	1224	UNK	ARG	conflict	UNP A0R1H7
D	1225	UNK	ARG	conflict	UNP A0R1H7
D	1226	UNK	ARG	conflict	UNP A0R1H7
D	1227	UNK	ASP	conflict	UNP A0R1H7
D	2076	UNK	GLY	conflict	UNP A0R1H7
D	2077	UNK	ASP	conflict	UNP A0R1H7
D	2078	UNK	ILE	conflict	UNP A0R1H7
D	2079	UNK	ASP	conflict	UNP A0R1H7
D	2080	UNK	ALA	conflict	UNP A0R1H7
D	2081	UNK	GLN	conflict	UNP A0R1H7
D	2082	UNK	TRP	conflict	UNP A0R1H7
D	2083	UNK	GLU	conflict	UNP A0R1H7
D	2084	UNK	GLN	conflict	UNP A0R1H7
D	2085	UNK	LEU	conflict	UNP A0R1H7
D	2086	UNK	SER	conflict	UNP A0R1H7
D	2087	UNK	GLN	conflict	UNP A0R1H7
D	2088	UNK	ARG	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	2089	UNK	PHE	conflict	UNP A0R1H7
D	2090	UNK	GLU	conflict	UNP A0R1H7
D	2091	UNK	GLY	conflict	UNP A0R1H7
D	2092	UNK	THR	conflict	UNP A0R1H7
D	2093	UNK	GLY	conflict	UNP A0R1H7
D	2094	UNK	HIS	conflict	UNP A0R1H7
D	2095	UNK	VAL	conflict	UNP A0R1H7
D	2096	UNK	VAL	conflict	UNP A0R1H7
D	2097	UNK	ALA	conflict	UNP A0R1H7
D	2098	UNK	THR	conflict	UNP A0R1H7
D	2099	UNK	GLN	conflict	UNP A0R1H7
D	2100	UNK	ALA	conflict	UNP A0R1H7
D	2101	UNK	ASN	conflict	UNP A0R1H7
D	2102	UNK	TRP	conflict	UNP A0R1H7
D	2103	UNK	TRP	conflict	UNP A0R1H7
D	2104	UNK	GLN	conflict	UNP A0R1H7
D	2105	UNK	GLY	conflict	UNP A0R1H7
D	2106	UNK	LYS	conflict	UNP A0R1H7
D	2107	UNK	ALA	conflict	UNP A0R1H7
D	2108	UNK	LEU	conflict	UNP A0R1H7
D	2109	UNK	ALA	conflict	UNP A0R1H7
D	2110	UNK	ALA	conflict	UNP A0R1H7
D	2111	UNK	GLY	conflict	UNP A0R1H7
D	2112	UNK	ARG	conflict	UNP A0R1H7
D	2113	UNK	ASN	conflict	UNP A0R1H7
D	2114	UNK	VAL	conflict	UNP A0R1H7
D	2115	UNK	HIS	conflict	UNP A0R1H7
D	2116	UNK	ALA	conflict	UNP A0R1H7
D	2117	UNK	SER	conflict	UNP A0R1H7
D	2118	UNK	LEU	conflict	UNP A0R1H7
D	2119	UNK	PHE	conflict	UNP A0R1H7
D	2120	UNK	GLY	conflict	UNP A0R1H7
D	2121	UNK	ARG	conflict	UNP A0R1H7
D	2122	UNK	ILE	conflict	UNP A0R1H7
D	2123	UNK	ALA	conflict	UNP A0R1H7
D	2124	UNK	ALA	conflict	UNP A0R1H7
D	2125	UNK	GLY	conflict	UNP A0R1H7
D	2126	UNK	ALA	conflict	UNP A0R1H7
D	2127	UNK	GLU	conflict	UNP A0R1H7
D	2128	UNK	ASN	conflict	UNP A0R1H7
D	2129	UNK	PRO	conflict	UNP A0R1H7
D	2130	UNK	GLY	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	2131	UNK	LYS	conflict	UNP A0R1H7
D	2132	UNK	GLY	conflict	UNP A0R1H7
D	2133	UNK	ARG	conflict	UNP A0R1H7
D	2134	UNK	TYR	conflict	UNP A0R1H7
D	2135	UNK	SER	conflict	UNP A0R1H7
D	2422	UNK	GLU	conflict	UNP A0R1H7
D	2423	UNK	SER	conflict	UNP A0R1H7
D	2424	UNK	ASP	conflict	UNP A0R1H7
D	2425	UNK	ASP	conflict	UNP A0R1H7
D	2426	UNK	GLU	conflict	UNP A0R1H7
D	2427	UNK	ALA	conflict	UNP A0R1H7
D	2428	UNK	PRO	conflict	UNP A0R1H7
D	2429	UNK	ALA	conflict	UNP A0R1H7
D	2430	UNK	GLY	conflict	UNP A0R1H7
D	2431	UNK	THR	conflict	UNP A0R1H7
D	2432	UNK	ILE	conflict	UNP A0R1H7
D	2433	UNK	ARG	conflict	UNP A0R1H7
D	2434	UNK	ALA	conflict	UNP A0R1H7
D	2435	UNK	LEU	conflict	UNP A0R1H7
D	2436	UNK	PRO	conflict	UNP A0R1H7
D	2437	UNK	SER	conflict	UNP A0R1H7
D	2438	UNK	PRO	conflict	UNP A0R1H7
D	2439	UNK	PRO	conflict	UNP A0R1H7
D	2440	UNK	ARG	conflict	UNP A0R1H7
D	2441	UNK	GLY	conflict	UNP A0R1H7
D	2442	UNK	TYR	conflict	UNP A0R1H7
D	2443	UNK	ASN	conflict	UNP A0R1H7
D	2444	UNK	PRO	conflict	UNP A0R1H7
D	2445	UNK	ALA	conflict	UNP A0R1H7
D	2446	UNK	PRO	conflict	UNP A0R1H7
D	2447	UNK	ALA	conflict	UNP A0R1H7
D	2448	UNK	PRO	conflict	UNP A0R1H7
D	2449	UNK	GLU	conflict	UNP A0R1H7
D	2450	UNK	TRP	conflict	UNP A0R1H7
D	2451	UNK	ASP	conflict	UNP A0R1H7
D	2452	UNK	ASP	conflict	UNP A0R1H7
D	2453	UNK	LEU	conflict	UNP A0R1H7
E	929	UNK	GLU	conflict	UNP A0R1H7
E	930	UNK	PRO	conflict	UNP A0R1H7
E	931	UNK	VAL	conflict	UNP A0R1H7
E	932	UNK	GLU	conflict	UNP A0R1H7
E	933	UNK	VAL	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	934	UNK	LEU	conflict	UNP A0R1H7
E	935	UNK	SER	conflict	UNP A0R1H7
E	936	UNK	ARG	conflict	UNP A0R1H7
E	937	UNK	ARG	conflict	UNP A0R1H7
E	938	UNK	GLN	conflict	UNP A0R1H7
E	939	UNK	ALA	conflict	UNP A0R1H7
E	940	UNK	ARG	conflict	UNP A0R1H7
E	941	UNK	ARG	conflict	UNP A0R1H7
E	942	UNK	ASP	conflict	UNP A0R1H7
E	943	UNK	ALA	conflict	UNP A0R1H7
E	944	UNK	SER	conflict	UNP A0R1H7
E	974	UNK	THR	conflict	UNP A0R1H7
E	975	UNK	GLU	conflict	UNP A0R1H7
E	976	UNK	TRP	conflict	UNP A0R1H7
E	977	UNK	GLN	conflict	UNP A0R1H7
E	978	UNK	VAL	conflict	UNP A0R1H7
E	979	UNK	ARG	conflict	UNP A0R1H7
E	980	UNK	GLU	conflict	UNP A0R1H7
E	981	UNK	GLY	conflict	UNP A0R1H7
E	982	UNK	SER	conflict	UNP A0R1H7
E	983	UNK	ASP	conflict	UNP A0R1H7
E	984	UNK	ASN	conflict	UNP A0R1H7
E	985	UNK	ARG	conflict	UNP A0R1H7
E	986	UNK	SER	conflict	UNP A0R1H7
E	987	UNK	ALA	conflict	UNP A0R1H7
E	988	UNK	SER	conflict	UNP A0R1H7
E	989	UNK	HIS	conflict	UNP A0R1H7
E	990	UNK	PRO	conflict	UNP A0R1H7
E	991	UNK	SER	conflict	UNP A0R1H7
E	992	UNK	THR	conflict	UNP A0R1H7
E	993	UNK	GLY	conflict	UNP A0R1H7
E	994	UNK	ALA	conflict	UNP A0R1H7
E	995	UNK	ARG	conflict	UNP A0R1H7
E	996	UNK	LEU	conflict	UNP A0R1H7
E	997	UNK	GLU	conflict	UNP A0R1H7
E	998	UNK	VAL	conflict	UNP A0R1H7
E	999	UNK	ALA	conflict	UNP A0R1H7
E	1000	UNK	ASP	conflict	UNP A0R1H7
E	1001	UNK	ASP	conflict	UNP A0R1H7
E	1002	UNK	GLN	conflict	UNP A0R1H7
E	1003	UNK	HIS	conflict	UNP A0R1H7
E	1004	UNK	VAL	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	1005	UNK	VAL	conflict	UNP A0R1H7
E	1006	UNK	LEU	conflict	UNP A0R1H7
E	1007	UNK	SER	conflict	UNP A0R1H7
E	1008	UNK	VAL	conflict	UNP A0R1H7
E	1009	UNK	PRO	conflict	UNP A0R1H7
E	1010	UNK	LEU	conflict	UNP A0R1H7
E	1011	UNK	SER	conflict	UNP A0R1H7
E	1012	UNK	GLY	conflict	UNP A0R1H7
E	1013	UNK	THR	conflict	UNP A0R1H7
E	1014	UNK	TRP	conflict	UNP A0R1H7
E	1196	UNK	GLY	conflict	UNP A0R1H7
E	1197	UNK	ARG	conflict	UNP A0R1H7
E	1198	UNK	THR	conflict	UNP A0R1H7
E	1199	UNK	GLY	conflict	UNP A0R1H7
E	1200	UNK	ALA	conflict	UNP A0R1H7
E	1201	UNK	ALA	conflict	UNP A0R1H7
E	1202	UNK	GLU	conflict	UNP A0R1H7
E	1203	UNK	LEU	conflict	UNP A0R1H7
E	1204	UNK	THR	conflict	UNP A0R1H7
E	1205	UNK	ASP	conflict	UNP A0R1H7
E	1206	UNK	PRO	conflict	UNP A0R1H7
E	1207	UNK	VAL	conflict	UNP A0R1H7
E	1208	UNK	ARG	conflict	UNP A0R1H7
E	1209	UNK	ALA	conflict	UNP A0R1H7
E	1210	UNK	GLY	conflict	UNP A0R1H7
E	1211	UNK	GLY	conflict	UNP A0R1H7
E	1212	UNK	ALA	conflict	UNP A0R1H7
E	1213	UNK	ILE	conflict	UNP A0R1H7
E	1214	UNK	SER	conflict	UNP A0R1H7
E	1215	UNK	ASP	conflict	UNP A0R1H7
E	1216	UNK	ASN	conflict	UNP A0R1H7
E	1217	UNK	ALA	conflict	UNP A0R1H7
E	1218	UNK	THR	conflict	UNP A0R1H7
E	1219	UNK	ASP	conflict	UNP A0R1H7
E	1220	UNK	THR	conflict	UNP A0R1H7
E	1221	UNK	PRO	conflict	UNP A0R1H7
E	1222	UNK	ARG	conflict	UNP A0R1H7
E	1223	UNK	ARG	conflict	UNP A0R1H7
E	1224	UNK	ARG	conflict	UNP A0R1H7
E	1225	UNK	ARG	conflict	UNP A0R1H7
E	1226	UNK	ARG	conflict	UNP A0R1H7
E	1227	UNK	ASP	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	2076	UNK	GLY	conflict	UNP A0R1H7
E	2077	UNK	ASP	conflict	UNP A0R1H7
E	2078	UNK	ILE	conflict	UNP A0R1H7
E	2079	UNK	ASP	conflict	UNP A0R1H7
E	2080	UNK	ALA	conflict	UNP A0R1H7
E	2081	UNK	GLN	conflict	UNP A0R1H7
E	2082	UNK	TRP	conflict	UNP A0R1H7
E	2083	UNK	GLU	conflict	UNP A0R1H7
E	2084	UNK	GLN	conflict	UNP A0R1H7
E	2085	UNK	LEU	conflict	UNP A0R1H7
E	2086	UNK	SER	conflict	UNP A0R1H7
E	2087	UNK	GLN	conflict	UNP A0R1H7
E	2088	UNK	ARG	conflict	UNP A0R1H7
E	2089	UNK	PHE	conflict	UNP A0R1H7
E	2090	UNK	GLU	conflict	UNP A0R1H7
E	2091	UNK	GLY	conflict	UNP A0R1H7
E	2092	UNK	THR	conflict	UNP A0R1H7
E	2093	UNK	GLY	conflict	UNP A0R1H7
E	2094	UNK	HIS	conflict	UNP A0R1H7
E	2095	UNK	VAL	conflict	UNP A0R1H7
E	2096	UNK	VAL	conflict	UNP A0R1H7
E	2097	UNK	ALA	conflict	UNP A0R1H7
E	2098	UNK	THR	conflict	UNP A0R1H7
E	2099	UNK	GLN	conflict	UNP A0R1H7
E	2100	UNK	ALA	conflict	UNP A0R1H7
E	2101	UNK	ASN	conflict	UNP A0R1H7
E	2102	UNK	TRP	conflict	UNP A0R1H7
E	2103	UNK	TRP	conflict	UNP A0R1H7
E	2104	UNK	GLN	conflict	UNP A0R1H7
E	2105	UNK	GLY	conflict	UNP A0R1H7
E	2106	UNK	LYS	conflict	UNP A0R1H7
E	2107	UNK	ALA	conflict	UNP A0R1H7
E	2108	UNK	LEU	conflict	UNP A0R1H7
E	2109	UNK	ALA	conflict	UNP A0R1H7
E	2110	UNK	ALA	conflict	UNP A0R1H7
E	2111	UNK	GLY	conflict	UNP A0R1H7
E	2112	UNK	ARG	conflict	UNP A0R1H7
E	2113	UNK	ASN	conflict	UNP A0R1H7
E	2114	UNK	VAL	conflict	UNP A0R1H7
E	2115	UNK	HIS	conflict	UNP A0R1H7
E	2116	UNK	ALA	conflict	UNP A0R1H7
E	2117	UNK	SER	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	2118	UNK	LEU	conflict	UNP A0R1H7
E	2119	UNK	PHE	conflict	UNP A0R1H7
E	2120	UNK	GLY	conflict	UNP A0R1H7
E	2121	UNK	ARG	conflict	UNP A0R1H7
E	2122	UNK	ILE	conflict	UNP A0R1H7
E	2123	UNK	ALA	conflict	UNP A0R1H7
E	2124	UNK	ALA	conflict	UNP A0R1H7
E	2125	UNK	GLY	conflict	UNP A0R1H7
E	2126	UNK	ALA	conflict	UNP A0R1H7
E	2127	UNK	GLU	conflict	UNP A0R1H7
E	2128	UNK	ASN	conflict	UNP A0R1H7
E	2129	UNK	PRO	conflict	UNP A0R1H7
E	2130	UNK	GLY	conflict	UNP A0R1H7
E	2131	UNK	LYS	conflict	UNP A0R1H7
E	2132	UNK	GLY	conflict	UNP A0R1H7
E	2133	UNK	ARG	conflict	UNP A0R1H7
E	2134	UNK	TYR	conflict	UNP A0R1H7
E	2135	UNK	SER	conflict	UNP A0R1H7
E	2422	UNK	GLU	conflict	UNP A0R1H7
E	2423	UNK	SER	conflict	UNP A0R1H7
E	2424	UNK	ASP	conflict	UNP A0R1H7
E	2425	UNK	ASP	conflict	UNP A0R1H7
E	2426	UNK	GLU	conflict	UNP A0R1H7
E	2427	UNK	ALA	conflict	UNP A0R1H7
E	2428	UNK	PRO	conflict	UNP A0R1H7
E	2429	UNK	ALA	conflict	UNP A0R1H7
E	2430	UNK	GLY	conflict	UNP A0R1H7
E	2431	UNK	THR	conflict	UNP A0R1H7
E	2432	UNK	ILE	conflict	UNP A0R1H7
E	2433	UNK	ARG	conflict	UNP A0R1H7
E	2434	UNK	ALA	conflict	UNP A0R1H7
E	2435	UNK	LEU	conflict	UNP A0R1H7
E	2436	UNK	PRO	conflict	UNP A0R1H7
E	2437	UNK	SER	conflict	UNP A0R1H7
E	2438	UNK	PRO	conflict	UNP A0R1H7
E	2439	UNK	PRO	conflict	UNP A0R1H7
E	2440	UNK	ARG	conflict	UNP A0R1H7
E	2441	UNK	GLY	conflict	UNP A0R1H7
E	2442	UNK	TYR	conflict	UNP A0R1H7
E	2443	UNK	ASN	conflict	UNP A0R1H7
E	2444	UNK	PRO	conflict	UNP A0R1H7
E	2445	UNK	ALA	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	2446	UNK	PRO	conflict	UNP A0R1H7
E	2447	UNK	ALA	conflict	UNP A0R1H7
E	2448	UNK	PRO	conflict	UNP A0R1H7
E	2449	UNK	GLU	conflict	UNP A0R1H7
E	2450	UNK	TRP	conflict	UNP A0R1H7
E	2451	UNK	ASP	conflict	UNP A0R1H7
E	2452	UNK	ASP	conflict	UNP A0R1H7
E	2453	UNK	LEU	conflict	UNP A0R1H7
F	929	UNK	GLU	conflict	UNP A0R1H7
F	930	UNK	PRO	conflict	UNP A0R1H7
F	931	UNK	VAL	conflict	UNP A0R1H7
F	932	UNK	GLU	conflict	UNP A0R1H7
F	933	UNK	VAL	conflict	UNP A0R1H7
F	934	UNK	LEU	conflict	UNP A0R1H7
F	935	UNK	SER	conflict	UNP A0R1H7
F	936	UNK	ARG	conflict	UNP A0R1H7
F	937	UNK	ARG	conflict	UNP A0R1H7
F	938	UNK	GLN	conflict	UNP A0R1H7
F	939	UNK	ALA	conflict	UNP A0R1H7
F	940	UNK	ARG	conflict	UNP A0R1H7
F	941	UNK	ARG	conflict	UNP A0R1H7
F	942	UNK	ASP	conflict	UNP A0R1H7
F	943	UNK	ALA	conflict	UNP A0R1H7
F	944	UNK	SER	conflict	UNP A0R1H7
F	974	UNK	THR	conflict	UNP A0R1H7
F	975	UNK	GLU	conflict	UNP A0R1H7
F	976	UNK	TRP	conflict	UNP A0R1H7
F	977	UNK	GLN	conflict	UNP A0R1H7
F	978	UNK	VAL	conflict	UNP A0R1H7
F	979	UNK	ARG	conflict	UNP A0R1H7
F	980	UNK	GLU	conflict	UNP A0R1H7
F	981	UNK	GLY	conflict	UNP A0R1H7
F	982	UNK	SER	conflict	UNP A0R1H7
F	983	UNK	ASP	conflict	UNP A0R1H7
F	984	UNK	ASN	conflict	UNP A0R1H7
F	985	UNK	ARG	conflict	UNP A0R1H7
F	986	UNK	SER	conflict	UNP A0R1H7
F	987	UNK	ALA	conflict	UNP A0R1H7
F	988	UNK	SER	conflict	UNP A0R1H7
F	989	UNK	HIS	conflict	UNP A0R1H7
F	990	UNK	PRO	conflict	UNP A0R1H7
F	991	UNK	SER	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	992	UNK	THR	conflict	UNP A0R1H7
F	993	UNK	GLY	conflict	UNP A0R1H7
F	994	UNK	ALA	conflict	UNP A0R1H7
F	995	UNK	ARG	conflict	UNP A0R1H7
F	996	UNK	LEU	conflict	UNP A0R1H7
F	997	UNK	GLU	conflict	UNP A0R1H7
F	998	UNK	VAL	conflict	UNP A0R1H7
F	999	UNK	ALA	conflict	UNP A0R1H7
F	1000	UNK	ASP	conflict	UNP A0R1H7
F	1001	UNK	ASP	conflict	UNP A0R1H7
F	1002	UNK	GLN	conflict	UNP A0R1H7
F	1003	UNK	HIS	conflict	UNP A0R1H7
F	1004	UNK	VAL	conflict	UNP A0R1H7
F	1005	UNK	VAL	conflict	UNP A0R1H7
F	1006	UNK	LEU	conflict	UNP A0R1H7
F	1007	UNK	SER	conflict	UNP A0R1H7
F	1008	UNK	VAL	conflict	UNP A0R1H7
F	1009	UNK	PRO	conflict	UNP A0R1H7
F	1010	UNK	LEU	conflict	UNP A0R1H7
F	1011	UNK	SER	conflict	UNP A0R1H7
F	1012	UNK	GLY	conflict	UNP A0R1H7
F	1013	UNK	THR	conflict	UNP A0R1H7
F	1014	UNK	TRP	conflict	UNP A0R1H7
F	1196	UNK	GLY	conflict	UNP A0R1H7
F	1197	UNK	ARG	conflict	UNP A0R1H7
F	1198	UNK	THR	conflict	UNP A0R1H7
F	1199	UNK	GLY	conflict	UNP A0R1H7
F	1200	UNK	ALA	conflict	UNP A0R1H7
F	1201	UNK	ALA	conflict	UNP A0R1H7
F	1202	UNK	GLU	conflict	UNP A0R1H7
F	1203	UNK	LEU	conflict	UNP A0R1H7
F	1204	UNK	THR	conflict	UNP A0R1H7
F	1205	UNK	ASP	conflict	UNP A0R1H7
F	1206	UNK	PRO	conflict	UNP A0R1H7
F	1207	UNK	VAL	conflict	UNP A0R1H7
F	1208	UNK	ARG	conflict	UNP A0R1H7
F	1209	UNK	ALA	conflict	UNP A0R1H7
F	1210	UNK	GLY	conflict	UNP A0R1H7
F	1211	UNK	GLY	conflict	UNP A0R1H7
F	1212	UNK	ALA	conflict	UNP A0R1H7
F	1213	UNK	ILE	conflict	UNP A0R1H7
F	1214	UNK	SER	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	1215	UNK	ASP	conflict	UNP A0R1H7
F	1216	UNK	ASN	conflict	UNP A0R1H7
F	1217	UNK	ALA	conflict	UNP A0R1H7
F	1218	UNK	THR	conflict	UNP A0R1H7
F	1219	UNK	ASP	conflict	UNP A0R1H7
F	1220	UNK	THR	conflict	UNP A0R1H7
F	1221	UNK	PRO	conflict	UNP A0R1H7
F	1222	UNK	ARG	conflict	UNP A0R1H7
F	1223	UNK	ARG	conflict	UNP A0R1H7
F	1224	UNK	ARG	conflict	UNP A0R1H7
F	1225	UNK	ARG	conflict	UNP A0R1H7
F	1226	UNK	ARG	conflict	UNP A0R1H7
F	1227	UNK	ASP	conflict	UNP A0R1H7
F	2076	UNK	GLY	conflict	UNP A0R1H7
F	2077	UNK	ASP	conflict	UNP A0R1H7
F	2078	UNK	ILE	conflict	UNP A0R1H7
F	2079	UNK	ASP	conflict	UNP A0R1H7
F	2080	UNK	ALA	conflict	UNP A0R1H7
F	2081	UNK	GLN	conflict	UNP A0R1H7
F	2082	UNK	TRP	conflict	UNP A0R1H7
F	2083	UNK	GLU	conflict	UNP A0R1H7
F	2084	UNK	GLN	conflict	UNP A0R1H7
F	2085	UNK	LEU	conflict	UNP A0R1H7
F	2086	UNK	SER	conflict	UNP A0R1H7
F	2087	UNK	GLN	conflict	UNP A0R1H7
F	2088	UNK	ARG	conflict	UNP A0R1H7
F	2089	UNK	PHE	conflict	UNP A0R1H7
F	2090	UNK	GLU	conflict	UNP A0R1H7
F	2091	UNK	GLY	conflict	UNP A0R1H7
F	2092	UNK	THR	conflict	UNP A0R1H7
F	2093	UNK	GLY	conflict	UNP A0R1H7
F	2094	UNK	HIS	conflict	UNP A0R1H7
F	2095	UNK	VAL	conflict	UNP A0R1H7
F	2096	UNK	VAL	conflict	UNP A0R1H7
F	2097	UNK	ALA	conflict	UNP A0R1H7
F	2098	UNK	THR	conflict	UNP A0R1H7
F	2099	UNK	GLN	conflict	UNP A0R1H7
F	2100	UNK	ALA	conflict	UNP A0R1H7
F	2101	UNK	ASN	conflict	UNP A0R1H7
F	2102	UNK	TRP	conflict	UNP A0R1H7
F	2103	UNK	TRP	conflict	UNP A0R1H7
F	2104	UNK	GLN	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	2105	UNK	GLY	conflict	UNP A0R1H7
F	2106	UNK	LYS	conflict	UNP A0R1H7
F	2107	UNK	ALA	conflict	UNP A0R1H7
F	2108	UNK	LEU	conflict	UNP A0R1H7
F	2109	UNK	ALA	conflict	UNP A0R1H7
F	2110	UNK	ALA	conflict	UNP A0R1H7
F	2111	UNK	GLY	conflict	UNP A0R1H7
F	2112	UNK	ARG	conflict	UNP A0R1H7
F	2113	UNK	ASN	conflict	UNP A0R1H7
F	2114	UNK	VAL	conflict	UNP A0R1H7
F	2115	UNK	HIS	conflict	UNP A0R1H7
F	2116	UNK	ALA	conflict	UNP A0R1H7
F	2117	UNK	SER	conflict	UNP A0R1H7
F	2118	UNK	LEU	conflict	UNP A0R1H7
F	2119	UNK	PHE	conflict	UNP A0R1H7
F	2120	UNK	GLY	conflict	UNP A0R1H7
F	2121	UNK	ARG	conflict	UNP A0R1H7
F	2122	UNK	ILE	conflict	UNP A0R1H7
F	2123	UNK	ALA	conflict	UNP A0R1H7
F	2124	UNK	ALA	conflict	UNP A0R1H7
F	2125	UNK	GLY	conflict	UNP A0R1H7
F	2126	UNK	ALA	conflict	UNP A0R1H7
F	2127	UNK	GLU	conflict	UNP A0R1H7
F	2128	UNK	ASN	conflict	UNP A0R1H7
F	2129	UNK	PRO	conflict	UNP A0R1H7
F	2130	UNK	GLY	conflict	UNP A0R1H7
F	2131	UNK	LYS	conflict	UNP A0R1H7
F	2132	UNK	GLY	conflict	UNP A0R1H7
F	2133	UNK	ARG	conflict	UNP A0R1H7
F	2134	UNK	TYR	conflict	UNP A0R1H7
F	2135	UNK	SER	conflict	UNP A0R1H7
F	2422	UNK	GLU	conflict	UNP A0R1H7
F	2423	UNK	SER	conflict	UNP A0R1H7
F	2424	UNK	ASP	conflict	UNP A0R1H7
F	2425	UNK	ASP	conflict	UNP A0R1H7
F	2426	UNK	GLU	conflict	UNP A0R1H7
F	2427	UNK	ALA	conflict	UNP A0R1H7
F	2428	UNK	PRO	conflict	UNP A0R1H7
F	2429	UNK	ALA	conflict	UNP A0R1H7
F	2430	UNK	GLY	conflict	UNP A0R1H7
F	2431	UNK	THR	conflict	UNP A0R1H7
F	2432	UNK	ILE	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	2433	UNK	ARG	conflict	UNP A0R1H7
F	2434	UNK	ALA	conflict	UNP A0R1H7
F	2435	UNK	LEU	conflict	UNP A0R1H7
F	2436	UNK	PRO	conflict	UNP A0R1H7
F	2437	UNK	SER	conflict	UNP A0R1H7
F	2438	UNK	PRO	conflict	UNP A0R1H7
F	2439	UNK	PRO	conflict	UNP A0R1H7
F	2440	UNK	ARG	conflict	UNP A0R1H7
F	2441	UNK	GLY	conflict	UNP A0R1H7
F	2442	UNK	TYR	conflict	UNP A0R1H7
F	2443	UNK	ASN	conflict	UNP A0R1H7
F	2444	UNK	PRO	conflict	UNP A0R1H7
F	2445	UNK	ALA	conflict	UNP A0R1H7
F	2446	UNK	PRO	conflict	UNP A0R1H7
F	2447	UNK	ALA	conflict	UNP A0R1H7
F	2448	UNK	PRO	conflict	UNP A0R1H7
F	2449	UNK	GLU	conflict	UNP A0R1H7
F	2450	UNK	TRP	conflict	UNP A0R1H7
F	2451	UNK	ASP	conflict	UNP A0R1H7
F	2452	UNK	ASP	conflict	UNP A0R1H7
F	2453	UNK	LEU	conflict	UNP A0R1H7
A	929	UNK	GLU	conflict	UNP A0R1H7
A	930	UNK	PRO	conflict	UNP A0R1H7
A	931	UNK	VAL	conflict	UNP A0R1H7
A	932	UNK	GLU	conflict	UNP A0R1H7
A	933	UNK	VAL	conflict	UNP A0R1H7
A	934	UNK	LEU	conflict	UNP A0R1H7
A	935	UNK	SER	conflict	UNP A0R1H7
A	936	UNK	ARG	conflict	UNP A0R1H7
A	937	UNK	ARG	conflict	UNP A0R1H7
A	938	UNK	GLN	conflict	UNP A0R1H7
A	939	UNK	ALA	conflict	UNP A0R1H7
A	940	UNK	ARG	conflict	UNP A0R1H7
A	941	UNK	ARG	conflict	UNP A0R1H7
A	942	UNK	ASP	conflict	UNP A0R1H7
A	943	UNK	ALA	conflict	UNP A0R1H7
A	944	UNK	SER	conflict	UNP A0R1H7
A	974	UNK	THR	conflict	UNP A0R1H7
A	975	UNK	GLU	conflict	UNP A0R1H7
A	976	UNK	TRP	conflict	UNP A0R1H7
A	977	UNK	GLN	conflict	UNP A0R1H7
A	978	UNK	VAL	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	979	UNK	ARG	conflict	UNP A0R1H7
A	980	UNK	GLU	conflict	UNP A0R1H7
A	981	UNK	GLY	conflict	UNP A0R1H7
A	982	UNK	SER	conflict	UNP A0R1H7
A	983	UNK	ASP	conflict	UNP A0R1H7
A	984	UNK	ASN	conflict	UNP A0R1H7
A	985	UNK	ARG	conflict	UNP A0R1H7
A	986	UNK	SER	conflict	UNP A0R1H7
A	987	UNK	ALA	conflict	UNP A0R1H7
A	988	UNK	SER	conflict	UNP A0R1H7
A	989	UNK	HIS	conflict	UNP A0R1H7
A	990	UNK	PRO	conflict	UNP A0R1H7
A	991	UNK	SER	conflict	UNP A0R1H7
A	992	UNK	THR	conflict	UNP A0R1H7
A	993	UNK	GLY	conflict	UNP A0R1H7
A	994	UNK	ALA	conflict	UNP A0R1H7
A	995	UNK	ARG	conflict	UNP A0R1H7
A	996	UNK	LEU	conflict	UNP A0R1H7
A	997	UNK	GLU	conflict	UNP A0R1H7
A	998	UNK	VAL	conflict	UNP A0R1H7
A	999	UNK	ALA	conflict	UNP A0R1H7
A	1000	UNK	ASP	conflict	UNP A0R1H7
A	1001	UNK	ASP	conflict	UNP A0R1H7
A	1002	UNK	GLN	conflict	UNP A0R1H7
A	1003	UNK	HIS	conflict	UNP A0R1H7
A	1004	UNK	VAL	conflict	UNP A0R1H7
A	1005	UNK	VAL	conflict	UNP A0R1H7
A	1006	UNK	LEU	conflict	UNP A0R1H7
A	1007	UNK	SER	conflict	UNP A0R1H7
A	1008	UNK	VAL	conflict	UNP A0R1H7
A	1009	UNK	PRO	conflict	UNP A0R1H7
A	1010	UNK	LEU	conflict	UNP A0R1H7
A	1011	UNK	SER	conflict	UNP A0R1H7
A	1012	UNK	GLY	conflict	UNP A0R1H7
A	1013	UNK	THR	conflict	UNP A0R1H7
A	1014	UNK	TRP	conflict	UNP A0R1H7
A	1196	UNK	GLY	conflict	UNP A0R1H7
A	1197	UNK	ARG	conflict	UNP A0R1H7
A	1198	UNK	THR	conflict	UNP A0R1H7
A	1199	UNK	GLY	conflict	UNP A0R1H7
A	1200	UNK	ALA	conflict	UNP A0R1H7
A	1201	UNK	ALA	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1202	UNK	GLU	conflict	UNP A0R1H7
A	1203	UNK	LEU	conflict	UNP A0R1H7
A	1204	UNK	THR	conflict	UNP A0R1H7
A	1205	UNK	ASP	conflict	UNP A0R1H7
A	1206	UNK	PRO	conflict	UNP A0R1H7
A	1207	UNK	VAL	conflict	UNP A0R1H7
A	1208	UNK	ARG	conflict	UNP A0R1H7
A	1209	UNK	ALA	conflict	UNP A0R1H7
A	1210	UNK	GLY	conflict	UNP A0R1H7
A	1211	UNK	GLY	conflict	UNP A0R1H7
A	1212	UNK	ALA	conflict	UNP A0R1H7
A	1213	UNK	ILE	conflict	UNP A0R1H7
A	1214	UNK	SER	conflict	UNP A0R1H7
A	1215	UNK	ASP	conflict	UNP A0R1H7
A	1216	UNK	ASN	conflict	UNP A0R1H7
A	1217	UNK	ALA	conflict	UNP A0R1H7
A	1218	UNK	THR	conflict	UNP A0R1H7
A	1219	UNK	ASP	conflict	UNP A0R1H7
A	1220	UNK	THR	conflict	UNP A0R1H7
A	1221	UNK	PRO	conflict	UNP A0R1H7
A	1222	UNK	ARG	conflict	UNP A0R1H7
A	1223	UNK	ARG	conflict	UNP A0R1H7
A	1224	UNK	ARG	conflict	UNP A0R1H7
A	1225	UNK	ARG	conflict	UNP A0R1H7
A	1226	UNK	ARG	conflict	UNP A0R1H7
A	1227	UNK	ASP	conflict	UNP A0R1H7
A	2076	UNK	GLY	conflict	UNP A0R1H7
A	2077	UNK	ASP	conflict	UNP A0R1H7
A	2078	UNK	ILE	conflict	UNP A0R1H7
A	2079	UNK	ASP	conflict	UNP A0R1H7
A	2080	UNK	ALA	conflict	UNP A0R1H7
A	2081	UNK	GLN	conflict	UNP A0R1H7
A	2082	UNK	TRP	conflict	UNP A0R1H7
A	2083	UNK	GLU	conflict	UNP A0R1H7
A	2084	UNK	GLN	conflict	UNP A0R1H7
A	2085	UNK	LEU	conflict	UNP A0R1H7
A	2086	UNK	SER	conflict	UNP A0R1H7
A	2087	UNK	GLN	conflict	UNP A0R1H7
A	2088	UNK	ARG	conflict	UNP A0R1H7
A	2089	UNK	PHE	conflict	UNP A0R1H7
A	2090	UNK	GLU	conflict	UNP A0R1H7
A	2091	UNK	GLY	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	2092	UNK	THR	conflict	UNP A0R1H7
A	2093	UNK	GLY	conflict	UNP A0R1H7
A	2094	UNK	HIS	conflict	UNP A0R1H7
A	2095	UNK	VAL	conflict	UNP A0R1H7
A	2096	UNK	VAL	conflict	UNP A0R1H7
A	2097	UNK	ALA	conflict	UNP A0R1H7
A	2098	UNK	THR	conflict	UNP A0R1H7
A	2099	UNK	GLN	conflict	UNP A0R1H7
A	2100	UNK	ALA	conflict	UNP A0R1H7
A	2101	UNK	ASN	conflict	UNP A0R1H7
A	2102	UNK	TRP	conflict	UNP A0R1H7
A	2103	UNK	TRP	conflict	UNP A0R1H7
A	2104	UNK	GLN	conflict	UNP A0R1H7
A	2105	UNK	GLY	conflict	UNP A0R1H7
A	2106	UNK	LYS	conflict	UNP A0R1H7
A	2107	UNK	ALA	conflict	UNP A0R1H7
A	2108	UNK	LEU	conflict	UNP A0R1H7
A	2109	UNK	ALA	conflict	UNP A0R1H7
A	2110	UNK	ALA	conflict	UNP A0R1H7
A	2111	UNK	GLY	conflict	UNP A0R1H7
A	2112	UNK	ARG	conflict	UNP A0R1H7
A	2113	UNK	ASN	conflict	UNP A0R1H7
A	2114	UNK	VAL	conflict	UNP A0R1H7
A	2115	UNK	HIS	conflict	UNP A0R1H7
A	2116	UNK	ALA	conflict	UNP A0R1H7
A	2117	UNK	SER	conflict	UNP A0R1H7
A	2118	UNK	LEU	conflict	UNP A0R1H7
A	2119	UNK	PHE	conflict	UNP A0R1H7
A	2120	UNK	GLY	conflict	UNP A0R1H7
A	2121	UNK	ARG	conflict	UNP A0R1H7
A	2122	UNK	ILE	conflict	UNP A0R1H7
A	2123	UNK	ALA	conflict	UNP A0R1H7
A	2124	UNK	ALA	conflict	UNP A0R1H7
A	2125	UNK	GLY	conflict	UNP A0R1H7
A	2126	UNK	ALA	conflict	UNP A0R1H7
A	2127	UNK	GLU	conflict	UNP A0R1H7
A	2128	UNK	ASN	conflict	UNP A0R1H7
A	2129	UNK	PRO	conflict	UNP A0R1H7
A	2130	UNK	GLY	conflict	UNP A0R1H7
A	2131	UNK	LYS	conflict	UNP A0R1H7
A	2132	UNK	GLY	conflict	UNP A0R1H7
A	2133	UNK	ARG	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	2134	UNK	TYR	conflict	UNP A0R1H7
A	2135	UNK	SER	conflict	UNP A0R1H7
A	2422	UNK	GLU	conflict	UNP A0R1H7
A	2423	UNK	SER	conflict	UNP A0R1H7
A	2424	UNK	ASP	conflict	UNP A0R1H7
A	2425	UNK	ASP	conflict	UNP A0R1H7
A	2426	UNK	GLU	conflict	UNP A0R1H7
A	2427	UNK	ALA	conflict	UNP A0R1H7
A	2428	UNK	PRO	conflict	UNP A0R1H7
A	2429	UNK	ALA	conflict	UNP A0R1H7
A	2430	UNK	GLY	conflict	UNP A0R1H7
A	2431	UNK	THR	conflict	UNP A0R1H7
A	2432	UNK	ILE	conflict	UNP A0R1H7
A	2433	UNK	ARG	conflict	UNP A0R1H7
A	2434	UNK	ALA	conflict	UNP A0R1H7
A	2435	UNK	LEU	conflict	UNP A0R1H7
A	2436	UNK	PRO	conflict	UNP A0R1H7
A	2437	UNK	SER	conflict	UNP A0R1H7
A	2438	UNK	PRO	conflict	UNP A0R1H7
A	2439	UNK	PRO	conflict	UNP A0R1H7
A	2440	UNK	ARG	conflict	UNP A0R1H7
A	2441	UNK	GLY	conflict	UNP A0R1H7
A	2442	UNK	TYR	conflict	UNP A0R1H7
A	2443	UNK	ASN	conflict	UNP A0R1H7
A	2444	UNK	PRO	conflict	UNP A0R1H7
A	2445	UNK	ALA	conflict	UNP A0R1H7
A	2446	UNK	PRO	conflict	UNP A0R1H7
A	2447	UNK	ALA	conflict	UNP A0R1H7
A	2448	UNK	PRO	conflict	UNP A0R1H7
A	2449	UNK	GLU	conflict	UNP A0R1H7
A	2450	UNK	TRP	conflict	UNP A0R1H7
A	2451	UNK	ASP	conflict	UNP A0R1H7
A	2452	UNK	ASP	conflict	UNP A0R1H7
A	2453	UNK	LEU	conflict	UNP A0R1H7
B	929	UNK	GLU	conflict	UNP A0R1H7
B	930	UNK	PRO	conflict	UNP A0R1H7
B	931	UNK	VAL	conflict	UNP A0R1H7
B	932	UNK	GLU	conflict	UNP A0R1H7
B	933	UNK	VAL	conflict	UNP A0R1H7
B	934	UNK	LEU	conflict	UNP A0R1H7
B	935	UNK	SER	conflict	UNP A0R1H7
B	936	UNK	ARG	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	937	UNK	ARG	conflict	UNP A0R1H7
B	938	UNK	GLN	conflict	UNP A0R1H7
B	939	UNK	ALA	conflict	UNP A0R1H7
B	940	UNK	ARG	conflict	UNP A0R1H7
B	941	UNK	ARG	conflict	UNP A0R1H7
B	942	UNK	ASP	conflict	UNP A0R1H7
B	943	UNK	ALA	conflict	UNP A0R1H7
B	944	UNK	SER	conflict	UNP A0R1H7
B	974	UNK	THR	conflict	UNP A0R1H7
B	975	UNK	GLU	conflict	UNP A0R1H7
B	976	UNK	TRP	conflict	UNP A0R1H7
B	977	UNK	GLN	conflict	UNP A0R1H7
B	978	UNK	VAL	conflict	UNP A0R1H7
B	979	UNK	ARG	conflict	UNP A0R1H7
B	980	UNK	GLU	conflict	UNP A0R1H7
B	981	UNK	GLY	conflict	UNP A0R1H7
B	982	UNK	SER	conflict	UNP A0R1H7
B	983	UNK	ASP	conflict	UNP A0R1H7
B	984	UNK	ASN	conflict	UNP A0R1H7
B	985	UNK	ARG	conflict	UNP A0R1H7
B	986	UNK	SER	conflict	UNP A0R1H7
B	987	UNK	ALA	conflict	UNP A0R1H7
B	988	UNK	SER	conflict	UNP A0R1H7
B	989	UNK	HIS	conflict	UNP A0R1H7
B	990	UNK	PRO	conflict	UNP A0R1H7
B	991	UNK	SER	conflict	UNP A0R1H7
B	992	UNK	THR	conflict	UNP A0R1H7
B	993	UNK	GLY	conflict	UNP A0R1H7
B	994	UNK	ALA	conflict	UNP A0R1H7
B	995	UNK	ARG	conflict	UNP A0R1H7
B	996	UNK	LEU	conflict	UNP A0R1H7
B	997	UNK	GLU	conflict	UNP A0R1H7
B	998	UNK	VAL	conflict	UNP A0R1H7
B	999	UNK	ALA	conflict	UNP A0R1H7
B	1000	UNK	ASP	conflict	UNP A0R1H7
B	1001	UNK	ASP	conflict	UNP A0R1H7
B	1002	UNK	GLN	conflict	UNP A0R1H7
B	1003	UNK	HIS	conflict	UNP A0R1H7
B	1004	UNK	VAL	conflict	UNP A0R1H7
B	1005	UNK	VAL	conflict	UNP A0R1H7
B	1006	UNK	LEU	conflict	UNP A0R1H7
B	1007	UNK	SER	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1008	UNK	VAL	conflict	UNP A0R1H7
B	1009	UNK	PRO	conflict	UNP A0R1H7
B	1010	UNK	LEU	conflict	UNP A0R1H7
B	1011	UNK	SER	conflict	UNP A0R1H7
B	1012	UNK	GLY	conflict	UNP A0R1H7
B	1013	UNK	THR	conflict	UNP A0R1H7
B	1014	UNK	TRP	conflict	UNP A0R1H7
B	1196	UNK	GLY	conflict	UNP A0R1H7
B	1197	UNK	ARG	conflict	UNP A0R1H7
B	1198	UNK	THR	conflict	UNP A0R1H7
B	1199	UNK	GLY	conflict	UNP A0R1H7
B	1200	UNK	ALA	conflict	UNP A0R1H7
B	1201	UNK	ALA	conflict	UNP A0R1H7
B	1202	UNK	GLU	conflict	UNP A0R1H7
B	1203	UNK	LEU	conflict	UNP A0R1H7
B	1204	UNK	THR	conflict	UNP A0R1H7
B	1205	UNK	ASP	conflict	UNP A0R1H7
B	1206	UNK	PRO	conflict	UNP A0R1H7
B	1207	UNK	VAL	conflict	UNP A0R1H7
B	1208	UNK	ARG	conflict	UNP A0R1H7
B	1209	UNK	ALA	conflict	UNP A0R1H7
B	1210	UNK	GLY	conflict	UNP A0R1H7
B	1211	UNK	GLY	conflict	UNP A0R1H7
B	1212	UNK	ALA	conflict	UNP A0R1H7
B	1213	UNK	ILE	conflict	UNP A0R1H7
B	1214	UNK	SER	conflict	UNP A0R1H7
B	1215	UNK	ASP	conflict	UNP A0R1H7
B	1216	UNK	ASN	conflict	UNP A0R1H7
B	1217	UNK	ALA	conflict	UNP A0R1H7
B	1218	UNK	THR	conflict	UNP A0R1H7
B	1219	UNK	ASP	conflict	UNP A0R1H7
B	1220	UNK	THR	conflict	UNP A0R1H7
B	1221	UNK	PRO	conflict	UNP A0R1H7
B	1222	UNK	ARG	conflict	UNP A0R1H7
B	1223	UNK	ARG	conflict	UNP A0R1H7
B	1224	UNK	ARG	conflict	UNP A0R1H7
B	1225	UNK	ARG	conflict	UNP A0R1H7
B	1226	UNK	ARG	conflict	UNP A0R1H7
B	1227	UNK	ASP	conflict	UNP A0R1H7
B	2076	UNK	GLY	conflict	UNP A0R1H7
B	2077	UNK	ASP	conflict	UNP A0R1H7
B	2078	UNK	ILE	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	2079	UNK	ASP	conflict	UNP A0R1H7
B	2080	UNK	ALA	conflict	UNP A0R1H7
B	2081	UNK	GLN	conflict	UNP A0R1H7
B	2082	UNK	TRP	conflict	UNP A0R1H7
B	2083	UNK	GLU	conflict	UNP A0R1H7
B	2084	UNK	GLN	conflict	UNP A0R1H7
B	2085	UNK	LEU	conflict	UNP A0R1H7
B	2086	UNK	SER	conflict	UNP A0R1H7
B	2087	UNK	GLN	conflict	UNP A0R1H7
B	2088	UNK	ARG	conflict	UNP A0R1H7
B	2089	UNK	PHE	conflict	UNP A0R1H7
B	2090	UNK	GLU	conflict	UNP A0R1H7
B	2091	UNK	GLY	conflict	UNP A0R1H7
B	2092	UNK	THR	conflict	UNP A0R1H7
B	2093	UNK	GLY	conflict	UNP A0R1H7
B	2094	UNK	HIS	conflict	UNP A0R1H7
B	2095	UNK	VAL	conflict	UNP A0R1H7
B	2096	UNK	VAL	conflict	UNP A0R1H7
B	2097	UNK	ALA	conflict	UNP A0R1H7
B	2098	UNK	THR	conflict	UNP A0R1H7
B	2099	UNK	GLN	conflict	UNP A0R1H7
B	2100	UNK	ALA	conflict	UNP A0R1H7
B	2101	UNK	ASN	conflict	UNP A0R1H7
B	2102	UNK	TRP	conflict	UNP A0R1H7
B	2103	UNK	TRP	conflict	UNP A0R1H7
B	2104	UNK	GLN	conflict	UNP A0R1H7
B	2105	UNK	GLY	conflict	UNP A0R1H7
B	2106	UNK	LYS	conflict	UNP A0R1H7
B	2107	UNK	ALA	conflict	UNP A0R1H7
B	2108	UNK	LEU	conflict	UNP A0R1H7
B	2109	UNK	ALA	conflict	UNP A0R1H7
B	2110	UNK	ALA	conflict	UNP A0R1H7
B	2111	UNK	GLY	conflict	UNP A0R1H7
B	2112	UNK	ARG	conflict	UNP A0R1H7
B	2113	UNK	ASN	conflict	UNP A0R1H7
B	2114	UNK	VAL	conflict	UNP A0R1H7
B	2115	UNK	HIS	conflict	UNP A0R1H7
B	2116	UNK	ALA	conflict	UNP A0R1H7
B	2117	UNK	SER	conflict	UNP A0R1H7
B	2118	UNK	LEU	conflict	UNP A0R1H7
B	2119	UNK	PHE	conflict	UNP A0R1H7
B	2120	UNK	GLY	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	2121	UNK	ARG	conflict	UNP A0R1H7
B	2122	UNK	ILE	conflict	UNP A0R1H7
B	2123	UNK	ALA	conflict	UNP A0R1H7
B	2124	UNK	ALA	conflict	UNP A0R1H7
B	2125	UNK	GLY	conflict	UNP A0R1H7
B	2126	UNK	ALA	conflict	UNP A0R1H7
B	2127	UNK	GLU	conflict	UNP A0R1H7
B	2128	UNK	ASN	conflict	UNP A0R1H7
B	2129	UNK	PRO	conflict	UNP A0R1H7
B	2130	UNK	GLY	conflict	UNP A0R1H7
B	2131	UNK	LYS	conflict	UNP A0R1H7
B	2132	UNK	GLY	conflict	UNP A0R1H7
B	2133	UNK	ARG	conflict	UNP A0R1H7
B	2134	UNK	TYR	conflict	UNP A0R1H7
B	2135	UNK	SER	conflict	UNP A0R1H7
B	2422	UNK	GLU	conflict	UNP A0R1H7
B	2423	UNK	SER	conflict	UNP A0R1H7
B	2424	UNK	ASP	conflict	UNP A0R1H7
B	2425	UNK	ASP	conflict	UNP A0R1H7
B	2426	UNK	GLU	conflict	UNP A0R1H7
B	2427	UNK	ALA	conflict	UNP A0R1H7
B	2428	UNK	PRO	conflict	UNP A0R1H7
B	2429	UNK	ALA	conflict	UNP A0R1H7
B	2430	UNK	GLY	conflict	UNP A0R1H7
B	2431	UNK	THR	conflict	UNP A0R1H7
B	2432	UNK	ILE	conflict	UNP A0R1H7
B	2433	UNK	ARG	conflict	UNP A0R1H7
B	2434	UNK	ALA	conflict	UNP A0R1H7
B	2435	UNK	LEU	conflict	UNP A0R1H7
B	2436	UNK	PRO	conflict	UNP A0R1H7
B	2437	UNK	SER	conflict	UNP A0R1H7
B	2438	UNK	PRO	conflict	UNP A0R1H7
B	2439	UNK	PRO	conflict	UNP A0R1H7
B	2440	UNK	ARG	conflict	UNP A0R1H7
B	2441	UNK	GLY	conflict	UNP A0R1H7
B	2442	UNK	TYR	conflict	UNP A0R1H7
B	2443	UNK	ASN	conflict	UNP A0R1H7
B	2444	UNK	PRO	conflict	UNP A0R1H7
B	2445	UNK	ALA	conflict	UNP A0R1H7
B	2446	UNK	PRO	conflict	UNP A0R1H7
B	2447	UNK	ALA	conflict	UNP A0R1H7
B	2448	UNK	PRO	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	2449	UNK	GLU	conflict	UNP A0R1H7
B	2450	UNK	TRP	conflict	UNP A0R1H7
B	2451	UNK	ASP	conflict	UNP A0R1H7
B	2452	UNK	ASP	conflict	UNP A0R1H7
B	2453	UNK	LEU	conflict	UNP A0R1H7
C	929	UNK	GLU	conflict	UNP A0R1H7
C	930	UNK	PRO	conflict	UNP A0R1H7
C	931	UNK	VAL	conflict	UNP A0R1H7
C	932	UNK	GLU	conflict	UNP A0R1H7
C	933	UNK	VAL	conflict	UNP A0R1H7
C	934	UNK	LEU	conflict	UNP A0R1H7
C	935	UNK	SER	conflict	UNP A0R1H7
C	936	UNK	ARG	conflict	UNP A0R1H7
C	937	UNK	ARG	conflict	UNP A0R1H7
C	938	UNK	GLN	conflict	UNP A0R1H7
C	939	UNK	ALA	conflict	UNP A0R1H7
C	940	UNK	ARG	conflict	UNP A0R1H7
C	941	UNK	ARG	conflict	UNP A0R1H7
C	942	UNK	ASP	conflict	UNP A0R1H7
C	943	UNK	ALA	conflict	UNP A0R1H7
C	944	UNK	SER	conflict	UNP A0R1H7
C	974	UNK	THR	conflict	UNP A0R1H7
C	975	UNK	GLU	conflict	UNP A0R1H7
C	976	UNK	TRP	conflict	UNP A0R1H7
C	977	UNK	GLN	conflict	UNP A0R1H7
C	978	UNK	VAL	conflict	UNP A0R1H7
C	979	UNK	ARG	conflict	UNP A0R1H7
C	980	UNK	GLU	conflict	UNP A0R1H7
C	981	UNK	GLY	conflict	UNP A0R1H7
C	982	UNK	SER	conflict	UNP A0R1H7
C	983	UNK	ASP	conflict	UNP A0R1H7
C	984	UNK	ASN	conflict	UNP A0R1H7
C	985	UNK	ARG	conflict	UNP A0R1H7
C	986	UNK	SER	conflict	UNP A0R1H7
C	987	UNK	ALA	conflict	UNP A0R1H7
C	988	UNK	SER	conflict	UNP A0R1H7
C	989	UNK	HIS	conflict	UNP A0R1H7
C	990	UNK	PRO	conflict	UNP A0R1H7
C	991	UNK	SER	conflict	UNP A0R1H7
C	992	UNK	THR	conflict	UNP A0R1H7
C	993	UNK	GLY	conflict	UNP A0R1H7
C	994	UNK	ALA	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	995	UNK	ARG	conflict	UNP A0R1H7
C	996	UNK	LEU	conflict	UNP A0R1H7
C	997	UNK	GLU	conflict	UNP A0R1H7
C	998	UNK	VAL	conflict	UNP A0R1H7
C	999	UNK	ALA	conflict	UNP A0R1H7
C	1000	UNK	ASP	conflict	UNP A0R1H7
C	1001	UNK	ASP	conflict	UNP A0R1H7
C	1002	UNK	GLN	conflict	UNP A0R1H7
C	1003	UNK	HIS	conflict	UNP A0R1H7
C	1004	UNK	VAL	conflict	UNP A0R1H7
C	1005	UNK	VAL	conflict	UNP A0R1H7
C	1006	UNK	LEU	conflict	UNP A0R1H7
C	1007	UNK	SER	conflict	UNP A0R1H7
C	1008	UNK	VAL	conflict	UNP A0R1H7
C	1009	UNK	PRO	conflict	UNP A0R1H7
C	1010	UNK	LEU	conflict	UNP A0R1H7
C	1011	UNK	SER	conflict	UNP A0R1H7
C	1012	UNK	GLY	conflict	UNP A0R1H7
C	1013	UNK	THR	conflict	UNP A0R1H7
C	1014	UNK	TRP	conflict	UNP A0R1H7
C	1196	UNK	GLY	conflict	UNP A0R1H7
C	1197	UNK	ARG	conflict	UNP A0R1H7
C	1198	UNK	THR	conflict	UNP A0R1H7
C	1199	UNK	GLY	conflict	UNP A0R1H7
C	1200	UNK	ALA	conflict	UNP A0R1H7
C	1201	UNK	ALA	conflict	UNP A0R1H7
C	1202	UNK	GLU	conflict	UNP A0R1H7
C	1203	UNK	LEU	conflict	UNP A0R1H7
C	1204	UNK	THR	conflict	UNP A0R1H7
C	1205	UNK	ASP	conflict	UNP A0R1H7
C	1206	UNK	PRO	conflict	UNP A0R1H7
C	1207	UNK	VAL	conflict	UNP A0R1H7
C	1208	UNK	ARG	conflict	UNP A0R1H7
C	1209	UNK	ALA	conflict	UNP A0R1H7
C	1210	UNK	GLY	conflict	UNP A0R1H7
C	1211	UNK	GLY	conflict	UNP A0R1H7
C	1212	UNK	ALA	conflict	UNP A0R1H7
C	1213	UNK	ILE	conflict	UNP A0R1H7
C	1214	UNK	SER	conflict	UNP A0R1H7
C	1215	UNK	ASP	conflict	UNP A0R1H7
C	1216	UNK	ASN	conflict	UNP A0R1H7
C	1217	UNK	ALA	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1218	UNK	THR	conflict	UNP A0R1H7
C	1219	UNK	ASP	conflict	UNP A0R1H7
C	1220	UNK	THR	conflict	UNP A0R1H7
C	1221	UNK	PRO	conflict	UNP A0R1H7
C	1222	UNK	ARG	conflict	UNP A0R1H7
C	1223	UNK	ARG	conflict	UNP A0R1H7
C	1224	UNK	ARG	conflict	UNP A0R1H7
C	1225	UNK	ARG	conflict	UNP A0R1H7
C	1226	UNK	ARG	conflict	UNP A0R1H7
C	1227	UNK	ASP	conflict	UNP A0R1H7
C	2076	UNK	GLY	conflict	UNP A0R1H7
C	2077	UNK	ASP	conflict	UNP A0R1H7
C	2078	UNK	ILE	conflict	UNP A0R1H7
C	2079	UNK	ASP	conflict	UNP A0R1H7
C	2080	UNK	ALA	conflict	UNP A0R1H7
C	2081	UNK	GLN	conflict	UNP A0R1H7
C	2082	UNK	TRP	conflict	UNP A0R1H7
C	2083	UNK	GLU	conflict	UNP A0R1H7
C	2084	UNK	GLN	conflict	UNP A0R1H7
C	2085	UNK	LEU	conflict	UNP A0R1H7
C	2086	UNK	SER	conflict	UNP A0R1H7
C	2087	UNK	GLN	conflict	UNP A0R1H7
C	2088	UNK	ARG	conflict	UNP A0R1H7
C	2089	UNK	PHE	conflict	UNP A0R1H7
C	2090	UNK	GLU	conflict	UNP A0R1H7
C	2091	UNK	GLY	conflict	UNP A0R1H7
C	2092	UNK	THR	conflict	UNP A0R1H7
C	2093	UNK	GLY	conflict	UNP A0R1H7
C	2094	UNK	HIS	conflict	UNP A0R1H7
C	2095	UNK	VAL	conflict	UNP A0R1H7
C	2096	UNK	VAL	conflict	UNP A0R1H7
C	2097	UNK	ALA	conflict	UNP A0R1H7
C	2098	UNK	THR	conflict	UNP A0R1H7
C	2099	UNK	GLN	conflict	UNP A0R1H7
C	2100	UNK	ALA	conflict	UNP A0R1H7
C	2101	UNK	ASN	conflict	UNP A0R1H7
C	2102	UNK	TRP	conflict	UNP A0R1H7
C	2103	UNK	TRP	conflict	UNP A0R1H7
C	2104	UNK	GLN	conflict	UNP A0R1H7
C	2105	UNK	GLY	conflict	UNP A0R1H7
C	2106	UNK	LYS	conflict	UNP A0R1H7
C	2107	UNK	ALA	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

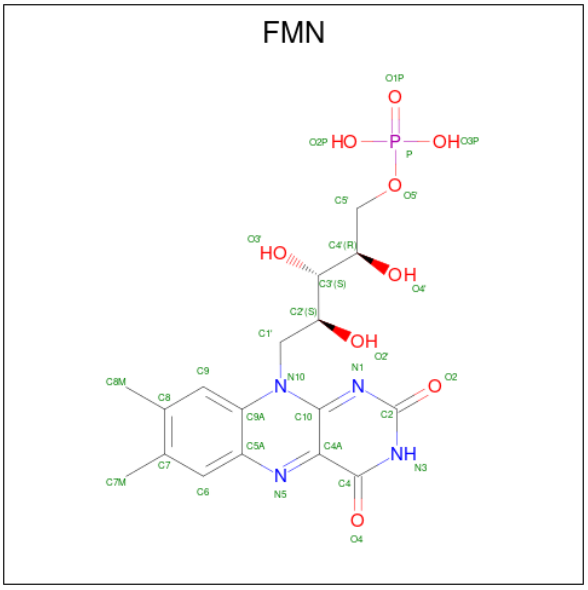
Chain	Residue	Modelled	Actual	Comment	Reference
C	2108	UNK	LEU	conflict	UNP A0R1H7
C	2109	UNK	ALA	conflict	UNP A0R1H7
C	2110	UNK	ALA	conflict	UNP A0R1H7
C	2111	UNK	GLY	conflict	UNP A0R1H7
C	2112	UNK	ARG	conflict	UNP A0R1H7
C	2113	UNK	ASN	conflict	UNP A0R1H7
C	2114	UNK	VAL	conflict	UNP A0R1H7
C	2115	UNK	HIS	conflict	UNP A0R1H7
C	2116	UNK	ALA	conflict	UNP A0R1H7
C	2117	UNK	SER	conflict	UNP A0R1H7
C	2118	UNK	LEU	conflict	UNP A0R1H7
C	2119	UNK	PHE	conflict	UNP A0R1H7
C	2120	UNK	GLY	conflict	UNP A0R1H7
C	2121	UNK	ARG	conflict	UNP A0R1H7
C	2122	UNK	ILE	conflict	UNP A0R1H7
C	2123	UNK	ALA	conflict	UNP A0R1H7
C	2124	UNK	ALA	conflict	UNP A0R1H7
C	2125	UNK	GLY	conflict	UNP A0R1H7
C	2126	UNK	ALA	conflict	UNP A0R1H7
C	2127	UNK	GLU	conflict	UNP A0R1H7
C	2128	UNK	ASN	conflict	UNP A0R1H7
C	2129	UNK	PRO	conflict	UNP A0R1H7
C	2130	UNK	GLY	conflict	UNP A0R1H7
C	2131	UNK	LYS	conflict	UNP A0R1H7
C	2132	UNK	GLY	conflict	UNP A0R1H7
C	2133	UNK	ARG	conflict	UNP A0R1H7
C	2134	UNK	TYR	conflict	UNP A0R1H7
C	2135	UNK	SER	conflict	UNP A0R1H7
C	2422	UNK	GLU	conflict	UNP A0R1H7
C	2423	UNK	SER	conflict	UNP A0R1H7
C	2424	UNK	ASP	conflict	UNP A0R1H7
C	2425	UNK	ASP	conflict	UNP A0R1H7
C	2426	UNK	GLU	conflict	UNP A0R1H7
C	2427	UNK	ALA	conflict	UNP A0R1H7
C	2428	UNK	PRO	conflict	UNP A0R1H7
C	2429	UNK	ALA	conflict	UNP A0R1H7
C	2430	UNK	GLY	conflict	UNP A0R1H7
C	2431	UNK	THR	conflict	UNP A0R1H7
C	2432	UNK	ILE	conflict	UNP A0R1H7
C	2433	UNK	ARG	conflict	UNP A0R1H7
C	2434	UNK	ALA	conflict	UNP A0R1H7
C	2435	UNK	LEU	conflict	UNP A0R1H7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	2436	UNK	PRO	conflict	UNP A0R1H7
C	2437	UNK	SER	conflict	UNP A0R1H7
C	2438	UNK	PRO	conflict	UNP A0R1H7
C	2439	UNK	PRO	conflict	UNP A0R1H7
C	2440	UNK	ARG	conflict	UNP A0R1H7
C	2441	UNK	GLY	conflict	UNP A0R1H7
C	2442	UNK	TYR	conflict	UNP A0R1H7
C	2443	UNK	ASN	conflict	UNP A0R1H7
C	2444	UNK	PRO	conflict	UNP A0R1H7
C	2445	UNK	ALA	conflict	UNP A0R1H7
C	2446	UNK	PRO	conflict	UNP A0R1H7
C	2447	UNK	ALA	conflict	UNP A0R1H7
C	2448	UNK	PRO	conflict	UNP A0R1H7
C	2449	UNK	GLU	conflict	UNP A0R1H7
C	2450	UNK	TRP	conflict	UNP A0R1H7
C	2451	UNK	ASP	conflict	UNP A0R1H7
C	2452	UNK	ASP	conflict	UNP A0R1H7
C	2453	UNK	LEU	conflict	UNP A0R1H7

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
2	D	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	E	1	Total	C	N	O	P	0
			31	17	4	9	1	

Continued on next page...

Continued from previous page...

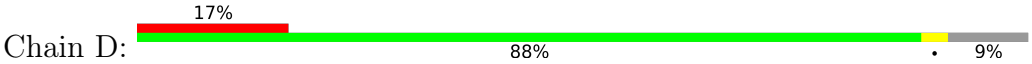
Mol	Chain	Residues	Atoms					AltConf
2	F	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	A	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	B	1	Total	C	N	O	P	0
			31	17	4	9	1	
2	C	1	Total	C	N	O	P	0
			31	17	4	9	1	

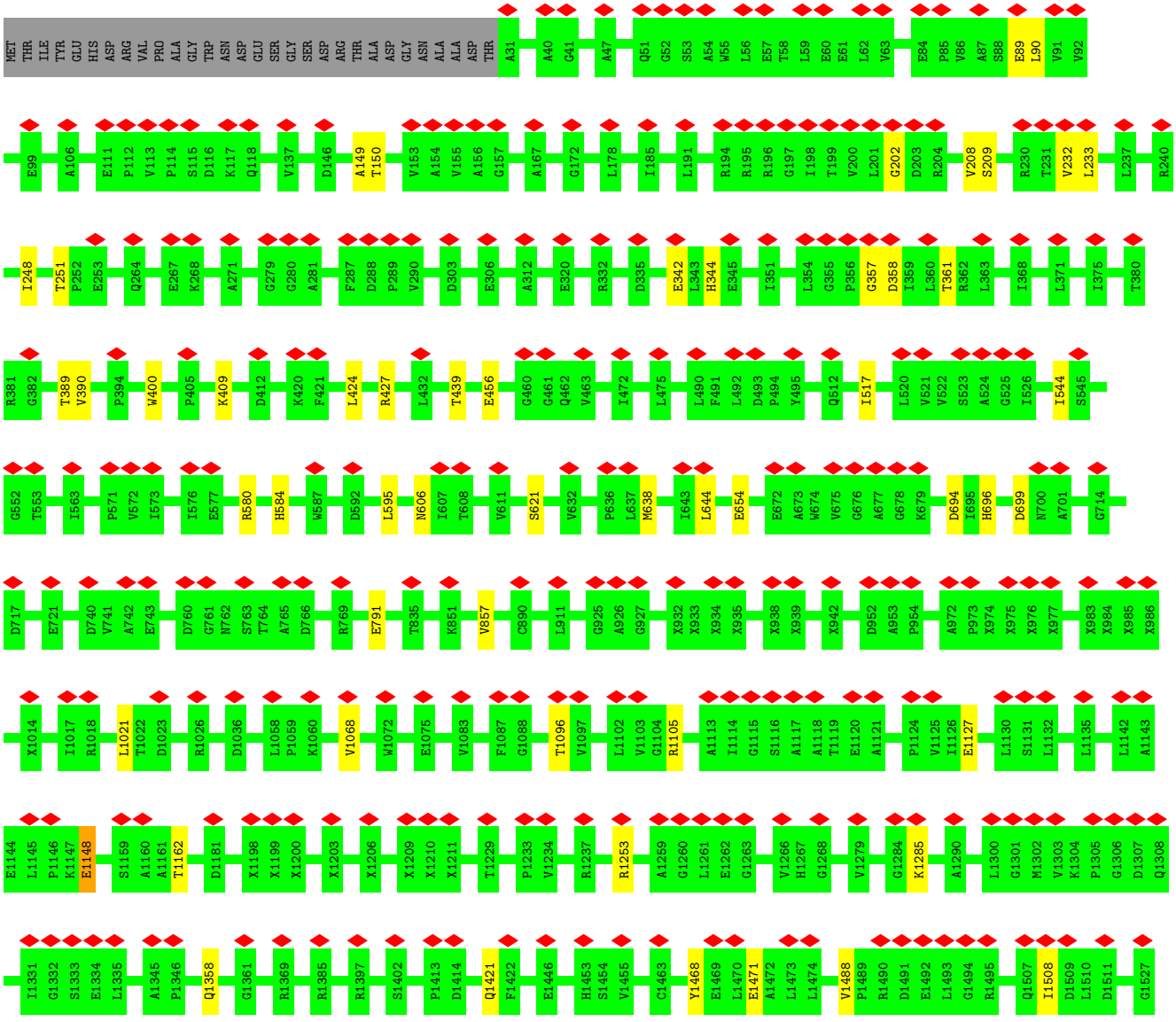
3 Residue-property plots (i)

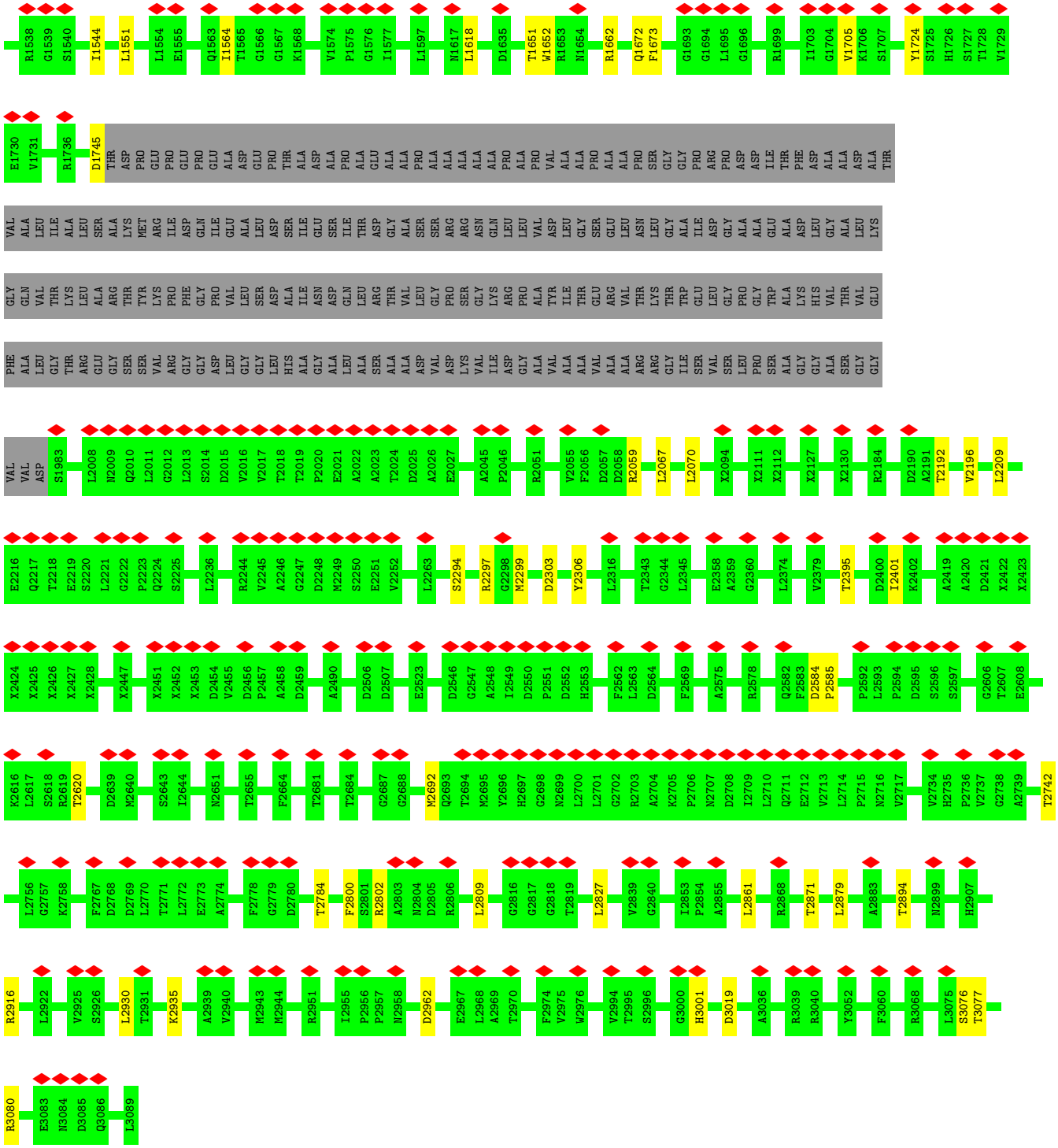
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: FATTY ACID SYNTHASE

Chain D:

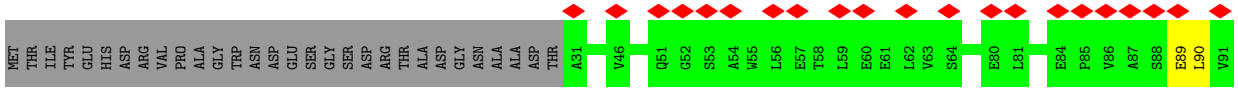


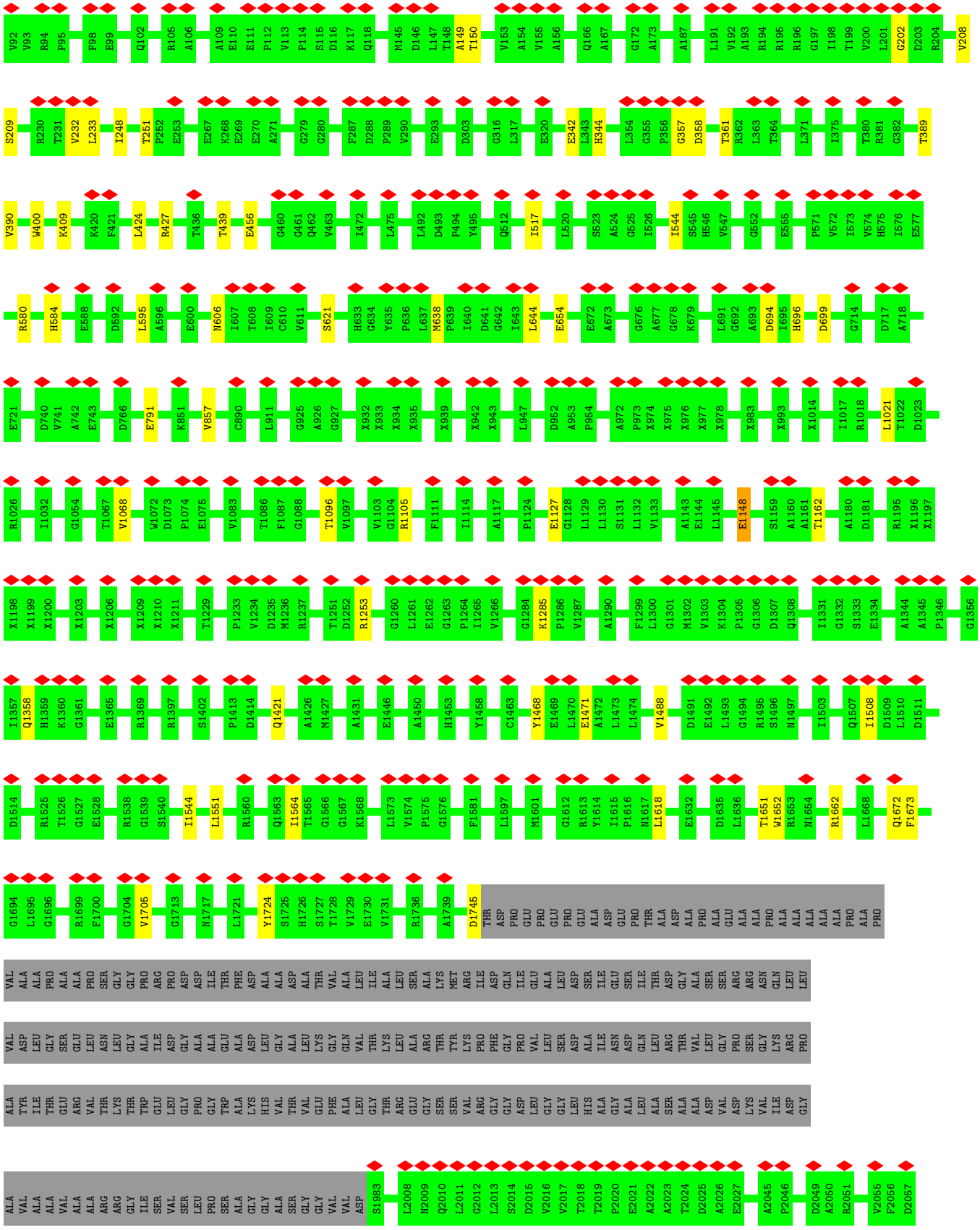


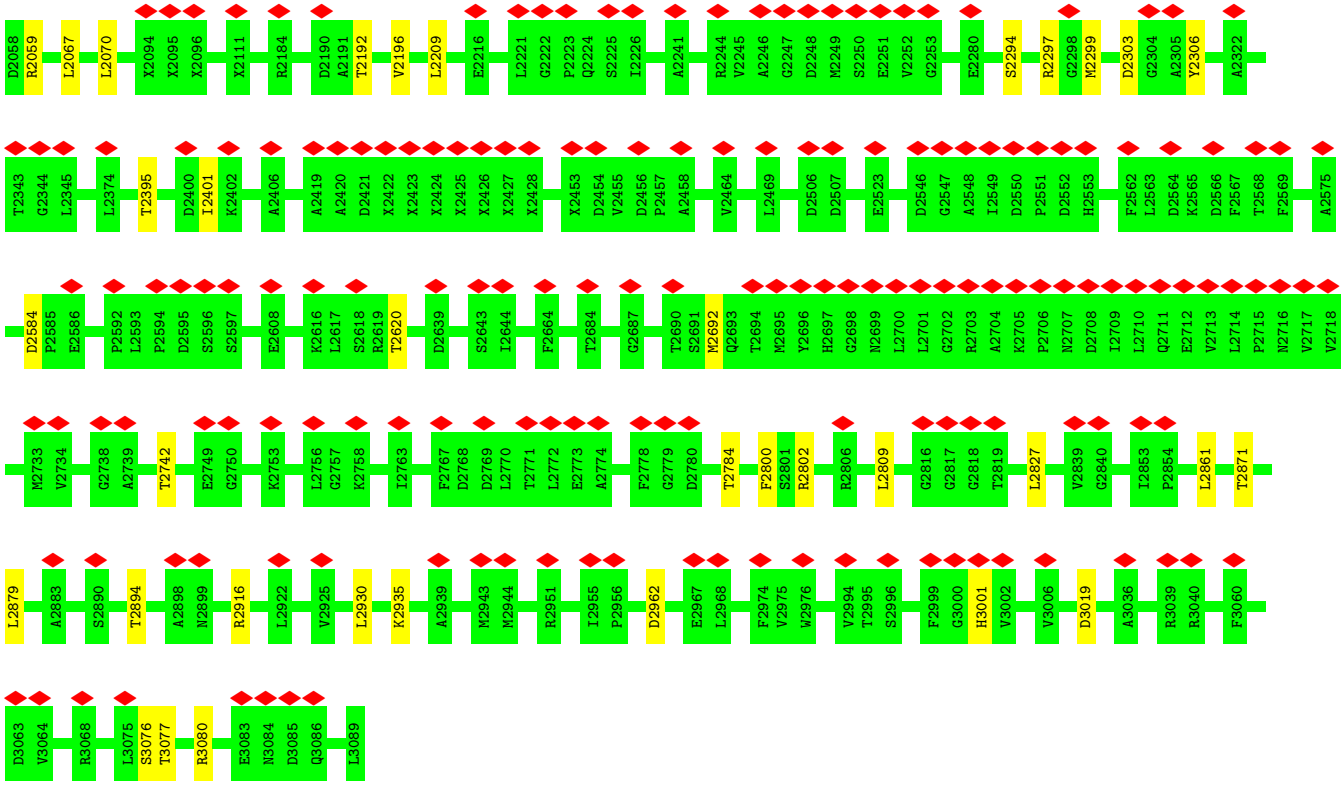


- Molecule 1: FATTY ACID SYNTHASE

Chain E:

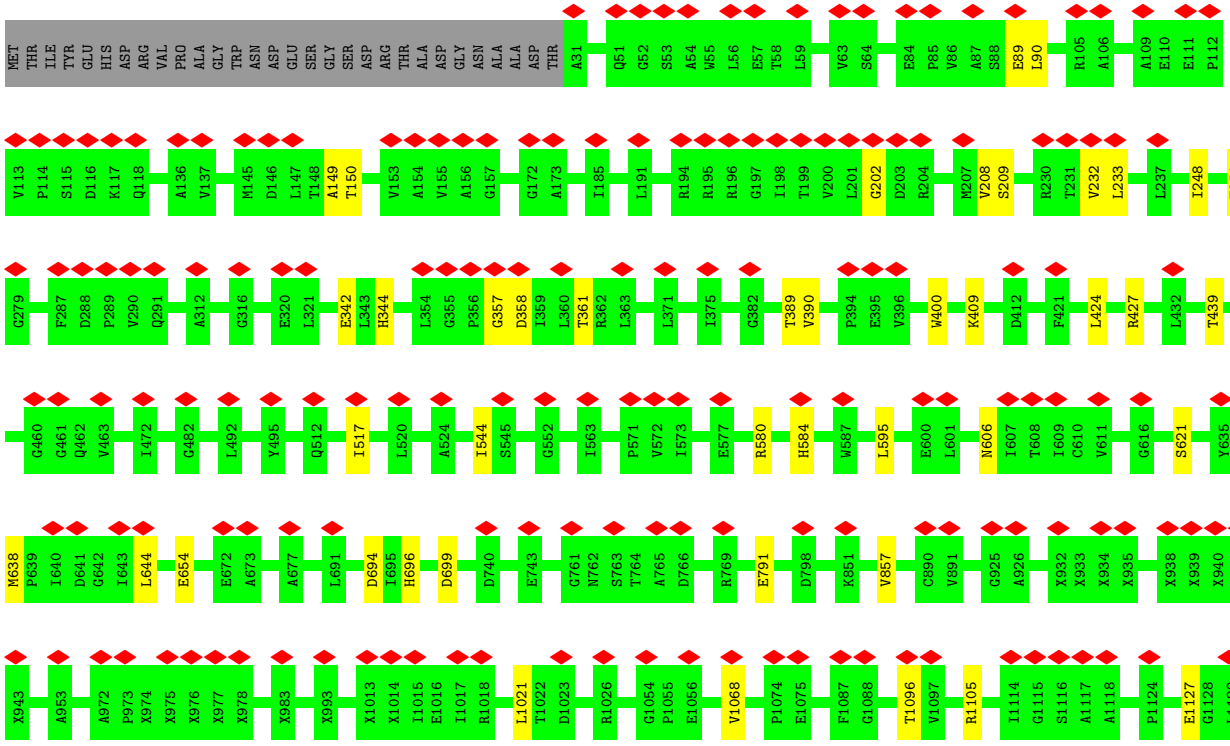


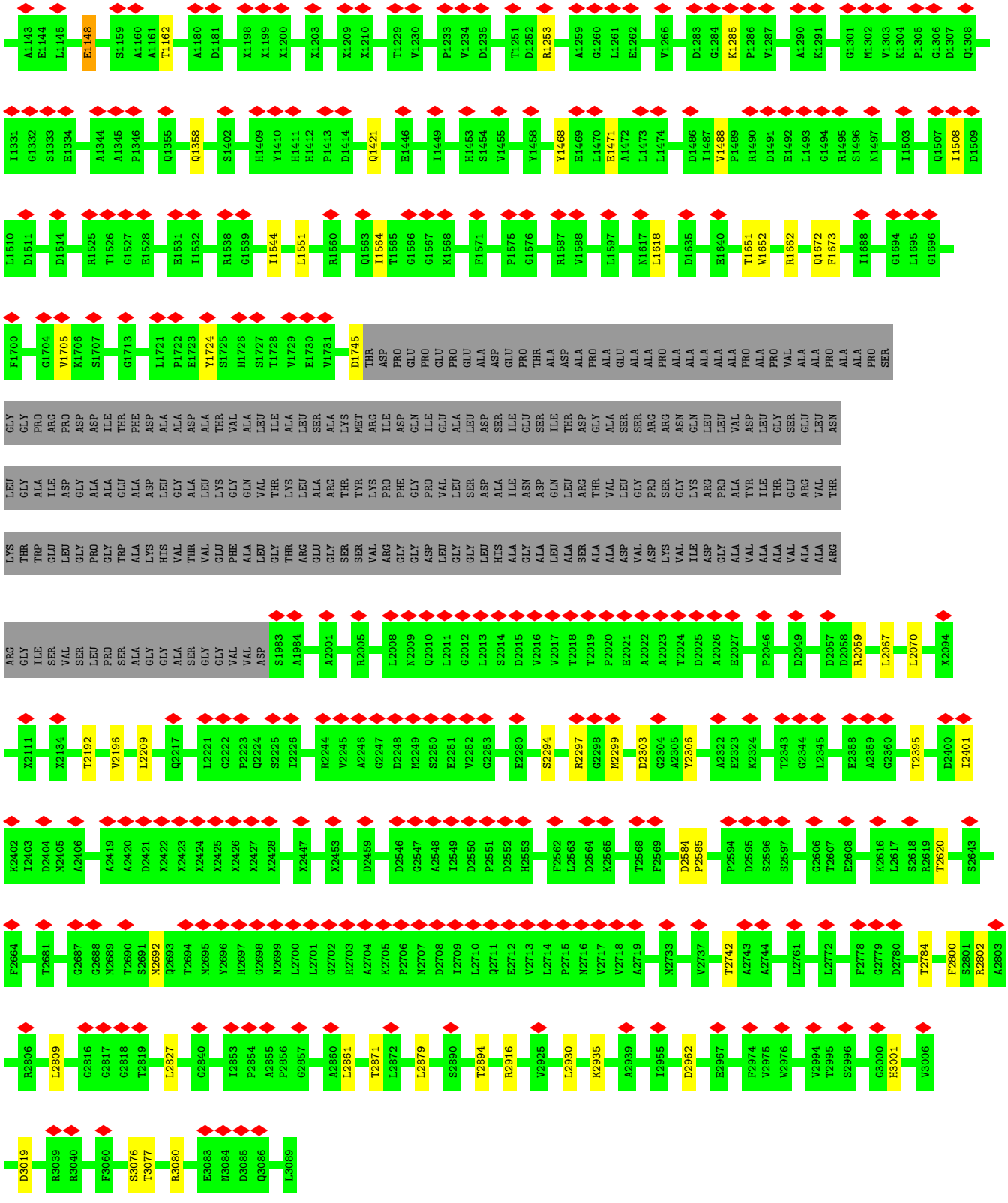

V92 V93 R94 P95 F98 E99 Q102 R105 A106 A109 E110 E111 P112 V113 P114 S115 D116 K117 Q118 M145 D146 L147 T148 A149 T150 V153 A154 V155 A156 Q166 A167 G172 A173 A187 L191 V192 A193 R194 R195 R196 G197 I198 T199 V200 L201 G202 D203 R204 V208
S209 R230 T231 V232 L233 I248 T251 F252 E253 E267 K268 E269 E270 A271 G279 G280 F287 D288 P289 V290 E293 D303 G316 L317 E320 E342 L343 H344 L354 G355 P356 G357 D358 T361 R362 L363 T364 L371 I375 T380 R381 G382 T389
V390 W400 K409 K420 F421 L424 R427 T436 T439 E456 G460 G461 Q462 V463 I472 L475 L492 D493 P494 Y495 Q512 I517 L520 S523 A524 G525 I526 I544 S545 H546 V547 G552 E555 P571 V572 I573 V574 H575 I576 E577
R580 H584 E588 D592 L595 A596 E600 N606 I607 T608 I609 C610 V611 S621 H633 G634 Y635 P636 L637 M638 P639 I640 D641 G642 I643 L644 E654 E672 A673 G676 A677 G678 K679 L691 G692 A693 D694 I695 H696 D699 G714 D717 A718
E721 D740 V741 A742 E743 D766 E791 K851 V857 G890 L911 G925 A926 G927 X932 X933 X934 X935 X939 X942 X943 L947 D952 A953 P954 A972 P973 X974 X975 X976 X977 X978 X983 X993 X1014 I1017 R1018 L1021 T1022 D1023
R1026 I1032 G1054 T1067 V1068 W1072 D1073 P1074 E1075 V1083 T1086 F1087 G1088 T1096 V1097 V1103 G1104 R1105 F1111 I1114 A1117 P1124 E1127 G1128 L1129 L1130 S1131 L1132 V1133 A1143 E1144 L1145 E1148 S1159 A1160 A1161 T1162 A1180 D1181 R1195 X1196 X1197
X1198 X1199 X1200 X1203 X1206 X1209 X1210 X1211 T1229 P1233 V1234 D1235 M1236 R1237 T1251 D1252 R1253 G1260 L1261 E1262 G1263 P1264 I1265 V1266 G1284 K1285 P1286 V1287 A1290 F1299 L1300 G1301 M1302 V1303 K1304 P1305 G1306 D1307 Q1308 I1331 G1332 S1333 E1334 A1344 A1345 P1346 G1356
I1357 Q1358 H1359 K1360 G1361 E1365 R1369 R1397 S1402 P1413 D1414 Q1421 A1426 M1427 A1431 E1446 A1450 H1453 Y1458 C1463 Y1468 E1469 L1470 E1471 A1472 L1473 L1474 V1488 D1491 E1492 L1493 G1494 R1495 S1496 N1497 I1503 Q1507 I1508 D1509 L1510 D1511
D1514 R1525 T1526 G1527 E1528 R1538 G1539 S1540 I1544 L1551 R1560 Q1563 I1564 T1565 G1566 G1567 K1568 L1573 V1574 P1575 G1576 F1581 L1597 M1601 G1612 R1613 Y1614 I1615 P1616 N1617 L1618 E1632 D1635 L1636 T1651 W1652 R1653 N1654 R1662 L1668 Q1672 F1673
G1694 L1695 G1696 R1699 F1700 G1704 V1705 G1713 N1717 L1721 Y1724 S1725 H1726 S1727 T1728 V1729 E1730 V1731 R1736 A1739 D1745 THR ASP PRO GLU PRO GLU PRO GLU ALA ASP GLU PRO THR ALA ASP ALA GLU ALA ALA ALA ALA ALA PRO ALA PRO
VAL ALA ALA PRO ALA ALA PRO SER GLY GLY PRO ARG PRO ASP ASP ILE THR PHE ASP ALA ALA ASP ALA THR VAL ALA LEU ILE ALA LEU SER ALA LYS MET ARG ILE ASP GLN ILE GLU ALA LEU ASP SER ILE GLU SER ILE THR ASP GLY ALA SER SER ARG ARG ASN GLN LEU LEU
VAL ASP LEU GLY SER GLU LEU ASN LEU GLY ALA ILE ASP GLY ALA ALA GLU ALA ASP LEU GLY ALA ALA LEU LYS GLY GLN VAL THR LYS LEU ALA ARG THR TYR LYS PRO PHE GLY PRO VAL LEU SER ASP ALA ILE ASN ASP GLN LEU ARG THR VAL LEU GLY PRO SER GLY LYS ARG PRO
ALA TYR ILE THR GLU ARG VAL THR LYS THR TRP GLU LEU GLY PRO GLY TRP ALA LYS HIS VAL THR VAL GLU PHE ALA LEU GLY THR ARG GLU GLY SER SER VAL ARG GLY GLY ASP LEU GLY GLY LEU HIS ALA SER ALA LEU ALA SER ALA ALA ASP VAL ASP LYS VAL ILE ASP GLY
ALA VAL ALA ALA VAL ALA ARG ARG GLY ILE SER VAL SER LEU PRO SER ALA GLY GLY ALA SER GLY GLY VAL VAL ASP S1983 L2008 N2009 Q2010 L2011 G2012 L2013 S2014 D2015 V2016 V2017 T2018 T2019 P2020 E2021 A2022 A2023 T2024 D2025 A2026 E2027 A2045 P2046 D2049 A2050 R2051 V2055 F2056 D2057



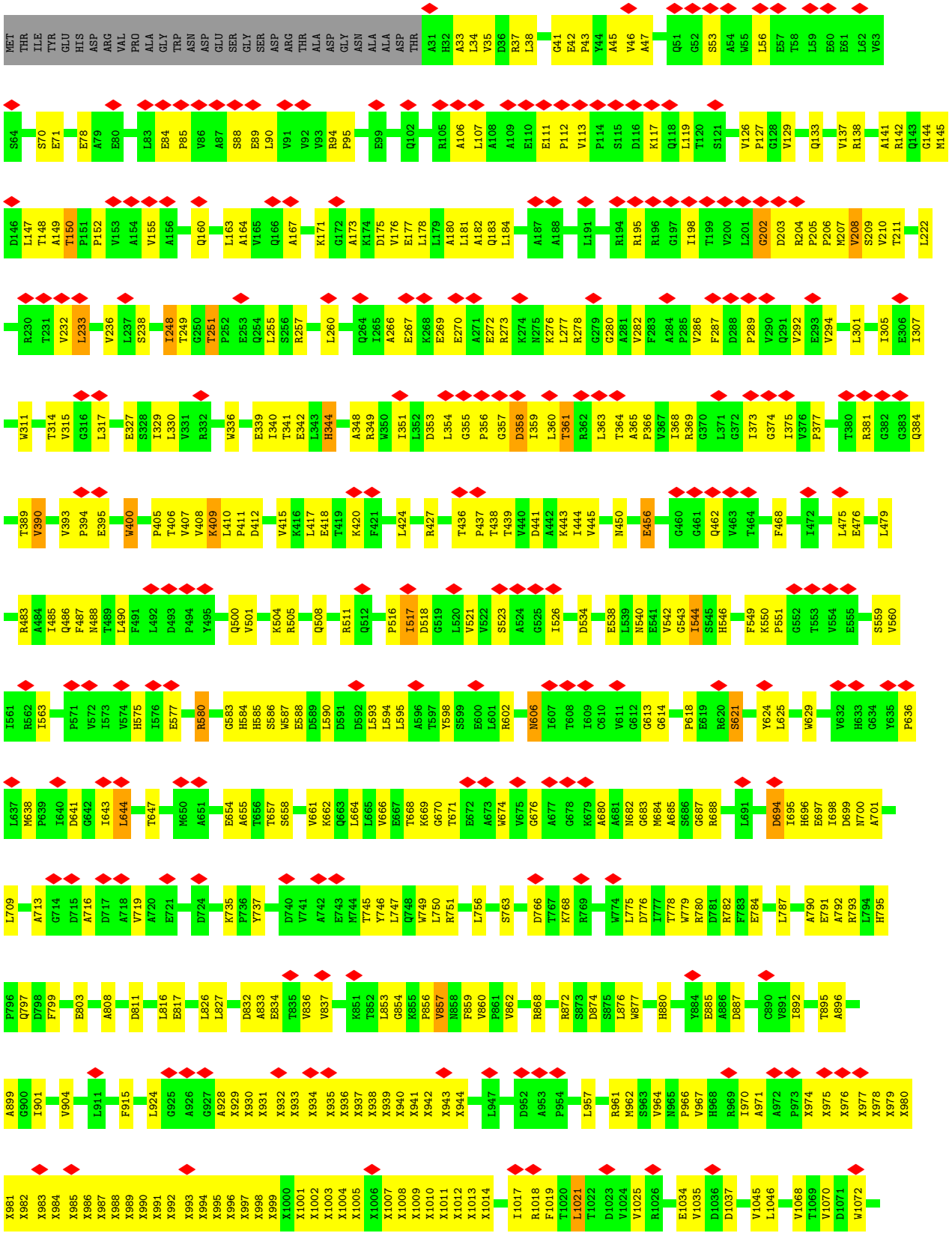
• Molecule 1: FATTY ACID SYNTHASE

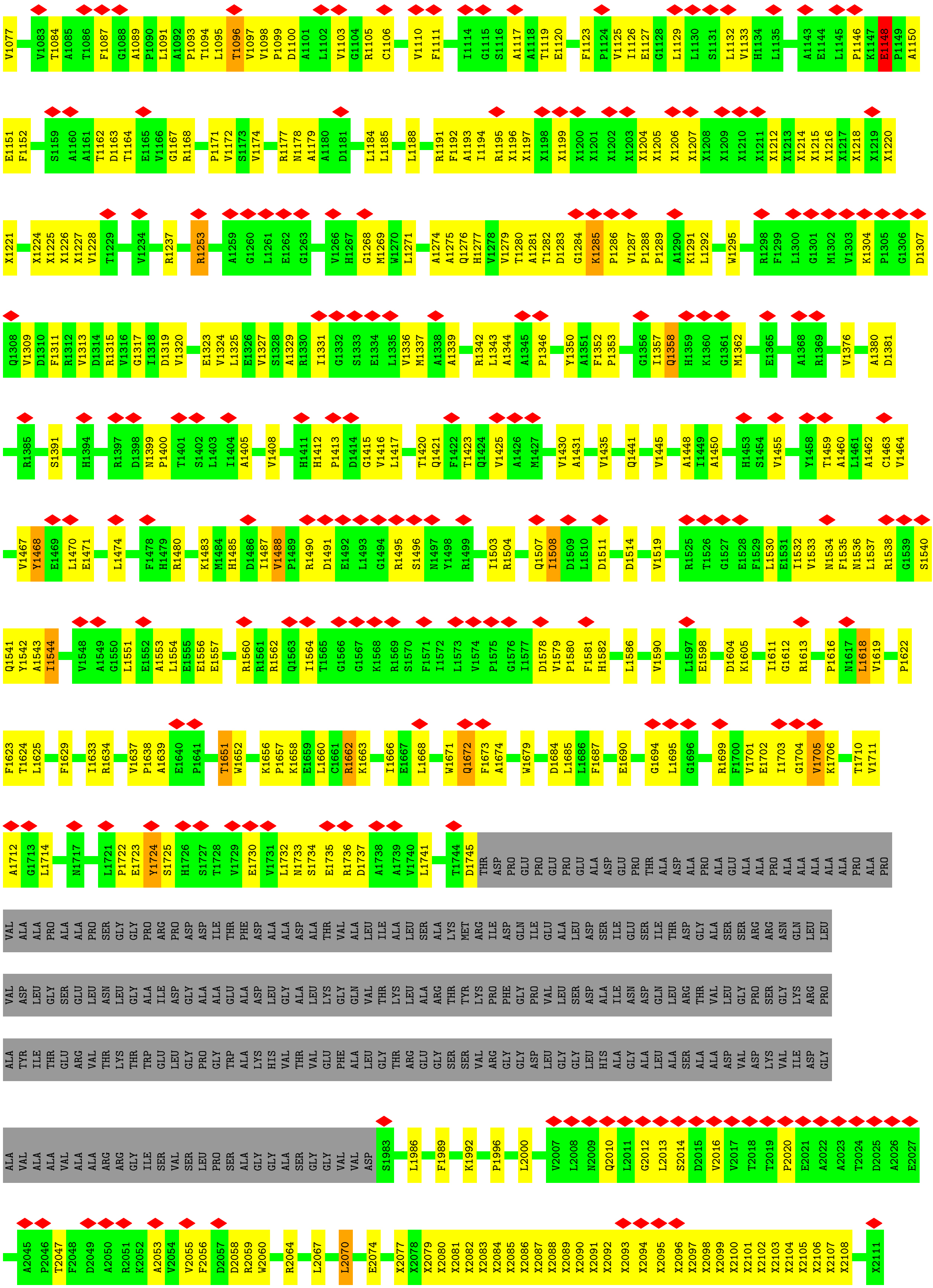
Chain F:

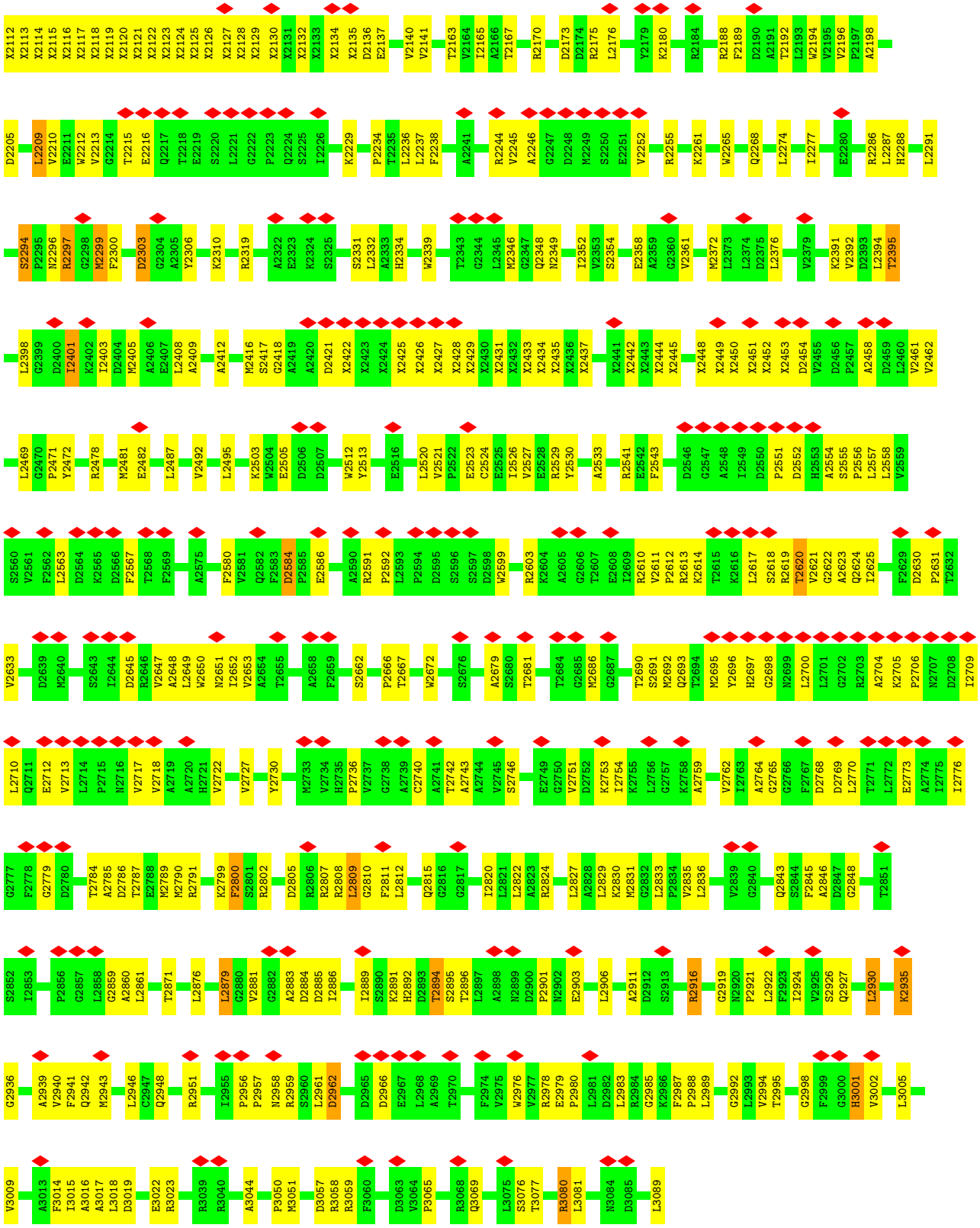




• Molecule 1: FATTY ACID SYNTHASE

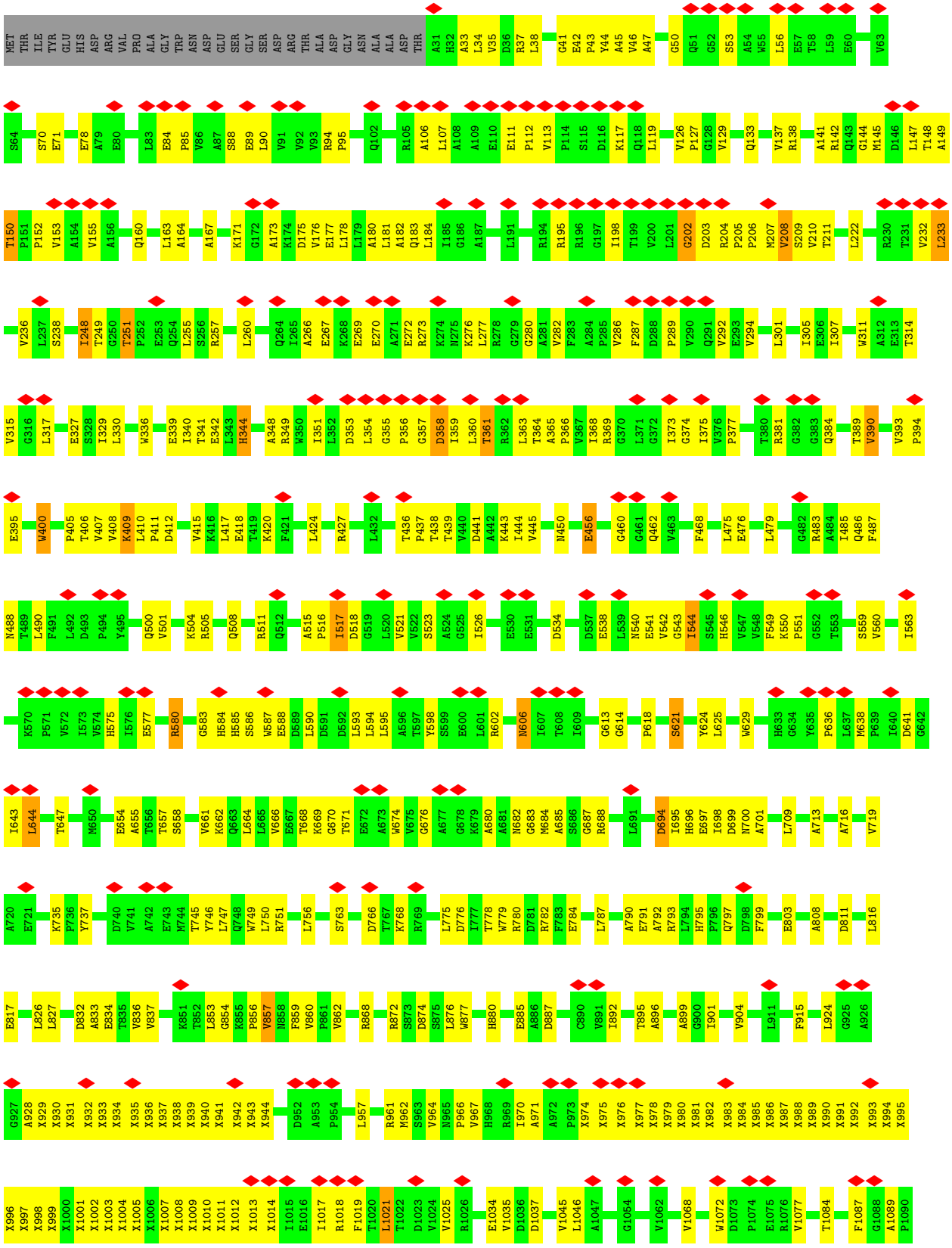


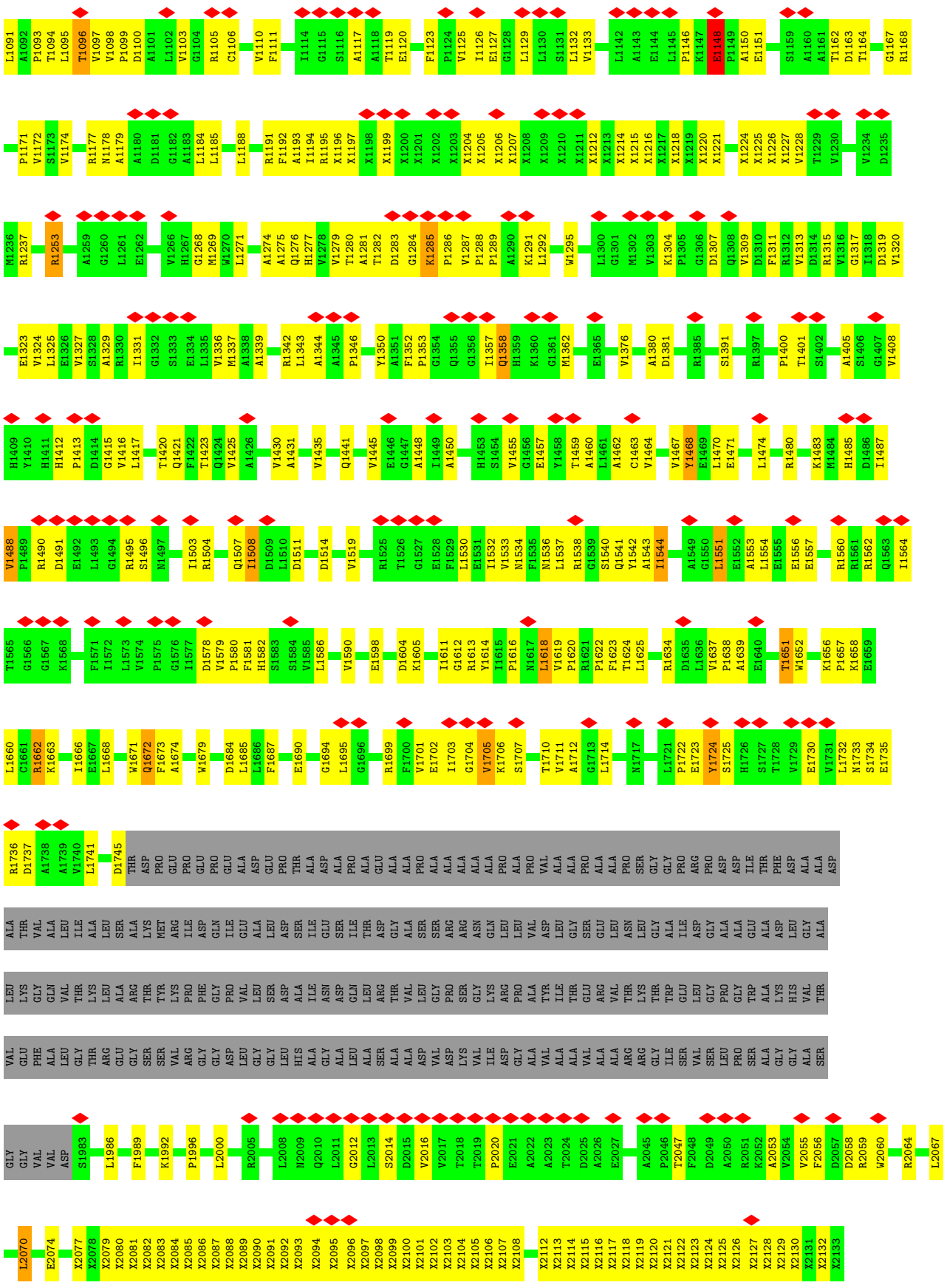

V1077 V1083 T1084 A1085 T1086 F1087 G1088 A1089 P1090 L1091 A1092 P1093 T1094 L1095 T1096 V1097 V1098 P1099 D1100 A1101 L1102 V1103 G1104 R1105 C1106 V1110 F1111 I1114 G1115 S1116 A1117 A1118 T1119 E1120 F1123 P1124 V1125 I1126 E1127 G1128 L1129 L1130 S1131 L1132 V1133 H1134 L1135 A1143 E1144 L1145 P1146 K1147 E1148 P1149 A1150
E1151 F1152 S1159 A1160 A1161 T1162 D1163 T1164 E1165 V1166 G1167 R1168 P1171 V1172 S1173 V1174 R1177 N1178 A1179 A1180 D1181 L1184 L1185 L1188 R1191 F1192 A1193 I1194 R1195 X1196 X1197 X1198 X1199 X1200 X1201 X1202 X1203 X1204 X1205 X1206 X1207 X1208 X1209 X1210 X1211 X1212 X1213 X1214 X1215 X1216 X1217 X1218 X1219 X1220
X1221 X1224 X1225 X1226 X1227 V1228 T1229 V1234 R1237 R1253 A1259 G1260 L1261 E1262 G1263 V1266 H1267 G1268 M1269 W1270 L1271 A1274 A1275 Q1276 H1277 V1278 V1279 T1280 A1281 T1282 D1283 G1284 K1285 P1286 V1287 P1288 P1289 A1290 K1291 L1292 W1295 R1298 F1299 L1300 G1301 M1302 V1303 K1304 P1305 G1306 D1307
Q1308 V1309 D1310 F1311 R1312 V1313 D1314 R1315 V1316 G1317 I1318 D1319 V1320 E1323 V1324 L1325 E1326 V1327 S1328 A1329 R1330 I1331 G1332 S1333 E1334 L1335 V1336 M1337 A1338 A1339 R1342 L1343 A1344 A1345 P1346 Y1350 A1351 F1352 P1353 G1356 I1357 Q1358 H1359 K1360 G1361 M1362 E1365 A1368 R1369 V1376 A1380 D1381
R1385 S1391 H1394 R1397 D1398 N1399 P1400 T1401 S1402 L1403 I1404 A1405 V1408 H1411 H1412 P1413 D1414 G1415 V1416 L1417 T1420 Q1421 F1422 T1423 Q1424 V1425 A1426 M1427 V1430 A1431 V1435 Q1441 V1445 A1448 I1449 A1450 H1453 S1454 V1455 Y1458 T1459 A1460 L1461 A1462 C1463 V1464
V1467 Y1468 E1469 L1470 E1471 L1474 F1478 H1479 R1480 K1483 M1484 H1485 D1486 I1487 V1488 P1489 R1490 D1491 E1492 L1493 G1494 R1495 S1496 N1497 Y1498 R1499 I1503 R1504 Q1507 I1508 D1509 L1510 D1511 D1514 V1519 R1525 T1526 G1527 E1528 F1529 L1530 E1531 I1532 V1533 N1534 F1535 N1536 L1537 R1538 G1539 S1540
Q1541 Y1542 A1543 I1544 V1548 A1549 G1550 L1551 E1552 A1553 L1554 E1555 E1556 E1557 R1560 R1561 R1562 Q1563 I1564 T1565 G1566 G1567 K1568 R1569 S1570 F1571 I1572 L1573 V1574 P1575 G1576 I1577 D1578 V1579 P1580 F1581 H1582 L1586 V1590 L1597 E1598 D1604 K1605 I1611 G1612 R1613 P1616 N1617 L1618 V1619 P1622
F1623 T1624 L1625 F1629 I1633 R1634 V1637 P1638 A1639 E1640 P1641 T1651 W1652 K1656 P1657 K1658 E1659 L1660 C1661 R1662 K1663 I1666 E1667 L1668 W1671 Q1672 F1673 A1674 W1679 D1684 L1685 L1686 F1687 E1690 G1694 L1695 G1696 R1699 F1700 V1701 E1702 I1703 G1704 V1705 K1706 T1710 V1711
A1712 G1713 L1714 N1717 L1721 P1722 E1723 Y1724 S1725 H1726 S1727 T1728 V1729 E1730 V1731 L1732 N1733 S1734 E1735 R1736 D1737 A1738 A1739 V1740 L1741 T1744 D1745 THR ASP PRO GLU PRO GLU PRO GLU ALA ASP GLU PRO THR ALA ASP ALA PRO ALA GLU ALA ALA PRO ALA ALA ALA ALA PRO ALA PRO
VAL ALA ALA PRO ALA ALA PRO SER GLY GLY PRO ARG PRO ASP ASP ILE THR PHE ASP ALA ALA ASP ALA THR VAL ALA LEU ILE ALA LEU SER ALA LYS MET ARG ILE ASP GLN ILE GLU ALA LEU ASP SER ILE GLU SER ILE THR ASP GLY ALA SER SER ARG ARG ASN GLN LEU LEU
VAL ASP LEU GLY SER GLU LEU ASN LEU GLY ALA ILE ASP GLY ALA ALA GLU ALA ASP LEU GLY ALA LEU LYS GLY GLN VAL THR LYS LEU ALA ARG THR TYR LYS PRO PHE GLY PRO VAL LEU SER ASP ALA ILE ASN ASP GLN LEU ARG THR VAL LEU GLY PRO SER GLY LYS ARG PRO
ALA TYR ILE THR GLU ARG VAL THR LYS THR TRP GLU LEU GLY PRO GLY TRP ALA LYS HIS VAL THR VAL GLU PHE ALA LEU GLY THR ARG GLU GLY SER SER VAL ARG GLY GLY ASP LEU GLY GLY LEU HIS ALA GLY ALA LEU ALA SER ALA ALA ASP VAL ASP LYS VAL ILE ASP GLY
ALA VAL ALA ALA VAL ALA ALA ARG ARG GLY ILE SER VAL SER LEU PRO SER ALA GLY GLY ALA SER GLY GLY VAL VAL ASP S1983 L1986 F1989 K1992 P1996 L2000 V2007 L2008 N2009 Q2010 L2011 G2012 L2013 S2014 D2015 V2016 V2017 T2018 T2019 P2020 E2021 A2022 A2023 T2024 D2025 A2026 E2027
A2045 P2046 T2047 F2048 D2049 A2050 R2051 K2052 A2053 V2054 V2055 F2056 D2057 D2058 R2059 W2060 R2064 L2067 L2070 E2074 X2077 X2078 X2079 X2080 X2081 X2082 X2083 X2084 X2085 X2086 X2087 X2088 X2089 X2090 X2091 X2092 X2093 X2094 X2095 X2096 X2097 X2098 X2099 X2100 X2101 X2102 X2103 X2104 X2105 X2106 X2107 X2108 X2111

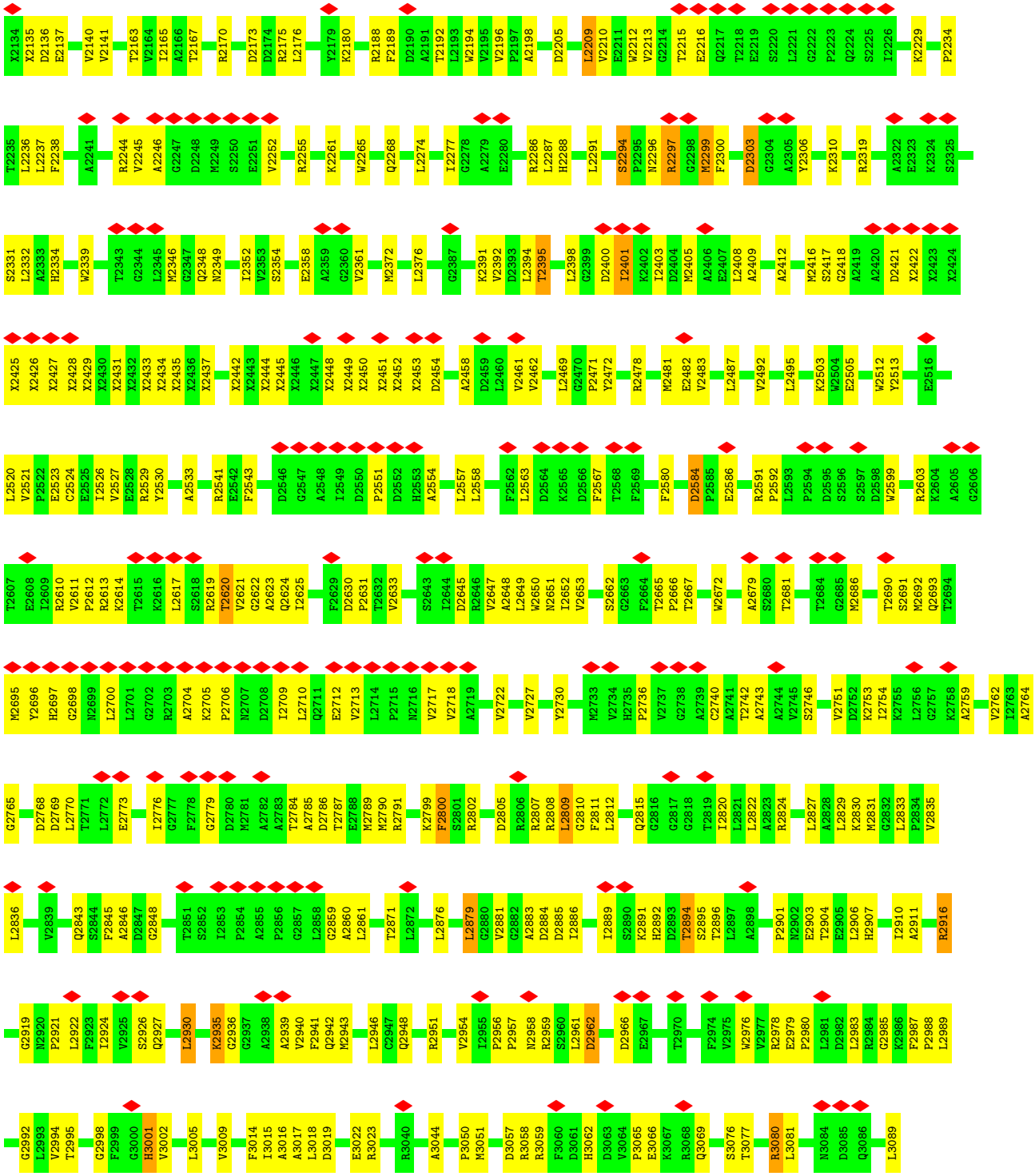


• Molecule 1: FATTY ACID SYNTHASE

Chain B: 17% 56% 33% • 9%

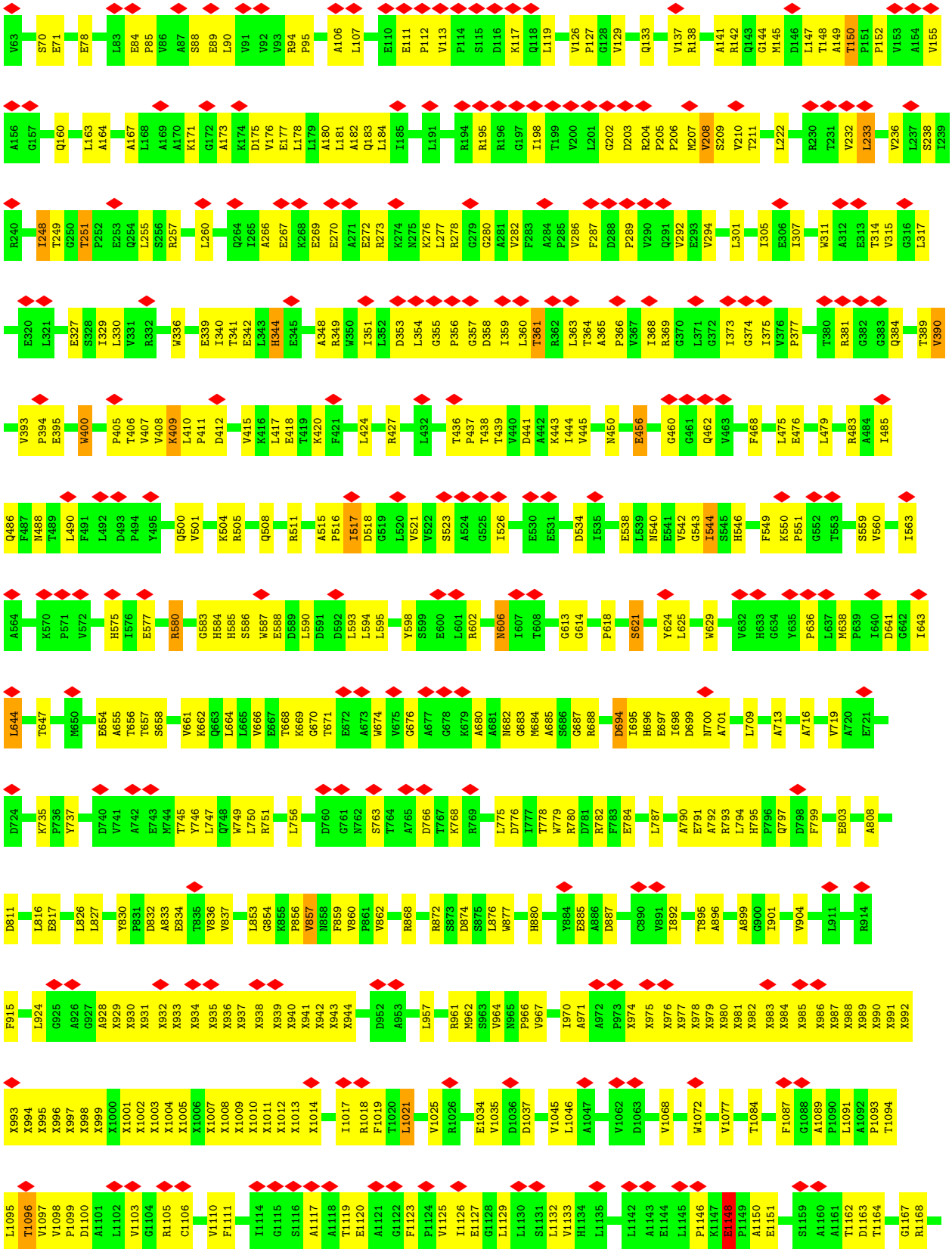

MET THR ILE TYR GLU HIS ASP ARG VAL PRO ALA GLY TRP ASN ASP GLU SER GLY SER ASP ARG THR ALA ASP GLY ASN ALA ALA ASP THR
A31 H32 A33 L34 V35 D36 R37 L38 G41 E42 P43 Y44 A45 V46 A47 G50 Q51 G52 S53 A54 W55 L56 E57 T58 L59 E60 V63
S64 S70 E71 E78 A79 E80 L83 E84 P85 V86 A87 S88 E89 L90 V91 V92 V93 R94 P95 Q102 R105 A106 L107 A108 A109 E110 E111 P112 V113 P114 S115 D116 K117 Q118 L119 V126 P127 G128 V129 Q133 V137 R138 A141 R142 Q143 G144 M145 D146 L147 T148 A149
T150 P151 P152 V153 A154 V155 A156 Q160 L163 A164 A167 K171 G172 A173 K174 D175 V176 E177 L178 L179 A180 L181 A182 Q183 L184 I185 G186 A187 L191 R194 R195 R196 G197 I198 T199 V200 L201 G202 D203 R204 P205 P206 M207 V208 S209 V210 T211 L222 R230 T231 V232 L233
V236 L237 S238 I248 T249 G250 T251 P252 E253 Q254 L255 S256 R257 L260 Q264 I265 A266 E267 K268 E269 E270 A271 E272 R273 K274 N275 K276 L277 R278 G279 G280 A281 V282 F283 A284 P285 V286 F287 D288 P289 V290 Q291 V292 E293 V294 L301 I305 E306 I307 W311 A312 E313 T314
V315 G316 L317 E327 S328 I329 L330 W336 E339 I340 T341 E342 L343 H344 A348 R349 W350 I351 L352 D353 L354 G355 P356 G357 D358 I359 L360 T361 R362 L363 T364 A365 P366 V367 I368 R369 G370 L371 G372 I373 G374 I375 V376 P377 T380 R381 G382 G383 Q384 T389 V390 V393 P394
E395 W400 P405 T406 V407 V408 K409 L410 P411 D412 V415 K416 L417 E418 T419 K420 F421 L424 R427 L432 T436 P437 T438 T439 Y440 D441 A442 K443 I444 V445 N450 E456 G460 G461 Q462 V463 F468 L475 E476 L479 G482 R483 A484 I485 Q486 F487
N488 T489 L490 F491 L492 D493 P494 Y495 Q500 V501 K504 R505 Q508 R511 Q512 A515 P516 I517 D518 G519 L520 V521 V522 S523 A524 G525 I526 E530 E531 D534 D537 E538 L539 N540 E541 V542 G543 T544 S545 H546 V547 V548 F549 K550 P551 G552 T553 S559 V560 I563
K570 P571 V572 I573 V574 H575 I576 E577 R580 G583 H584 H585 S586 W587 E588 D589 L590 D591 D592 L593 L594 L595 A596 T597 Y598 S599 E600 L601 R602 N606 I607 T608 I609 G613 G614 P618 S621 Y624 L625 W629 H633 G634 Y635 P636 L637 M638 P639 I640 D641 G642
I643 L644 T647 M650 E654 A655 T656 T657 S658 V661 K662 Q663 L664 L665 V666 E667 T668 K669 G670 T671 E672 A673 W674 V675 G676 A677 G678 K679 A680 A681 N682 G683 M684 A685 S686 G687 R688 L691 D694 I695 H696 E697 I698 D699 N700 A701 L709 A713 A716 V719
A720 E721 K735 P736 Y737 D740 V741 A742 E743 M744 T745 Y746 L747 Q748 W749 L750 R751 L756 S763 D766 T767 K768 R769 L775 D776 I777 T778 W779 R780 D781 R782 F783 E784 L787 A790 E791 A792 R793 L794 H795 P796 Q797 D798 F799 E803 A808 D811 L816
E817 L826 L827 D832 A833 E834 T835 V836 V837 K851 T852 L853 G854 K855 P856 V857 N858 F859 V860 P861 V862 R868 R872 S873 D874 S875 L876 W877 H880 E885 A886 D887 C890 V891 I892 T895 A896 A899 G900 I901 V904 L911 F915 L924 G925 A926
G927 A928 X929 X930 X931 X932 X933 X934 X935 X936 X937 X938 X939 X940 X941 X942 X943 X944 D952 A953 P954 L957 R961 M962 S963 V964 N965 P966 V967 H968 R969 I970 A971 A972 P973 X974 X975 X976 X977 X978 X979 X980 X981 X982 X983 X984 X985 X986 X987 X988 X989 X990 X991 X992 X993 X994 X995
X996 X997 X998 X999 X1000 X1001 X1002 X1003 X1004 X1005 X1006 X1007 X1008 X1009 X1010 X1011 X1012 X1013 X1014 I1015 E1016 I1017 R1018 F1019 T1020 L1021 T1022 D1023 V1024 V1025 R1026 E1034 V1035 D1036 D1037 V1045 L1046 A1047 G1054 V1062 V1068 W1072 D1073 P1074 E1075 R1076 V1077 T1084 F1087 G1088 A1089 P1090

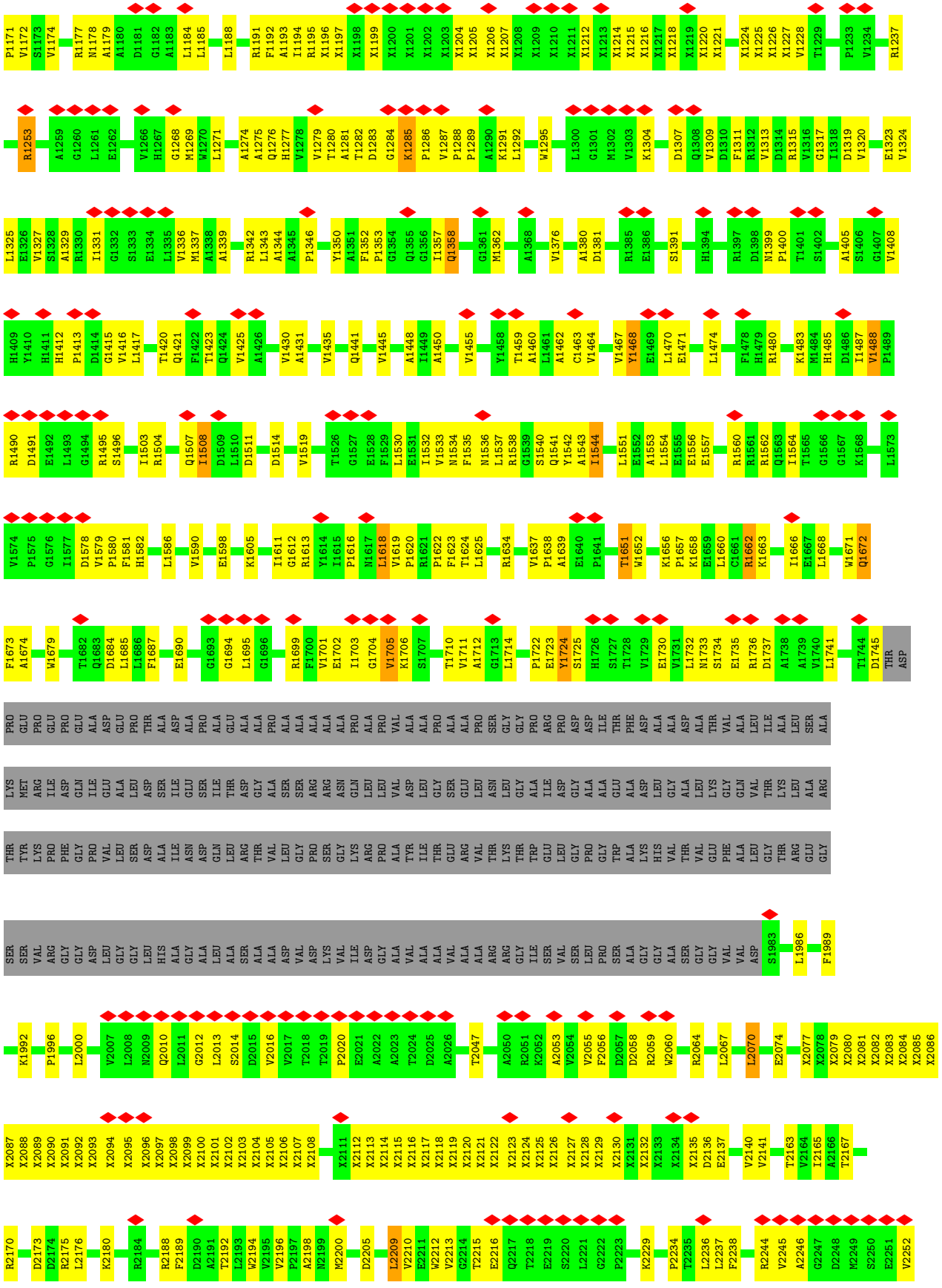

L1091 A1092 P1093 T1094 L1095 T1096 V1097 V1098 P1099 D1100 A1101 L1102 V1103 G1104 R1105 C1106 V1110 F1111 I1114 G1115 S1116 A1117 A1118 T1119 E1120 F1123 P1124 V1125 I1126 E1127 G1128 L1129 L1130 S1131 L1132 V1133 L1142 A1143 E1144 L1145 P1146 K1147 E1148 P1149 A1150 E1151 S1159 A1160 A1161 T1162 D1163 T1164 G1167 R1168
P1171 V1172 S1173 V1174 R1177 N1178 A1179 A1180 D1181 G1182 A1183 L1184 L1185 L1188 R1191 F1192 A1193 I1194 R1195 X1196 X1197 X1198 X1199 X1200 X1201 X1202 X1203 X1204 X1205 X1206 X1207 X1208 X1209 X1210 X1211 X1212 X1213 X1214 X1215 X1216 X1217 X1218 X1219 X1220 X1221 X1224 X1225 X1226 X1227 V1228 T1229 V1230 V1234 D1235
M1236 R1237 R1253 A1259 G1260 L1261 E1262 V1266 H1267 G1268 M1269 W1270 L1271 A1274 A1275 Q1276 H1277 V1278 V1279 T1280 A1281 T1282 D1283 G1284 K1285 P1286 V1287 P1288 P1289 A1290 K1291 L1292 W1295 L1300 G1301 M1302 V1303 K1304 P1305 G1306 D1307 Q1308 V1309 D1310 F1311 R1312 V1313 D1314 R1315 V1316 G1317 I1318 D1319 V1320
E1323 V1324 L1325 E1326 V1327 S1328 A1329 R1330 I1331 G1332 S1333 E1334 L1335 V1336 M1337 A1338 A1339 R1342 L1343 A1344 A1345 P1346 Y1350 A1351 F1352 P1353 G1354 Q1355 G1356 I1357 Q1358 H1359 K1360 G1361 M1362 E1365 V1376 A1380 D1381 R1385 S1391 R1397 P1400 T1401 S1402 A1405 S1406 G1407 V1408
H1409 Y1410 H1411 H1412 P1413 D1414 G1415 V1416 L1417 T1420 Q1421 F1422 T1423 Q1424 V1425 A1426 V1430 A1431 V1435 Q1441 V1445 E1446 G1447 A1448 I1449 A1450 H1453 S1454 V1455 G1456 E1457 Y1458 T1459 A1460 L1461 A1462 C1463 V1464 V1467 Y1468 E1469 L1470 E1471 L1474 R1480 K1483 M1484 H1485 D1486 I1487
V1488 P1489 R1490 D1491 E1492 L1493 G1494 R1495 S1496 N1497 I1503 R1504 Q1507 I1508 D1509 L1510 D1511 D1514 V1519 R1525 T1526 G1527 E1528 F1529 L1530 E1531 I1532 V1533 N1534 F1535 N1536 L1537 R1538 G1539 S1540 Q1541 Y1542 A1543 I1544 A1549 G1550 L1551 E1552 A1553 L1554 E1555 E1556 E1557 R1560 R1561 R1562 Q1563 I1564
T1565 G1566 G1567 K1568 F1571 I1572 L1573 V1574 P1575 G1576 I1577 D1578 V1579 P1580 F1581 H1582 S1583 S1584 V1585 L1586 V1590 E1598 D1604 K1605 I1611 G1612 R1613 Y1614 I1615 P1616 N1617 L1618 V1619 P1620 R1621 P1622 F1623 T1624 L1625 R1634 D1635 L1636 V1637 P1638 A1639 E1640 T1651 W1652 K1656 P1657 K1658 E1659
L1660 C1661 R1662 K1663 I1666 E1667 L1668 W1671 Q1672 F1673 A1674 W1679 D1684 L1685 L1686 F1687 E1690 G1694 L1695 G1696 R1699 F1700 V1701 E1702 I1703 G1704 V1705 K1706 S1707 T1710 V1711 A1712 G1713 L1714 N1717 L1721 P1722 E1723 Y1724 S1725 H1726 S1727 T1728 V1729 E1730 V1731 L1732 N1733 S1734 E1735
R1736 D1737 A1738 A1739 V1740 L1741 D1745 THR ASP PRO GLU PRO GLU PRO GLU ALA ASP GLU PRO THR ALA ASP ALA PRO ALA GLU ALA ALA PRO ALA ALA ALA ALA ALA PRO ALA PRO VAL ALA ALA PRO ALA ALA PRO SER GLY GLY PRO ARG PRO ASP ASP ILE THR PHE ASP ALA ALA ASP
ALA THR VAL ALA LEU ILE ALA LEU SER ALA LYS MET ARG ILE ASP GLN ILE GLU ALA LEU ASP SER ILE GLU SER ILE THR ASP GLY ALA SER SER ARG ARG ASN GLN LEU LEU LEU VAL ASP LEU GLY SER GLU LEU ASN LEU GLY ALA ILE ASP GLY ALA ALA GLU LEU THR ILE LEU GLY PRO
LEU LYS GLY GLN VAL THR LYS LEU ALA ARG THR TYR LYS PRO PHE GLY PRO VAL LEU SER ASP ALA ILE ASN ASP GLN LEU ARG THR VAL LEU GLY PRO SER GLY LYS ARG PRO ALA TYR ILE THR GLU ARG VAL THR LYS THR TRP GLU LEU GLY PRO PRO GLY TRP ALA LYS HIS VAL THR
VAL GLU PHE ALA LEU GLY THR ARG GLU GLY SER SER VAL ARG GLY GLY ASP LEU GLY GLY LEU HIS ALA GLY LEU ALA SER ALA ILE ALA GLY LEU ALA ASP VAL ASP LYS VAL ILE ASP GLY PRO ALA VAL ALA ILE THR ALA VAL ALA ALA ARG ARG GLY ILE SER VAL SER LEU PRO SER ALA GLY GLY ALA SER
GLY GLY VAL VAL ASP S1983 L1986 F1989 K1992 P1996 L2000 R2005 L2008 N2009 Q2010 L2011 G2012 L2013 S2014 D2015 V2016 V2017 T2018 T2019 P2020 E2021 A2022 A2023 T2024 D2025 A2026 E2027 A2045 P2046 T2047 F2048 D2049 A2050 R2051 K2052 A2053 V2054 V2055 F2056 D2057 D2058 R2059 W2060 R2064 L2067
L2070 E2074 X2077 X2078 X2079 X2080 X2081 X2082 X2083 X2084 X2085 X2086 X2087 X2088 X2089 X2090 X2091 X2092 X2093 X2094 X2095 X2096 X2097 X2098 X2099 X2100 X2101 X2102 X2103 X2104 X2105 X2106 X2107 X2108 X2112 X2113 X2114 X2115 X2116 X2117 X2118 X2119 X2120 X2121 X2122 X2123 X2124 X2125 X2126 X2127 X2128 X2129 X2130 X2131 X2132 X2133

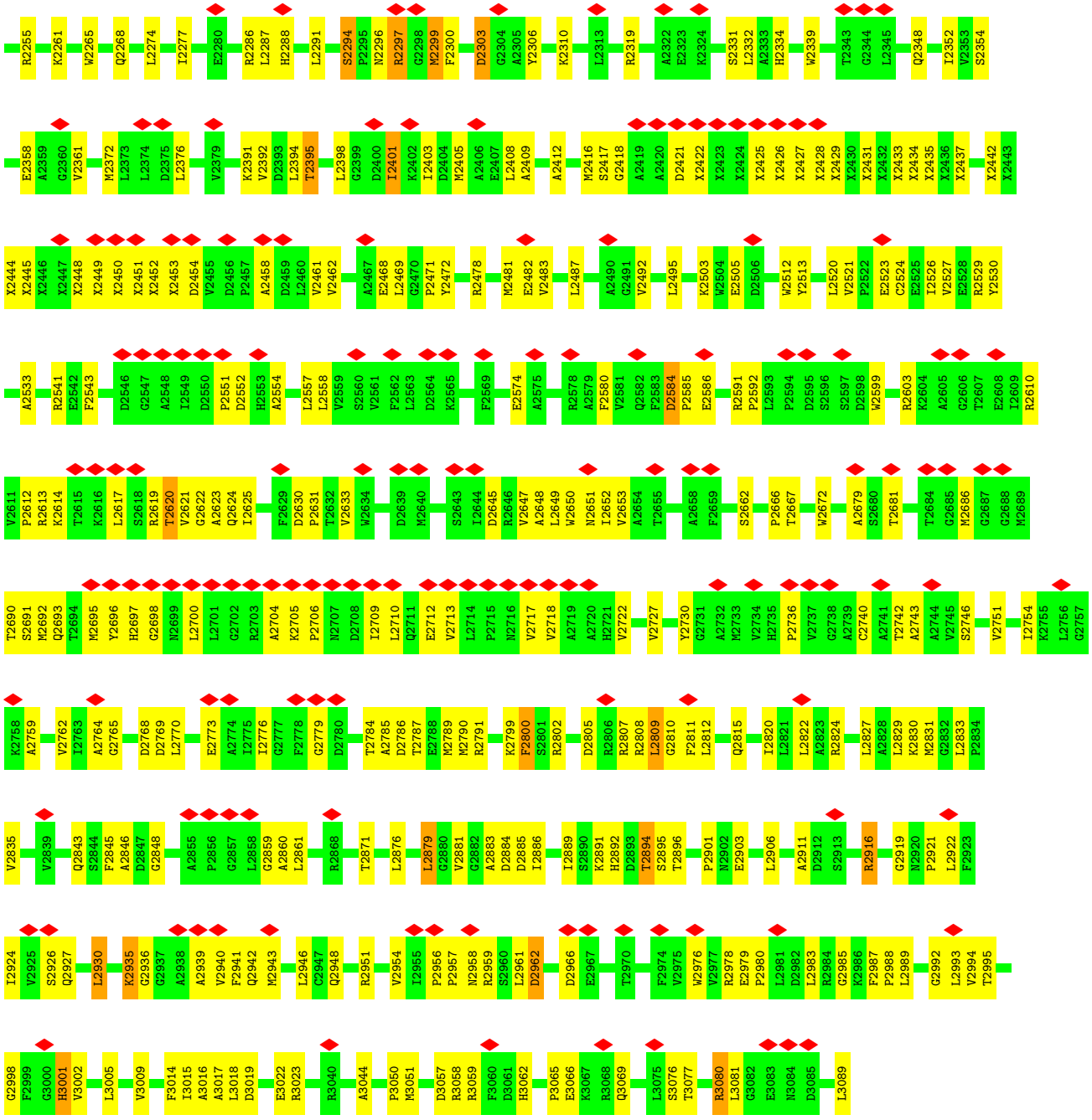


• Molecule 1: FATTY ACID SYNTHASE

Chain C:






R2255 K2261 W2265 Q2268 L2274 I2277 E2280 R2286 L2287 H2288 L2291 S2294 P2295 N2296 R2297 G2298 M2299 F2300 D2303 G2304 A2305 Y2306 K2310 L2313 R2319 A2322 E2323 K2324 S2331 L2332 A2333 H2334 W2339 T2343 G2344 L2345 Q2348 I2352 V2353 S2354
E2358 A2359 G2360 V2361 M2372 L2373 L2374 D2375 L2376 V2379 K2391 V2392 D2393 L2394 T2395 L2398 G2399 D2400 I2401 K2402 I2403 D2404 M2405 A2406 E2407 L2408 A2409 A2412 M2416 S2417 G2418 A2419 A2420 D2421 X2422 X2423 X2424 X2425 X2426 X2427 X2428 X2429 X2430 X2431 X2432 X2433 X2434 X2435 X2436 X2437 X2442 X2443
X2444 X2445 X2446 X2447 X2448 X2449 X2450 X2451 X2452 X2453 D2454 D2455 D2456 P2457 A2458 D2459 L2460 V2461 V2462 A2467 E2468 L2469 G2470 P2471 Y2472 R2478 M2481 E2482 V2483 L2487 A2490 G2491 V2492 L2495 K2503 W2504 E2505 D2506 W2512 Y2513 L2520 V2521 P2522 E2523 C2524 E2525 I2526 V2527 E2528 R2529 Y2530
A2533 R2541 E2542 F2543 D2546 G2547 A2548 I2549 D2550 P2551 D2552 H2553 A2554 L2557 L2558 V2559 S2560 V2561 F2562 L2563 D2564 K2565 F2569 E2574 A2575 R2578 A2579 F2580 V2581 Q2582 F2583 D2584 P2585 E2586 R2591 P2592 L2593 P2594 D2595 S2596 S2597 D2598 W2599 R2603 K2604 A2605 G2606 T2607 E2608 I2609 R2610
V2611 P2612 R2613 K2614 T2615 K2616 L2617 S2618 R2619 T2620 V2621 G2622 A2623 Q2624 I2625 F2629 D2630 P2631 T2632 V2633 W2634 D2639 M2640 S2643 I2644 D2645 R2646 V2647 A2648 L2649 W2650 N2651 I2652 V2653 A2654 T2655 A2658 F2659 S2662 P2666 T2667 W2672 A2679 S2680 T2681 T2684 G2685 M2686 G2687 G2688 M2689
T2690 S2691 M2692 Q2693 T2694 M2695 Y2696 H2697 G2698 N2699 L2700 L2701 G2702 R2703 A2704 K2705 P2706 N2707 D2708 I2709 L2710 Q2711 E2712 V2713 L2714 P2715 N2716 V2717 V2718 A2719 A2720 H2721 V2722 V2727 Y2730 G2731 A2732 M2733 V2734 H2735 P2736 V2737 G2738 A2739 C2740 A2741 T2742 A2743 A2744 V2745 S2746 V2751 I2754 K2755 L2756 G2757
K2758 A2759 V2762 I2763 A2764 G2765 D2768 D2769 L2770 E2773 A2774 I2775 I2776 G2777 F2778 G2779 D2780 T2784 A2785 D2786 T2787 E2788 M2789 M2790 R2791 K2799 P2800 S2801 R2802 D2805 R2806 R2807 R2808 L2809 G2810 P2811 L2812 Q2815 I2820 L2821 L2822 A2823 R2824 L2827 A2828 L2829 K2830 M2831 G2832 L2833 P2834
V2835 V2839 Q2843 S2844 F2845 A2846 D2847 G2848 A2855 P2856 G2857 L2858 G2859 A2860 L2861 R2868 T2871 L2876 L2879 G2880 V2881 G2882 A2883 D2884 D2885 I2886 I2889 S2890 K2891 H2892 D2893 T2894 S2895 T2896 P2901 N2902 E2903 L2906 A2911 D2912 S2913 R2916 G2919 N2920 P2921 L2922 F2923
I2924 V2925 S2926 Q2927 L2930 K2935 G2936 G2937 A2938 A2939 V2940 F2941 Q2942 M2943 L2946 C2947 Q2948 R2951 V2954 I2955 P2956 P2957 N2958 R2959 S2960 L2961 D2962 D2966 E2967 T2970 F2974 V2975 W2976 V2977 R2978 E2979 P2980 L2981 D2982 L2983 R2984 G2985 K2986 F2987 P2988 L2989 G2992 L2993 V2994 T2995
G2998 F2999 G3000 H3001 V3002 L3005 V3009 F3014 I3015 A3016 A3017 L3018 D3019 E3022 R3023 R3040 A3044 P3050 M3051 D3057 R3058 R3059 F3060 D3061 H3062 P3065 E3066 K3067 R3068 Q3069 L3075 S3076 T3077 R3080 L3081 G3082 E3083 N3084 D3085 L3089

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	106884	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH IMAGE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	100000	Depositor
Image detector	FEI FALCON I (4k x 4k)	Depositor
Maximum map value	14.936	Depositor
Minimum map value	-7.793	Depositor
Average map value	-0.133	Depositor
Map value standard deviation	1.076	Depositor
Recommended contour level	2.7	Depositor
Map size (Å)	392.0, 392.0, 392.0	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.45, 2.45, 2.45	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.24	0/20319	0.48	0/27667
1	B	0.24	0/20319	0.48	0/27667
1	C	0.24	0/20319	0.48	0/27667
1	D	0.24	0/20319	0.48	0/27667
1	E	0.24	0/20319	0.48	0/27667
1	F	0.24	0/20319	0.48	0/27667
All	All	0.24	0/121914	0.48	0/166002

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	5
1	C	0	5
1	D	0	5
1	E	0	5
1	F	0	5
All	All	0	30

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1148	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	150	THR	Peptide
1	A	202	GLY	Peptide
1	A	2584	ASP	Peptide
1	A	357	GLY	Peptide
1	B	1148	GLU	Peptide
1	B	150	THR	Peptide
1	B	202	GLY	Peptide
1	B	2584	ASP	Peptide
1	B	357	GLY	Peptide
1	C	1148	GLU	Peptide
1	C	150	THR	Peptide
1	C	202	GLY	Peptide
1	C	2584	ASP	Peptide
1	C	357	GLY	Peptide
1	D	1148	GLU	Peptide
1	D	150	THR	Peptide
1	D	202	GLY	Peptide
1	D	2584	ASP	Peptide
1	D	357	GLY	Peptide
1	E	1148	GLU	Peptide
1	E	150	THR	Peptide
1	E	202	GLY	Peptide
1	E	2584	ASP	Peptide
1	E	357	GLY	Peptide
1	F	1148	GLU	Peptide
1	F	150	THR	Peptide
1	F	202	GLY	Peptide
1	F	2584	ASP	Peptide
1	F	357	GLY	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	21020	0	20990	1056	0
1	B	21020	0	20990	1067	0
1	C	21020	0	20990	1051	0
1	D	21020	0	20990	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	21020	0	20990	0	0
1	F	21020	0	20990	0	0
2	A	31	0	19	5	0
2	B	31	0	19	5	0
2	C	31	0	19	4	0
2	D	31	0	19	0	0
2	E	31	0	19	0	0
2	F	31	0	19	0	0
All	All	126306	0	126054	3117	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (3117) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:ARG:O	1:A:2435:UNK:HG2	1.31	1.30
1:B:793:ARG:O	1:B:2435:UNK:HG2	1.31	1.28
1:B:2100:UNK:O	1:B:2103:UNK:HG3	1.36	1.26
1:A:2105:UNK:O	1:A:2108:UNK:HG3	1.34	1.25
1:B:2105:UNK:O	1:B:2108:UNK:HG3	1.34	1.25
1:C:2100:UNK:O	1:C:2103:UNK:HG3	1.36	1.23
1:C:793:ARG:O	1:C:2435:UNK:HG2	1.31	1.23
1:A:2093:UNK:HG1	1:A:2129:UNK:O	1.40	1.22
1:A:2100:UNK:O	1:A:2103:UNK:HG3	1.36	1.21
1:C:2093:UNK:HG1	1:C:2129:UNK:O	1.39	1.21
1:C:2105:UNK:O	1:C:2108:UNK:HG3	1.34	1.21
1:B:992:UNK:CG	1:B:996:UNK:HG3	1.72	1.20
1:C:992:UNK:CG	1:C:996:UNK:HG3	1.72	1.18
1:B:2093:UNK:HG1	1:B:2129:UNK:O	1.39	1.18
1:A:992:UNK:CG	1:A:996:UNK:HG3	1.72	1.18
1:B:2451:UNK:HG1	1:B:2454:ASP:OD2	1.44	1.17
1:C:2451:UNK:HG1	1:C:2454:ASP:OD2	1.44	1.16
1:A:2451:UNK:HG1	1:A:2454:ASP:OD2	1.44	1.15
1:C:2094:UNK:HG2	1:C:2096:UNK:HG3	1.32	1.12
1:C:2450:UNK:HG1	1:C:3016:ALA:HB1	1.23	1.11
1:A:2450:UNK:HG1	1:A:3016:ALA:HB1	1.23	1.11
1:B:2097:UNK:O	1:B:2100:UNK:HG3	1.51	1.10
1:B:2450:UNK:HG1	1:B:3016:ALA:HB1	1.23	1.09
1:A:2097:UNK:O	1:A:2100:UNK:HG3	1.51	1.09
1:B:975:UNK:HG3	1:B:993:UNK:CG	1.83	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2097:UNK:O	1:C:2100:UNK:HG3	1.51	1.09
1:A:975:UNK:HG3	1:A:993:UNK:CG	1.82	1.08
1:A:2094:UNK:HG2	1:A:2096:UNK:HG3	1.32	1.08
1:C:975:UNK:HG3	1:C:993:UNK:CG	1.83	1.07
1:B:2094:UNK:HG2	1:B:2096:UNK:HG3	1.32	1.07
1:A:981:UNK:HG1	1:A:987:UNK:HG2	1.37	1.06
1:C:934:UNK:O	1:C:937:UNK:HG3	1.57	1.04
1:C:981:UNK:HG1	1:C:987:UNK:HG2	1.37	1.04
1:A:934:UNK:O	1:A:937:UNK:HG3	1.58	1.03
1:B:934:UNK:O	1:B:937:UNK:HG3	1.57	1.02
1:B:981:UNK:HG1	1:B:987:UNK:HG2	1.37	1.02
1:B:2094:UNK:CG	1:B:2096:UNK:HG3	1.90	1.02
1:C:975:UNK:CG	1:C:993:UNK:HG1	1.90	1.01
1:C:992:UNK:CG	1:C:996:UNK:CG	2.39	1.01
1:B:975:UNK:CG	1:B:993:UNK:HG1	1.90	1.01
1:A:975:UNK:CG	1:A:993:UNK:HG1	1.89	1.01
1:C:2094:UNK:CG	1:C:2096:UNK:HG3	1.90	1.01
1:A:2094:UNK:CG	1:A:2096:UNK:HG3	1.90	1.00
1:C:932:UNK:O	1:C:936:UNK:HG2	1.61	1.00
1:B:2088:UNK:O	1:B:2091:UNK:HG3	1.61	1.00
1:A:992:UNK:CG	1:A:996:UNK:CG	2.39	1.00
1:A:2113:UNK:O	1:A:2116:UNK:HG3	1.62	1.00
1:C:2113:UNK:O	1:C:2116:UNK:HG3	1.62	1.00
1:B:992:UNK:CG	1:B:996:UNK:CG	2.39	0.99
1:B:1220:UNK:HG3	1:B:1221:UNK:N	1.78	0.99
1:B:2433:UNK:HA	1:B:2524:CYS:HB3	1.44	0.99
1:A:2088:UNK:O	1:A:2091:UNK:HG3	1.61	0.99
1:B:976:UNK:HG3	1:B:993:UNK:HB1	1.43	0.99
1:B:932:UNK:O	1:B:936:UNK:HG2	1.61	0.99
1:C:2088:UNK:O	1:C:2091:UNK:HG3	1.61	0.99
1:A:992:UNK:HG1	1:A:996:UNK:HG3	1.41	0.98
1:B:792:ALA:O	1:B:2433:UNK:CG	2.12	0.98
1:A:932:UNK:O	1:A:936:UNK:HG2	1.61	0.98
1:A:792:ALA:O	1:A:2433:UNK:CG	2.12	0.98
1:B:2113:UNK:O	1:B:2116:UNK:HG3	1.62	0.98
1:C:1220:UNK:HG3	1:C:1221:UNK:N	1.78	0.98
1:C:792:ALA:O	1:C:2433:UNK:CG	2.12	0.98
1:C:992:UNK:HG1	1:C:996:UNK:HG3	1.41	0.98
1:A:976:UNK:HG3	1:A:993:UNK:HB1	1.43	0.98
1:B:992:UNK:HG1	1:B:996:UNK:HG3	1.41	0.97
1:C:975:UNK:HG3	1:C:993:UNK:HG1	0.99	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2096:UNK:O	1:B:2099:UNK:HG3	1.65	0.97
1:A:2433:UNK:HA	1:A:2524:CYS:HB3	1.44	0.97
1:C:1003:UNK:HG2	1:C:1004:UNK:N	1.78	0.97
1:B:975:UNK:HG3	1:B:993:UNK:HG1	0.99	0.97
1:C:407:VAL:HB	1:C:933:UNK:HG1	1.47	0.96
1:A:3080:ARG:HH11	1:A:3080:ARG:HG3	1.29	0.96
1:B:1003:UNK:HG2	1:B:1004:UNK:N	1.78	0.96
1:C:2096:UNK:O	1:C:2099:UNK:HG3	1.65	0.96
1:C:2433:UNK:HA	1:C:2524:CYS:HB3	1.44	0.96
1:A:2096:UNK:O	1:A:2099:UNK:HG3	1.65	0.96
1:B:407:VAL:HB	1:B:933:UNK:HG1	1.47	0.96
1:C:3080:ARG:HH11	1:C:3080:ARG:HG3	1.29	0.96
1:A:407:VAL:HB	1:A:933:UNK:HG1	1.47	0.96
1:A:1220:UNK:HG3	1:A:1221:UNK:N	1.78	0.95
1:A:793:ARG:HD3	1:A:2435:UNK:HG1	1.48	0.95
1:C:976:UNK:HG3	1:C:993:UNK:HB1	1.43	0.95
1:A:975:UNK:HG3	1:A:993:UNK:HG1	0.99	0.95
1:B:3080:ARG:HH11	1:B:3080:ARG:HG3	1.29	0.95
1:A:792:ALA:O	1:A:2433:UNK:HG1	1.67	0.94
1:C:792:ALA:O	1:C:2433:UNK:HG1	1.67	0.94
1:A:1003:UNK:HG2	1:A:1004:UNK:N	1.79	0.94
1:B:792:ALA:O	1:B:2433:UNK:HG1	1.67	0.94
1:B:793:ARG:HD3	1:B:2435:UNK:HG1	1.48	0.94
1:B:992:UNK:HG1	1:B:996:UNK:CG	1.97	0.93
1:C:793:ARG:HD3	1:C:2435:UNK:HG1	1.48	0.93
1:A:793:ARG:O	1:A:2435:UNK:CG	2.16	0.93
1:C:793:ARG:O	1:C:2435:UNK:CG	2.17	0.93
1:A:992:UNK:HG1	1:A:996:UNK:CG	1.97	0.93
1:B:793:ARG:O	1:B:2435:UNK:CG	2.17	0.93
1:C:1212:UNK:HG2	1:C:1342:ARG:HH21	1.32	0.93
1:A:929:UNK:O	1:A:930:UNK:HG3	1.69	0.93
1:A:2127:UNK:O	1:A:2130:UNK:HG3	1.69	0.93
1:B:2127:UNK:O	1:B:2130:UNK:HG3	1.70	0.92
1:B:929:UNK:O	1:B:930:UNK:HG3	1.69	0.92
1:B:1225:UNK:HG1	1:B:1283:ASP:OD1	1.70	0.92
1:C:992:UNK:HG1	1:C:996:UNK:CG	1.97	0.92
1:C:1225:UNK:HG1	1:C:1283:ASP:OD1	1.70	0.92
1:A:1013:UNK:HG2	1:A:1014:UNK:N	1.84	0.91
1:A:939:UNK:O	1:A:940:UNK:HG3	1.70	0.91
1:C:939:UNK:O	1:C:940:UNK:HG3	1.70	0.91
1:C:1012:UNK:O	1:C:1013:UNK:HG3	1.69	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1212:UNK:HG2	1:A:1342:ARG:HH21	1.32	0.91
1:B:1212:UNK:HG2	1:B:1342:ARG:HH21	1.32	0.91
1:A:1225:UNK:HG1	1:A:1283:ASP:OD1	1.70	0.91
1:C:2127:UNK:O	1:C:2130:UNK:HG3	1.69	0.91
1:B:1012:UNK:O	1:B:1013:UNK:HG3	1.69	0.91
1:A:2112:UNK:O	1:A:2115:UNK:HG3	1.70	0.91
1:B:2112:UNK:O	1:B:2115:UNK:HG3	1.70	0.91
1:A:943:UNK:O	1:A:944:UNK:HG3	1.71	0.91
1:C:929:UNK:O	1:C:930:UNK:HG3	1.69	0.91
1:C:943:UNK:O	1:C:944:UNK:HG3	1.71	0.90
1:C:1013:UNK:HG2	1:C:1014:UNK:N	1.84	0.90
1:C:2112:UNK:O	1:C:2115:UNK:HG3	1.70	0.90
1:A:1012:UNK:O	1:A:1013:UNK:HG3	1.69	0.90
1:B:939:UNK:O	1:B:940:UNK:HG3	1.70	0.90
1:B:943:UNK:O	1:B:944:UNK:HG3	1.71	0.90
1:B:1013:UNK:HG2	1:B:1014:UNK:N	1.84	0.90
1:C:2093:UNK:HA	1:C:2097:UNK:HG1	1.52	0.90
1:C:981:UNK:CG	1:C:987:UNK:HG2	2.02	0.89
1:B:2093:UNK:HA	1:B:2097:UNK:HG1	1.52	0.89
1:A:2093:UNK:HA	1:A:2097:UNK:HG1	1.52	0.89
1:A:981:UNK:CG	1:A:987:UNK:HG2	2.02	0.89
1:C:1002:UNK:O	1:C:1003:UNK:HG3	1.73	0.89
1:C:2434:UNK:HG3	1:C:2524:CYS:HA	1.54	0.89
1:B:1002:UNK:O	1:B:1003:UNK:HG3	1.73	0.89
1:B:981:UNK:CG	1:B:987:UNK:HG2	2.02	0.88
1:B:2103:UNK:HG2	1:B:2104:UNK:N	1.89	0.88
1:B:2100:UNK:O	1:B:2103:UNK:CG	2.22	0.88
1:C:2100:UNK:O	1:C:2103:UNK:CG	2.22	0.88
1:C:928:ALA:HB1	1:C:931:UNK:HB1	1.55	0.88
1:A:1002:UNK:O	1:A:1003:UNK:HG3	1.73	0.88
1:B:2112:UNK:H	1:B:2115:UNK:CG	1.87	0.88
1:A:2103:UNK:HG2	1:A:2104:UNK:N	1.89	0.87
1:A:2451:UNK:CG	1:A:2454:ASP:OD2	2.22	0.87
1:B:2112:UNK:H	1:B:2115:UNK:HG1	1.40	0.87
1:A:2434:UNK:HG3	1:A:2524:CYS:HA	1.54	0.87
1:B:928:ALA:HB1	1:B:931:UNK:HB1	1.55	0.87
1:B:2434:UNK:HG3	1:B:2524:CYS:HA	1.54	0.87
1:C:2112:UNK:H	1:C:2115:UNK:HG1	1.40	0.87
1:B:2086:UNK:O	1:B:2089:UNK:HG3	1.74	0.87
1:A:928:ALA:HB1	1:A:931:UNK:HB1	1.55	0.87
1:B:2126:UNK:O	1:B:2129:UNK:HG3	1.75	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2086:UNK:O	1:A:2089:UNK:HG3	1.74	0.86
1:A:2112:UNK:H	1:A:2115:UNK:CG	1.87	0.86
1:C:992:UNK:CG	1:C:994:UNK:HG3	2.05	0.86
1:A:2112:UNK:H	1:A:2115:UNK:HG1	1.40	0.86
1:C:2112:UNK:H	1:C:2115:UNK:CG	1.87	0.86
1:C:2451:UNK:CG	1:C:2454:ASP:OD2	2.22	0.86
1:A:992:UNK:CG	1:A:994:UNK:HG3	2.05	0.86
1:A:2126:UNK:O	1:A:2129:UNK:HG3	1.75	0.86
1:C:2086:UNK:O	1:C:2089:UNK:HG3	1.74	0.86
1:B:992:UNK:CG	1:B:994:UNK:CG	2.53	0.86
1:A:2100:UNK:O	1:A:2103:UNK:CG	2.22	0.86
1:B:2451:UNK:CG	1:B:2454:ASP:OD2	2.22	0.86
1:A:931:UNK:HG1	1:A:933:UNK:CG	2.06	0.86
1:A:992:UNK:CG	1:A:994:UNK:CG	2.53	0.86
1:C:2126:UNK:O	1:C:2129:UNK:HG3	1.75	0.86
1:C:992:UNK:CG	1:C:994:UNK:CG	2.53	0.85
1:A:2085:UNK:O	1:A:2088:UNK:HG3	1.76	0.85
1:B:992:UNK:CG	1:B:994:UNK:HG3	2.05	0.85
1:B:2081:UNK:O	1:B:2084:UNK:HG3	1.76	0.85
1:C:2103:UNK:HG2	1:C:2104:UNK:N	1.89	0.85
1:B:1218:UNK:HG2	1:B:1441:GLN:OE1	1.77	0.85
1:B:2085:UNK:O	1:B:2088:UNK:HG3	1.76	0.85
1:B:935:UNK:O	1:B:939:UNK:HG3	1.77	0.85
1:C:2081:UNK:O	1:C:2084:UNK:HG3	1.76	0.85
1:C:1218:UNK:HG2	1:C:1441:GLN:OE1	1.77	0.85
1:C:2085:UNK:O	1:C:2088:UNK:HG3	1.76	0.85
1:A:935:UNK:O	1:A:939:UNK:HG3	1.77	0.85
1:A:1218:UNK:HG2	1:A:1441:GLN:OE1	1.77	0.85
1:A:2118:UNK:O	1:A:2122:UNK:HG3	1.76	0.85
1:B:2118:UNK:O	1:B:2122:UNK:HG3	1.76	0.84
1:A:2081:UNK:O	1:A:2084:UNK:HG3	1.76	0.84
1:A:992:UNK:HG3	1:A:996:UNK:CG	2.07	0.84
1:B:931:UNK:HG1	1:B:933:UNK:CG	2.06	0.84
1:A:999:UNK:HG2	1:A:1007:UNK:CG	2.07	0.84
1:C:2118:UNK:O	1:C:2122:UNK:HG3	1.76	0.84
1:B:1538:ARG:HH11	1:B:1722:PRO:HB3	1.43	0.84
1:C:935:UNK:O	1:C:939:UNK:HG3	1.77	0.84
1:B:999:UNK:HG2	1:B:1007:UNK:CG	2.07	0.84
1:C:931:UNK:HG1	1:C:933:UNK:CG	2.06	0.83
1:A:43:PRO:HG2	1:A:348:ALA:HA	1.60	0.83
1:C:992:UNK:HG3	1:C:996:UNK:CG	2.07	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2105:UNK:O	1:B:2108:UNK:CG	2.24	0.83
1:A:992:UNK:HG1	1:A:994:UNK:CG	2.09	0.83
1:C:999:UNK:O	1:C:1007:UNK:HG3	1.80	0.82
1:C:1538:ARG:HH11	1:C:1722:PRO:HB3	1.43	0.82
1:C:2097:UNK:O	1:C:2100:UNK:CG	2.27	0.82
1:B:992:UNK:HG3	1:B:996:UNK:CG	2.07	0.82
1:B:992:UNK:HG1	1:B:994:UNK:CG	2.09	0.82
1:C:999:UNK:HG2	1:C:1007:UNK:CG	2.07	0.82
1:A:2097:UNK:O	1:A:2100:UNK:CG	2.27	0.82
1:C:992:UNK:HG1	1:C:994:UNK:CG	2.09	0.82
1:A:2016:VAL:HG13	1:A:2020:PRO:HG3	1.62	0.82
1:B:2097:UNK:O	1:B:2100:UNK:CG	2.27	0.82
1:C:2016:VAL:HG13	1:C:2020:PRO:HG3	1.62	0.82
1:A:2093:UNK:CG	1:A:2129:UNK:O	2.27	0.81
1:A:2105:UNK:O	1:A:2108:UNK:CG	2.25	0.81
1:B:43:PRO:HG2	1:B:348:ALA:HA	1.60	0.81
1:B:999:UNK:O	1:B:1007:UNK:HG3	1.80	0.81
1:B:2730:TYR:OH	1:B:3059:ARG:NH1	2.14	0.81
1:B:2016:VAL:HG13	1:B:2020:PRO:HG3	1.62	0.81
1:A:967:VAL:HA	1:A:970:ILE:HB	1.63	0.81
1:C:2091:UNK:O	1:C:2132:UNK:HG1	1.80	0.81
1:C:43:PRO:HG2	1:C:348:ALA:HA	1.60	0.81
1:C:138:ARG:NH2	1:C:175:ASP:OD2	2.14	0.81
1:A:2091:UNK:O	1:A:2132:UNK:HG1	1.80	0.81
1:A:2730:TYR:OH	1:A:3059:ARG:NH1	2.14	0.81
1:B:2091:UNK:O	1:B:2132:UNK:HG1	1.80	0.81
1:A:138:ARG:NH2	1:A:175:ASP:OD2	2.14	0.80
1:B:2093:UNK:CG	1:B:2129:UNK:O	2.27	0.80
1:C:46:VAL:HB	1:C:155:VAL:HG13	1.63	0.80
1:A:995:UNK:HB1	1:A:1011:UNK:HG3	1.63	0.80
1:A:1538:ARG:HH11	1:A:1722:PRO:HB3	1.43	0.80
1:C:2093:UNK:CG	1:C:2129:UNK:O	2.27	0.80
1:B:995:UNK:HB1	1:B:1011:UNK:HG3	1.63	0.80
1:C:2730:TYR:OH	1:C:3059:ARG:NH1	2.14	0.80
1:A:931:UNK:CG	1:A:933:UNK:CG	2.60	0.80
1:C:2123:UNK:O	1:C:2126:UNK:HG3	1.82	0.80
1:B:138:ARG:NH2	1:B:175:ASP:OD2	2.14	0.80
1:C:967:VAL:HA	1:C:970:ILE:HB	1.63	0.80
1:A:1001:UNK:HG1	1:A:1018:ARG:NH2	1.97	0.80
1:B:46:VAL:HB	1:B:155:VAL:HG13	1.63	0.80
1:A:999:UNK:O	1:A:1007:UNK:HG3	1.80	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:ARG:HB2	1:C:282:VAL:H	1.47	0.80
1:C:1001:UNK:HG1	1:C:1018:ARG:NH2	1.97	0.79
1:A:46:VAL:HB	1:A:155:VAL:HG13	1.63	0.79
1:B:931:UNK:CG	1:B:933:UNK:CG	2.60	0.79
1:C:2105:UNK:O	1:C:2108:UNK:CG	2.24	0.79
1:C:1220:UNK:CG	1:C:1221:UNK:N	2.46	0.79
1:A:2098:UNK:O	1:A:2102:UNK:HG3	1.82	0.79
1:B:1001:UNK:HG1	1:B:1018:ARG:NH2	1.97	0.79
1:B:2610:ARG:HH12	1:B:2700:LEU:HD11	1.47	0.79
1:C:931:UNK:CG	1:C:933:UNK:CG	2.60	0.79
1:A:273:ARG:HB2	1:A:282:VAL:H	1.47	0.79
1:B:2084:UNK:O	1:B:2087:UNK:HG3	1.82	0.79
1:B:2098:UNK:O	1:B:2102:UNK:HG3	1.82	0.78
1:C:2077:UNK:HG2	1:C:2079:UNK:HG3	1.65	0.78
1:B:2077:UNK:HG2	1:B:2079:UNK:HG3	1.65	0.78
1:B:2123:UNK:O	1:B:2126:UNK:HG3	1.82	0.78
1:A:931:UNK:HG1	1:A:933:UNK:HG2	1.65	0.78
1:C:995:UNK:HB1	1:C:1011:UNK:HG3	1.63	0.78
1:C:2610:ARG:HH12	1:C:2700:LEU:HD11	1.47	0.78
1:A:2084:UNK:O	1:A:2087:UNK:HG3	1.82	0.78
1:B:930:UNK:O	1:B:930:UNK:HG2	1.83	0.78
1:B:967:VAL:HA	1:B:970:ILE:HB	1.63	0.78
1:B:273:ARG:HB2	1:B:282:VAL:H	1.47	0.78
1:C:2098:UNK:O	1:C:2102:UNK:HG3	1.82	0.78
1:C:930:UNK:HG2	1:C:930:UNK:O	1.83	0.78
1:A:971:ALA:O	1:A:974:UNK:HG3	1.84	0.78
1:A:2077:UNK:HG2	1:A:2079:UNK:HG3	1.65	0.78
1:A:2123:UNK:O	1:A:2126:UNK:HG3	1.82	0.78
1:C:2084:UNK:O	1:C:2087:UNK:HG3	1.82	0.78
1:B:2135:UNK:HG3	1:B:2136:ASP:N	1.99	0.77
1:C:971:ALA:O	1:C:974:UNK:HG3	1.84	0.77
1:B:1220:UNK:CG	1:B:1221:UNK:N	2.46	0.77
1:A:930:UNK:O	1:A:930:UNK:HG2	1.83	0.77
1:A:1329:ALA:HB3	1:A:1337:MET:H	1.48	0.77
1:A:2135:UNK:HG3	1:A:2136:ASP:N	1.99	0.77
1:B:1329:ALA:HB3	1:B:1337:MET:H	1.49	0.77
1:C:2135:UNK:HG3	1:C:2136:ASP:N	1.99	0.77
1:C:2100:UNK:HG2	1:C:2101:UNK:N	2.00	0.77
1:C:931:UNK:HG1	1:C:933:UNK:HG2	1.65	0.77
1:C:1329:ALA:HB3	1:C:1337:MET:H	1.49	0.77
1:B:971:ALA:O	1:B:974:UNK:HG3	1.84	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:931:UNK:CG	1:C:933:UNK:HG2	2.15	0.77
1:B:931:UNK:CG	1:B:933:UNK:HG2	2.15	0.77
1:A:257:ARG:HH12	1:C:1695:LEU:HD23	1.51	0.76
1:A:931:UNK:CG	1:A:933:UNK:HG2	2.15	0.76
1:A:2610:ARG:HH12	1:A:2700:LEU:HD11	1.47	0.76
1:B:1695:LEU:HD23	1:C:257:ARG:HH12	1.50	0.76
1:A:1695:LEU:HD23	1:B:257:ARG:HH12	1.51	0.76
1:A:2557:LEU:O	1:A:2613:ARG:N	2.18	0.76
1:A:944:UNK:HG2	1:A:944:UNK:O	1.85	0.76
1:B:931:UNK:HG1	1:B:933:UNK:HG2	1.65	0.76
1:C:934:UNK:O	1:C:937:UNK:CG	2.34	0.76
1:A:1097:VAL:HB	1:A:1146:PRO:HB2	1.68	0.76
1:B:1097:VAL:HB	1:B:1146:PRO:HB2	1.68	0.76
1:A:1220:UNK:CG	1:A:1221:UNK:N	2.46	0.76
1:A:2100:UNK:HG2	1:A:2101:UNK:N	2.00	0.76
1:B:2557:LEU:O	1:B:2613:ARG:N	2.18	0.76
1:A:995:UNK:HB1	1:A:1011:UNK:CG	2.17	0.75
1:B:2124:UNK:O	1:B:2127:UNK:HG3	1.86	0.75
1:C:2452:UNK:HG2	1:C:2453:UNK:N	2.01	0.75
1:A:940:UNK:O	1:A:940:UNK:HG2	1.86	0.75
1:B:2126:UNK:C	1:B:2129:UNK:HG3	2.16	0.75
1:B:2452:UNK:HG2	1:B:2453:UNK:N	2.00	0.75
1:B:944:UNK:O	1:B:944:UNK:HG2	1.85	0.75
1:B:2418:GLY:O	1:B:2422:UNK:HG3	1.87	0.75
1:C:2124:UNK:O	1:C:2127:UNK:HG3	1.87	0.75
1:A:2452:UNK:HG2	1:A:2453:UNK:N	2.00	0.75
1:A:2418:GLY:O	1:A:2422:UNK:HG3	1.87	0.75
1:B:2645:ASP:OD2	1:B:2691:SER:N	2.19	0.75
1:A:1212:UNK:HG2	1:A:1342:ARG:NH2	2.02	0.75
1:B:995:UNK:HB1	1:B:1011:UNK:CG	2.17	0.75
1:B:2088:UNK:O	1:B:2091:UNK:CG	2.35	0.75
1:B:2100:UNK:HG2	1:B:2101:UNK:N	2.00	0.75
1:C:2122:UNK:O	1:C:2125:UNK:HG3	1.87	0.75
1:A:2122:UNK:O	1:A:2125:UNK:HG3	1.87	0.74
1:C:445:VAL:HG13	1:C:475:LEU:HD21	1.69	0.74
1:C:944:UNK:HG2	1:C:944:UNK:O	1.85	0.74
1:C:995:UNK:HB1	1:C:1011:UNK:CG	2.17	0.74
1:C:2418:GLY:O	1:C:2422:UNK:HG3	1.87	0.74
1:C:1097:VAL:HB	1:C:1146:PRO:HB2	1.68	0.74
1:C:2088:UNK:O	1:C:2091:UNK:CG	2.35	0.74
1:B:445:VAL:HG13	1:B:475:LEU:HD21	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1212:UNK:HG2	1:B:1342:ARG:NH2	2.02	0.74
1:A:2124:UNK:O	1:A:2127:UNK:HG3	1.86	0.74
1:C:33:ALA:HB2	1:C:390:VAL:HA	1.70	0.74
1:A:33:ALA:HB2	1:A:390:VAL:HA	1.70	0.74
1:A:1556:GLU:OE2	1:A:1560:ARG:NH2	2.20	0.74
1:B:940:UNK:O	1:B:940:UNK:HG2	1.86	0.74
1:A:934:UNK:O	1:A:937:UNK:CG	2.34	0.74
1:C:940:UNK:HG2	1:C:940:UNK:O	1.86	0.74
1:A:994:UNK:HG2	1:A:996:UNK:HG3	1.70	0.74
1:A:2087:UNK:HA	1:A:2090:UNK:HG3	1.70	0.74
1:A:2126:UNK:C	1:A:2129:UNK:HG3	2.17	0.74
1:A:2645:ASP:OD2	1:A:2691:SER:N	2.19	0.74
1:B:2122:UNK:O	1:B:2125:UNK:HG3	1.87	0.74
1:C:1212:UNK:CG	1:C:1342:ARG:HE	2.01	0.74
1:C:2557:LEU:O	1:C:2613:ARG:N	2.18	0.74
1:B:33:ALA:HB2	1:B:390:VAL:HA	1.69	0.74
1:B:1212:UNK:CG	1:B:1342:ARG:HE	2.01	0.74
1:C:1212:UNK:HG2	1:C:1342:ARG:NH2	2.02	0.74
1:A:799:PHE:CZ	1:A:2433:UNK:HG3	2.23	0.74
1:A:992:UNK:HG3	1:A:996:UNK:HG3	1.66	0.74
1:B:1001:UNK:O	1:B:1002:UNK:HG3	1.88	0.74
1:B:1556:GLU:OE2	1:B:1560:ARG:NH2	2.20	0.74
1:C:1168:ARG:N	1:C:1194:ILE:O	2.21	0.74
1:C:1556:GLU:OE2	1:C:1560:ARG:NH2	2.20	0.74
1:A:1212:UNK:CG	1:A:1342:ARG:HE	2.01	0.73
1:B:934:UNK:O	1:B:937:UNK:CG	2.34	0.73
1:B:1226:UNK:HG3	1:B:1313:VAL:HG12	1.70	0.73
1:B:2087:UNK:HA	1:B:2090:UNK:HG3	1.70	0.73
1:C:2126:UNK:C	1:C:2129:UNK:HG3	2.17	0.73
1:A:992:UNK:HG2	1:A:994:UNK:CG	2.17	0.73
1:A:1168:ARG:N	1:A:1194:ILE:O	2.21	0.73
1:B:992:UNK:HG2	1:B:994:UNK:CG	2.17	0.73
1:C:994:UNK:HG2	1:C:996:UNK:HG3	1.70	0.73
1:B:3015:ILE:HG12	1:B:3023:ARG:HG3	1.69	0.73
1:C:2096:UNK:O	1:C:2099:UNK:CG	2.37	0.73
1:B:799:PHE:CZ	1:B:2433:UNK:HG3	2.23	0.73
1:C:799:PHE:CZ	1:C:2433:UNK:HG3	2.23	0.73
1:B:994:UNK:HG2	1:B:996:UNK:HG3	1.70	0.73
1:C:3015:ILE:HG12	1:C:3023:ARG:HG3	1.69	0.73
1:A:2883:ALA:O	1:A:2916:ARG:NH1	2.22	0.73
1:B:2053:ALA:O	1:B:2807:ARG:NH2	2.21	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2096:UNK:O	1:B:2099:UNK:CG	2.36	0.73
1:C:437:PRO:HG3	1:C:876:LEU:HB3	1.70	0.73
1:C:980:UNK:O	1:C:981:UNK:HG3	1.89	0.73
1:C:2053:ALA:O	1:C:2807:ARG:NH2	2.21	0.73
1:B:2093:UNK:HA	1:B:2097:UNK:CG	2.19	0.73
1:C:992:UNK:HG2	1:C:994:UNK:CG	2.17	0.73
1:C:1001:UNK:O	1:C:1002:UNK:HG3	1.88	0.73
1:A:2053:ALA:O	1:A:2807:ARG:NH2	2.21	0.72
1:B:437:PRO:HG3	1:B:876:LEU:HB3	1.70	0.72
1:C:976:UNK:HG3	1:C:993:UNK:CB	2.19	0.72
1:B:1168:ARG:N	1:B:1194:ILE:O	2.21	0.72
1:C:936:UNK:HB1	1:C:941:UNK:HB1	1.71	0.72
1:C:2883:ALA:O	1:C:2916:ARG:NH1	2.22	0.72
1:A:1226:UNK:HG3	1:A:1313:VAL:HG12	1.70	0.72
1:B:1253:ARG:HH11	1:B:1253:ARG:HG3	1.55	0.72
1:C:1226:UNK:HG3	1:C:1313:VAL:HG12	1.70	0.72
1:C:1253:ARG:HH11	1:C:1253:ARG:HG3	1.54	0.72
1:C:1400:PRO:HD2	1:C:1416:VAL:HG22	1.72	0.72
1:A:2093:UNK:HA	1:A:2097:UNK:CG	2.19	0.72
1:B:1400:PRO:HD2	1:B:1416:VAL:HG22	1.72	0.72
1:A:1001:UNK:O	1:A:1002:UNK:HG3	1.88	0.72
1:C:70:SER:OG	1:C:142:ARG:NH2	2.23	0.72
1:C:2645:ASP:OD2	1:C:2691:SER:N	2.19	0.72
1:A:95:PRO:HB2	1:C:1237:ARG:NH1	2.05	0.72
1:A:980:UNK:O	1:A:981:UNK:HG3	1.89	0.72
1:A:2088:UNK:O	1:A:2091:UNK:CG	2.35	0.72
1:B:936:UNK:HB1	1:B:941:UNK:HB1	1.71	0.72
1:B:2121:UNK:O	1:B:2124:UNK:HG3	1.90	0.72
1:A:70:SER:OG	1:A:142:ARG:NH2	2.23	0.72
1:A:445:VAL:HG13	1:A:475:LEU:HD21	1.69	0.72
1:A:2113:UNK:O	1:A:2116:UNK:CG	2.38	0.72
1:A:3015:ILE:HG12	1:A:3023:ARG:HG3	1.69	0.72
1:B:1218:UNK:CG	1:B:1441:GLN:OE1	2.38	0.72
1:C:2093:UNK:HA	1:C:2097:UNK:CG	2.19	0.72
1:A:992:UNK:HG2	1:A:994:UNK:HG3	1.72	0.72
1:B:980:UNK:O	1:B:981:UNK:HG3	1.89	0.72
1:A:1253:ARG:HH11	1:A:1253:ARG:HG3	1.55	0.72
1:A:1400:PRO:HD2	1:A:1416:VAL:HG22	1.72	0.72
1:B:2883:ALA:O	1:B:2916:ARG:NH1	2.22	0.72
1:C:992:UNK:HG2	1:C:994:UNK:HG3	1.72	0.72
1:C:2087:UNK:HA	1:C:2090:UNK:HG3	1.70	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2268:GLN:OE1	1:C:2319:ARG:NH1	2.23	0.71
1:A:1237:ARG:NH1	1:B:95:PRO:HB2	2.05	0.71
1:A:2121:UNK:O	1:A:2124:UNK:HG3	1.90	0.71
1:B:70:SER:OG	1:B:142:ARG:NH2	2.23	0.71
1:B:1237:ARG:NH1	1:C:95:PRO:HB2	2.05	0.71
1:B:2268:GLN:OE1	1:B:2319:ARG:NH1	2.23	0.71
1:A:981:UNK:HG1	1:A:987:UNK:CG	2.19	0.71
1:C:1218:UNK:CG	1:C:1441:GLN:OE1	2.38	0.71
1:C:2113:UNK:O	1:C:2116:UNK:CG	2.38	0.71
1:A:976:UNK:HG3	1:A:993:UNK:CB	2.19	0.71
1:A:982:UNK:HG2	1:A:983:UNK:N	2.05	0.71
1:B:976:UNK:HG3	1:B:993:UNK:CB	2.19	0.71
1:B:982:UNK:HG2	1:B:983:UNK:N	2.05	0.71
1:B:2998:GLY:N	1:B:3002:VAL:O	2.23	0.71
1:A:981:UNK:HB2	1:A:984:UNK:CG	2.21	0.71
1:A:936:UNK:HB1	1:A:941:UNK:HB1	1.71	0.71
1:C:1634:ARG:HH11	1:C:1639:ALA:H	1.39	0.71
1:C:2121:UNK:O	1:C:2124:UNK:HG3	1.90	0.71
1:A:2096:UNK:O	1:A:2099:UNK:CG	2.37	0.70
1:C:982:UNK:HG2	1:C:983:UNK:N	2.05	0.70
1:C:1507:GLN:O	1:C:1562:ARG:NH1	2.24	0.70
1:A:437:PRO:HG3	1:A:876:LEU:HB3	1.70	0.70
1:C:2112:UNK:O	1:C:2115:UNK:CG	2.38	0.70
1:A:1218:UNK:CG	1:A:1441:GLN:OE1	2.38	0.70
1:A:2268:GLN:OE1	1:A:2319:ARG:NH1	2.23	0.70
1:A:2558:LEU:HG	1:A:2612:PRO:HA	1.73	0.70
1:A:1507:GLN:O	1:A:1562:ARG:NH1	2.24	0.70
1:B:981:UNK:HB2	1:B:984:UNK:CG	2.21	0.70
1:C:981:UNK:HG1	1:C:987:UNK:CG	2.19	0.70
1:B:137:VAL:HG22	1:B:354:LEU:HD13	1.74	0.70
1:B:1634:ARG:HH11	1:B:1639:ALA:H	1.39	0.70
1:A:2743:ALA:HB1	1:A:2940:VAL:HG23	1.73	0.70
1:A:2998:GLY:N	1:A:3002:VAL:O	2.23	0.70
1:C:981:UNK:HB2	1:C:984:UNK:CG	2.21	0.70
1:C:2558:LEU:HG	1:C:2612:PRO:HA	1.73	0.70
1:B:580:ARG:HD2	1:B:614:GLY:HA3	1.73	0.70
1:C:974:UNK:HG1	1:C:977:UNK:HB1	1.74	0.70
1:B:992:UNK:HG2	1:B:994:UNK:HG3	1.72	0.70
1:B:2112:UNK:O	1:B:2115:UNK:CG	2.38	0.70
1:B:2743:ALA:HB1	1:B:2940:VAL:HG23	1.73	0.70
1:A:1634:ARG:HH11	1:A:1639:ALA:H	1.39	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2112:UNK:O	1:A:2115:UNK:CG	2.38	0.69
1:C:580:ARG:HD2	1:C:614:GLY:HA3	1.72	0.69
1:C:1035:VAL:HG12	1:C:1037:ASP:H	1.57	0.69
1:A:580:ARG:HD2	1:A:614:GLY:HA3	1.73	0.69
1:A:1035:VAL:HG12	1:A:1037:ASP:H	1.57	0.69
1:A:2860:ALA:HB3	1:A:2906:LEU:HD21	1.73	0.69
1:B:2860:ALA:HB3	1:B:2906:LEU:HD21	1.73	0.69
1:C:2860:ALA:HB3	1:C:2906:LEU:HD21	1.73	0.69
1:B:2215:THR:HB	1:B:2229:LYS:HB2	1.74	0.69
1:C:2085:UNK:O	1:C:2088:UNK:CG	2.41	0.69
1:A:1012:UNK:O	1:A:1013:UNK:CG	2.41	0.69
1:B:1177:ARG:HB2	1:B:1184:LEU:HD23	1.74	0.69
1:A:137:VAL:HG22	1:A:354:LEU:HD13	1.74	0.69
1:B:1164:THR:N	1:B:1167:GLY:O	2.25	0.69
1:B:2558:LEU:HG	1:B:2612:PRO:HA	1.74	0.69
1:C:2122:UNK:HA	1:C:2125:UNK:HG3	1.75	0.69
1:A:2215:THR:HB	1:A:2229:LYS:HB2	1.74	0.69
1:B:2122:UNK:HA	1:B:2125:UNK:HG3	1.75	0.69
1:C:2647:VAL:HG22	1:C:2769:ASP:HB2	1.75	0.69
1:A:1046:LEU:HD13	1:A:1129:LEU:HD22	1.75	0.69
1:B:1046:LEU:HD13	1:B:1129:LEU:HD22	1.75	0.69
1:B:1507:GLN:O	1:B:1562:ARG:NH1	2.24	0.69
1:C:1046:LEU:HD13	1:C:1129:LEU:HD22	1.75	0.69
1:C:2445:UNK:HG2	1:C:2985:GLY:O	1.93	0.69
1:C:2743:ALA:HB1	1:C:2940:VAL:HG23	1.73	0.69
1:C:2998:GLY:N	1:C:3002:VAL:O	2.23	0.69
1:C:2112:UNK:C	1:C:2115:UNK:HG3	2.22	0.69
1:B:2085:UNK:O	1:B:2088:UNK:CG	2.40	0.69
1:B:2946:LEU:HD11	1:B:2992:GLY:HA3	1.75	0.69
1:A:2445:UNK:HG2	1:A:2985:GLY:O	1.93	0.68
1:C:992:UNK:HG3	1:C:996:UNK:HG3	1.66	0.68
1:B:2113:UNK:C	1:B:2116:UNK:HG3	2.23	0.68
1:A:511:ARG:HD3	1:A:543:GLY:HA3	1.76	0.68
1:A:1177:ARG:HB2	1:A:1184:LEU:HD23	1.74	0.68
1:B:2112:UNK:C	1:B:2115:UNK:HG3	2.22	0.68
1:B:2113:UNK:O	1:B:2116:UNK:CG	2.37	0.68
1:C:2093:UNK:CG	1:C:2132:UNK:HB1	2.24	0.68
1:B:340:ILE:HD13	1:B:364:THR:HG21	1.75	0.68
1:B:1035:VAL:HG12	1:B:1037:ASP:H	1.57	0.68
1:C:1164:THR:N	1:C:1167:GLY:O	2.25	0.68
1:C:1177:ARG:HB2	1:C:1184:LEU:HD23	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ILE:HD13	1:A:364:THR:HG21	1.75	0.68
1:A:2112:UNK:C	1:A:2115:UNK:HG3	2.22	0.68
1:C:511:ARG:HD3	1:C:543:GLY:HA3	1.76	0.68
1:C:2113:UNK:C	1:C:2116:UNK:HG3	2.23	0.68
1:A:2093:UNK:CG	1:A:2132:UNK:HB1	2.24	0.68
1:B:2093:UNK:CG	1:B:2132:UNK:HB1	2.24	0.68
1:B:2647:VAL:HG22	1:B:2769:ASP:HB2	1.75	0.68
1:C:137:VAL:HG22	1:C:354:LEU:HD13	1.74	0.68
1:C:2215:THR:HB	1:C:2229:LYS:HB2	1.74	0.68
1:A:2080:UNK:HB2	1:A:2082:UNK:HG3	1.75	0.68
1:A:2946:LEU:HD11	1:A:2992:GLY:HA3	1.75	0.68
1:C:269:GLU:HB3	1:C:282:VAL:HA	1.75	0.68
1:A:2085:UNK:O	1:A:2088:UNK:CG	2.40	0.68
1:B:2445:UNK:HG2	1:B:2985:GLY:O	1.93	0.68
1:C:1488:VAL:HG21	1:C:1580:PRO:HD2	1.76	0.68
1:C:2097:UNK:C	1:C:2100:UNK:HG3	2.24	0.68
1:A:992:UNK:HG3	1:A:996:UNK:HG2	1.76	0.68
1:A:1724:TYR:OH	1:B:267:GLU:OE2	2.08	0.68
1:B:511:ARG:HD3	1:B:543:GLY:HA3	1.76	0.68
1:C:2080:UNK:HB2	1:C:2082:UNK:HG3	1.75	0.68
1:A:974:UNK:HG1	1:A:977:UNK:HB1	1.74	0.67
1:A:2112:UNK:HG2	1:A:2114:UNK:HG3	1.77	0.67
1:A:2122:UNK:HA	1:A:2125:UNK:HG3	1.75	0.67
1:C:2946:LEU:HD11	1:C:2992:GLY:HA3	1.75	0.67
1:C:3080:ARG:HH11	1:C:3080:ARG:CG	2.07	0.67
1:A:2113:UNK:C	1:A:2116:UNK:HG3	2.23	0.67
1:B:974:UNK:HG1	1:B:977:UNK:HB1	1.74	0.67
1:B:1163:ASP:HB3	1:B:1199:UNK:HG3	1.76	0.67
1:A:1164:THR:N	1:A:1167:GLY:O	2.25	0.67
1:B:2103:UNK:CG	1:B:2104:UNK:N	2.58	0.67
1:C:2112:UNK:HG2	1:C:2114:UNK:HG3	1.77	0.67
1:B:792:ALA:HA	1:B:799:PHE:HE2	1.60	0.67
1:B:2086:UNK:C	1:B:2089:UNK:HG3	2.25	0.67
1:B:2093:UNK:HG3	1:B:2132:UNK:HB1	1.77	0.67
1:B:3080:ARG:HH11	1:B:3080:ARG:CG	2.07	0.67
1:C:340:ILE:HD13	1:C:364:THR:HG21	1.75	0.67
1:C:2093:UNK:HG3	1:C:2132:UNK:HB1	1.77	0.67
1:C:2103:UNK:CG	1:C:2104:UNK:N	2.58	0.67
1:A:2112:UNK:N	1:A:2115:UNK:CG	2.57	0.67
1:A:2126:UNK:O	1:A:2129:UNK:CG	2.43	0.67
1:B:269:GLU:HB3	1:B:282:VAL:HA	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2080:UNK:HB2	1:B:2082:UNK:HG3	1.75	0.67
1:A:2081:UNK:O	1:A:2084:UNK:CG	2.43	0.67
1:A:2097:UNK:C	1:A:2100:UNK:HG3	2.24	0.67
1:B:2080:UNK:O	1:B:2083:UNK:HG3	1.94	0.67
1:B:931:UNK:CG	1:B:933:UNK:HG3	2.25	0.67
1:A:1008:UNK:HG3	1:A:1019:PHE:HB3	1.76	0.67
1:A:2103:UNK:CG	1:A:2104:UNK:N	2.58	0.67
1:B:1488:VAL:HG12	1:B:1490:ARG:NH1	2.10	0.67
1:A:269:GLU:HB3	1:A:282:VAL:HA	1.75	0.66
1:A:1488:VAL:HG21	1:A:1580:PRO:HD2	1.76	0.66
1:A:2084:UNK:C	1:A:2087:UNK:HG3	2.25	0.66
1:A:2647:VAL:HG22	1:A:2769:ASP:HB2	1.75	0.66
1:C:970:ILE:HG12	1:C:996:UNK:HG1	1.76	0.66
1:C:1008:UNK:HG3	1:C:1019:PHE:HB3	1.76	0.66
1:A:511:ARG:HB2	1:A:540:ASN:HB2	1.77	0.66
1:A:792:ALA:HA	1:A:799:PHE:HE2	1.60	0.66
1:A:2080:UNK:O	1:A:2083:UNK:HG3	1.95	0.66
1:A:2093:UNK:HG3	1:A:2132:UNK:HB1	1.77	0.66
1:B:1012:UNK:O	1:B:1013:UNK:CG	2.41	0.66
1:B:1168:ARG:HB2	1:B:1197:UNK:HB2	1.77	0.66
1:B:2084:UNK:C	1:B:2087:UNK:HG3	2.25	0.66
1:C:981:UNK:O	1:C:981:UNK:HG2	1.95	0.66
1:C:992:UNK:HG3	1:C:996:UNK:HG2	1.76	0.66
1:C:1163:ASP:HB3	1:C:1199:UNK:HG3	1.76	0.66
1:B:992:UNK:HG3	1:B:996:UNK:HG2	1.76	0.66
1:B:2097:UNK:C	1:B:2100:UNK:HG3	2.24	0.66
1:C:1358:GLN:HG2	1:C:1423:THR:HG23	1.78	0.66
1:B:2081:UNK:O	1:B:2084:UNK:CG	2.43	0.66
1:B:2126:UNK:O	1:B:2129:UNK:CG	2.43	0.66
1:C:511:ARG:HB2	1:C:540:ASN:HB2	1.78	0.66
1:C:2080:UNK:O	1:C:2083:UNK:HG3	1.94	0.66
1:A:1412:HIS:HD2	1:A:1413:PRO:HD2	1.61	0.66
1:B:511:ARG:HB2	1:B:540:ASN:HB2	1.77	0.66
1:B:981:UNK:HG1	1:B:987:UNK:CG	2.19	0.66
1:C:683:GLY:HA2	1:C:700:ASN:HB2	1.78	0.66
1:C:2126:UNK:O	1:C:2129:UNK:CG	2.43	0.66
1:A:1163:ASP:HB3	1:A:1199:UNK:HG3	1.76	0.66
1:B:1167:GLY:HA3	1:B:1195:ARG:HA	1.77	0.66
1:B:1412:HIS:HD2	1:B:1413:PRO:HD2	1.61	0.66
1:C:1168:ARG:HB2	1:C:1197:UNK:HB2	1.77	0.66
1:A:2591:ARG:HH12	1:C:2012:GLY:C	1.99	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1008:UNK:HG3	1:B:1019:PHE:HB3	1.76	0.66
1:C:792:ALA:HA	1:C:799:PHE:HE2	1.60	0.66
1:A:1084:THR:HG21	1:A:1274:ALA:HA	1.78	0.66
1:A:1358:GLN:HG2	1:A:1423:THR:HG23	1.78	0.66
1:B:35:VAL:HG11	1:B:147:LEU:HB3	1.78	0.66
1:B:2112:UNK:HG2	1:B:2114:UNK:HG3	1.77	0.66
1:C:931:UNK:CG	1:C:933:UNK:HG3	2.24	0.66
1:C:1132:LEU:HD11	1:C:1192:PHE:HB3	1.78	0.66
1:A:931:UNK:CG	1:A:933:UNK:HG3	2.25	0.66
1:B:2012:GLY:C	1:C:2591:ARG:HH12	1.99	0.66
1:C:1084:THR:HG21	1:C:1274:ALA:HA	1.78	0.66
1:C:2081:UNK:O	1:C:2084:UNK:CG	2.43	0.66
1:C:2112:UNK:N	1:C:2115:UNK:CG	2.57	0.66
1:A:2086:UNK:C	1:A:2089:UNK:HG3	2.25	0.66
1:B:666:VAL:HG21	1:B:904:VAL:HB	1.78	0.66
1:B:1358:GLN:HG2	1:B:1423:THR:HG23	1.78	0.66
1:B:2112:UNK:N	1:B:2115:UNK:CG	2.57	0.66
1:C:997:UNK:O	1:C:1009:UNK:N	2.29	0.66
1:A:997:UNK:O	1:A:1009:UNK:N	2.29	0.65
1:A:1167:GLY:HA3	1:A:1195:ARG:HA	1.78	0.65
1:A:2112:UNK:N	1:A:2115:UNK:HG1	2.11	0.65
1:A:2679:ALA:HB3	1:A:2762:VAL:HG12	1.78	0.65
1:B:970:ILE:HG12	1:B:996:UNK:HG1	1.76	0.65
1:B:1488:VAL:HG21	1:B:1580:PRO:HD2	1.77	0.65
1:B:1534:ASN:HB2	1:B:1543:ALA:HB3	1.78	0.65
1:B:2123:UNK:C	1:B:2126:UNK:HG3	2.26	0.65
1:A:970:ILE:HG12	1:A:996:UNK:HG1	1.76	0.65
1:A:1488:VAL:HG12	1:A:1490:ARG:NH1	2.10	0.65
1:B:2706:PRO:HG2	1:B:2709:ILE:HG23	1.79	0.65
1:C:2123:UNK:C	1:C:2126:UNK:HG3	2.26	0.65
1:A:2012:GLY:C	1:B:2591:ARG:HH12	1.99	0.65
1:A:2123:UNK:C	1:A:2126:UNK:HG3	2.26	0.65
1:B:683:GLY:HA2	1:B:700:ASN:HB2	1.78	0.65
1:C:1534:ASN:HB2	1:C:1543:ALA:HB3	1.79	0.65
1:C:2084:UNK:C	1:C:2087:UNK:HG3	2.25	0.65
1:B:1417:LEU:O	1:B:1423:THR:OG1	2.14	0.65
1:C:203:ASP:OD1	1:C:204:ARG:N	2.29	0.65
1:C:924:LEU:O	1:C:929:UNK:N	2.30	0.65
1:C:2876:LEU:HD11	1:C:2886:ILE:HD11	1.79	0.65
1:A:981:UNK:O	1:A:981:UNK:HG2	1.95	0.65
1:B:2112:UNK:N	1:B:2115:UNK:HG1	2.11	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2679:ALA:HB3	1:B:2762:VAL:HG12	1.78	0.65
1:C:1488:VAL:HG12	1:C:1490:ARG:NH1	2.10	0.65
1:C:2086:UNK:C	1:C:2089:UNK:HG3	2.25	0.65
1:A:35:VAL:HG11	1:A:147:LEU:HB3	1.78	0.65
1:A:450:ASN:HA	1:A:483:ARG:HH11	1.62	0.65
1:B:3080:ARG:HG3	1:B:3080:ARG:NH1	2.09	0.65
1:C:1012:UNK:O	1:C:1013:UNK:CG	2.41	0.65
1:A:2876:LEU:HD11	1:A:2886:ILE:HD11	1.79	0.65
1:B:1132:LEU:HD11	1:B:1192:PHE:HB3	1.78	0.65
1:C:666:VAL:HG21	1:C:904:VAL:HB	1.78	0.65
1:C:1412:HIS:HD2	1:C:1413:PRO:HD2	1.61	0.65
1:C:1417:LEU:O	1:C:1423:THR:OG1	2.14	0.65
1:A:666:VAL:HG21	1:A:904:VAL:HB	1.78	0.65
1:A:1168:ARG:HB2	1:A:1197:UNK:HB2	1.77	0.65
1:B:500:GLN:O	1:B:504:LYS:N	2.24	0.65
1:B:1084:THR:HG21	1:B:1274:ALA:HA	1.78	0.65
1:B:2876:LEU:HD11	1:B:2886:ILE:HD11	1.79	0.65
1:A:943:UNK:O	1:A:944:UNK:CG	2.44	0.65
1:A:999:UNK:CG	1:A:1007:UNK:CG	2.75	0.65
1:A:1536:ASN:HA	1:A:1679:TRP:HB3	1.79	0.65
1:A:3080:ARG:HH11	1:A:3080:ARG:CG	2.07	0.65
1:B:203:ASP:OD1	1:B:204:ARG:N	2.29	0.65
1:B:997:UNK:O	1:B:1009:UNK:N	2.29	0.65
1:C:999:UNK:CG	1:C:1007:UNK:CG	2.75	0.65
1:C:1167:GLY:HA3	1:C:1195:ARG:HA	1.78	0.65
1:A:2652:ILE:HG12	1:A:2722:VAL:HG22	1.79	0.65
1:B:943:UNK:O	1:B:944:UNK:CG	2.44	0.65
1:C:2652:ILE:HG12	1:C:2722:VAL:HG22	1.79	0.65
1:C:2706:PRO:HG2	1:C:2709:ILE:HG23	1.79	0.65
1:C:35:VAL:HG11	1:C:147:LEU:HB3	1.77	0.64
1:C:1536:ASN:HA	1:C:1679:TRP:HB3	1.78	0.64
1:A:56:LEU:HD22	1:A:119:LEU:HD13	1.79	0.64
1:A:408:VAL:HG13	1:A:943:UNK:HG1	1.80	0.64
1:A:1417:LEU:O	1:A:1423:THR:OG1	2.14	0.64
1:B:238:SER:HG	1:B:249:THR:HG1	1.42	0.64
1:B:981:UNK:HG2	1:B:981:UNK:O	1.95	0.64
1:A:924:LEU:O	1:A:929:UNK:N	2.30	0.64
1:A:2120:UNK:O	1:A:2123:UNK:HG3	1.97	0.64
1:A:2706:PRO:HG2	1:A:2709:ILE:HG23	1.78	0.64
1:A:1534:ASN:HB2	1:A:1543:ALA:HB3	1.78	0.64
1:B:924:LEU:O	1:B:929:UNK:N	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:ASN:HA	1:C:483:ARG:HH11	1.62	0.64
1:C:943:UNK:O	1:C:944:UNK:CG	2.44	0.64
1:A:34:LEU:O	1:A:38:LEU:N	2.25	0.64
1:A:643:ILE:HD12	1:A:915:PHE:HZ	1.62	0.64
1:B:42:GLU:HB3	1:B:349:ARG:HG3	1.79	0.64
1:B:999:UNK:CG	1:B:1007:UNK:CG	2.75	0.64
1:B:2120:UNK:O	1:B:2123:UNK:HG3	1.97	0.64
1:B:2428:UNK:HG2	1:B:2428:UNK:O	1.98	0.64
1:C:2449:UNK:O	1:C:2449:UNK:HG2	1.98	0.64
1:C:2679:ALA:HB3	1:C:2762:VAL:HG12	1.78	0.64
1:C:408:VAL:HG13	1:C:943:UNK:HG1	1.79	0.64
1:A:683:GLY:HA2	1:A:700:ASN:HB2	1.78	0.64
1:A:792:ALA:O	1:A:2433:UNK:HG2	1.96	0.64
1:A:1132:LEU:HD11	1:A:1192:PHE:HB3	1.78	0.64
1:A:1214:UNK:HB1	1:A:1320:VAL:HB	1.80	0.64
1:B:2080:UNK:HG2	1:B:2083:UNK:HG3	1.79	0.64
1:C:2120:UNK:O	1:C:2123:UNK:HG3	1.97	0.64
1:B:56:LEU:HD22	1:B:119:LEU:HD13	1.79	0.64
1:A:203:ASP:OD1	1:A:204:ARG:N	2.30	0.64
1:A:2252:VAL:HA	1:A:2255:ARG:HE	1.62	0.64
1:B:1536:ASN:HA	1:B:1679:TRP:HB3	1.78	0.64
1:B:2252:VAL:HA	1:B:2255:ARG:HE	1.62	0.64
1:C:803:GLU:OE1	1:C:2431:UNK:HG3	1.98	0.64
1:B:2449:UNK:HG2	1:B:2449:UNK:O	1.98	0.64
1:A:42:GLU:HB3	1:A:349:ARG:HG3	1.79	0.63
1:C:42:GLU:HB3	1:C:349:ARG:HG3	1.79	0.63
1:C:2080:UNK:HG2	1:C:2083:UNK:HG3	1.79	0.63
1:A:974:UNK:CG	1:A:977:UNK:HB1	2.29	0.63
1:C:643:ILE:HD12	1:C:915:PHE:HZ	1.62	0.63
1:A:892:ILE:HG22	2:A:4000:FMN:HM82	1.80	0.63
1:A:2428:UNK:O	1:A:2428:UNK:HG2	1.98	0.63
1:B:450:ASN:HA	1:B:483:ARG:HH11	1.62	0.63
1:B:643:ILE:HD12	1:B:915:PHE:HZ	1.62	0.63
1:B:974:UNK:CG	1:B:977:UNK:HB1	2.29	0.63
1:B:2176:LEU:HG	1:B:2180:LYS:HE3	1.80	0.63
1:C:360:LEU:HD12	1:C:363:LEU:HD23	1.80	0.63
1:A:2080:UNK:HG2	1:A:2083:UNK:HG3	1.79	0.63
1:A:2422:UNK:HG2	1:A:2422:UNK:O	1.98	0.63
1:C:1214:UNK:HB1	1:C:1320:VAL:HB	1.80	0.63
1:C:2252:VAL:HA	1:C:2255:ARG:HE	1.62	0.63
1:C:2428:UNK:O	1:C:2428:UNK:HG2	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1072:TRP:NE1	1:A:1077:VAL:HG22	2.14	0.63
1:A:2092:UNK:HA	1:A:2189:PHE:HB2	1.81	0.63
1:B:2297:ARG:HD3	1:B:2297:ARG:H	1.64	0.63
1:C:1072:TRP:NE1	1:C:1077:VAL:HG22	2.14	0.63
1:C:2094:UNK:CG	1:C:2096:UNK:CG	2.75	0.63
1:A:2135:UNK:HG3	1:A:2136:ASP:H	1.64	0.63
1:B:408:VAL:HG13	1:B:943:UNK:HG1	1.79	0.63
1:B:585:HIS:CD2	1:B:586:SER:H	2.17	0.63
1:B:1072:TRP:NE1	1:B:1077:VAL:HG22	2.14	0.63
1:B:1212:UNK:HG2	1:B:1212:UNK:O	1.99	0.63
1:B:2125:UNK:HA	1:B:2128:UNK:HG3	1.81	0.63
1:B:2652:ILE:HG12	1:B:2722:VAL:HG22	1.79	0.63
1:A:2948:GLN:HG2	1:A:2951:ARG:HH21	1.64	0.63
1:B:1215:UNK:HG2	1:B:1216:UNK:N	2.14	0.63
1:C:1212:UNK:HG2	1:C:1212:UNK:O	1.99	0.63
1:C:2092:UNK:O	1:C:2092:UNK:HG2	1.99	0.63
1:A:980:UNK:C	1:A:981:UNK:HG3	2.29	0.63
1:A:1212:UNK:HG2	1:A:1212:UNK:O	1.99	0.63
1:A:2047:THR:OG1	1:A:2205:ASP:OD2	2.17	0.63
1:A:2117:UNK:O	1:A:2121:UNK:HG3	1.98	0.63
1:B:360:LEU:HD12	1:B:363:LEU:HD23	1.80	0.63
1:B:2117:UNK:O	1:B:2121:UNK:HG3	1.98	0.63
1:A:360:LEU:HD12	1:A:363:LEU:HD23	1.80	0.63
1:A:803:GLU:OE1	1:A:2431:UNK:HG3	1.98	0.63
1:A:2173:ASP:OD2	1:A:2799:LYS:NZ	2.32	0.63
1:A:2297:ARG:H	1:A:2297:ARG:HD3	1.64	0.63
1:B:750:LEU:HD12	1:B:827:LEU:HD11	1.81	0.63
1:B:803:GLU:OE1	1:B:2431:UNK:HG3	1.98	0.63
1:B:1212:UNK:HG2	1:B:1342:ARG:HE	1.64	0.63
1:B:2047:THR:OG1	1:B:2205:ASP:OD2	2.17	0.63
1:A:750:LEU:HD12	1:A:827:LEU:HD11	1.81	0.62
1:A:1215:UNK:HG2	1:A:1216:UNK:N	2.14	0.62
1:A:1315:ARG:HH21	1:A:1323:GLU:HG2	1.64	0.62
1:A:1412:HIS:ND1	1:A:1415:GLY:O	2.26	0.62
1:A:2125:UNK:HA	1:A:2128:UNK:HG3	1.81	0.62
1:C:974:UNK:CG	1:C:977:UNK:HB1	2.29	0.62
1:C:1126:ILE:HG22	1:C:1196:UNK:HG1	1.81	0.62
1:C:1412:HIS:ND1	1:C:1415:GLY:O	2.26	0.62
1:C:2422:UNK:HG2	1:C:2422:UNK:O	1.98	0.62
1:A:664:LEU:HD13	1:A:701:ALA:HB1	1.81	0.62
1:B:34:LEU:O	1:B:38:LEU:N	2.25	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:980:UNK:C	1:B:981:UNK:HG3	2.29	0.62
1:B:1126:ILE:HG22	1:B:1196:UNK:HG1	1.81	0.62
1:B:2422:UNK:O	1:B:2422:UNK:HG2	1.98	0.62
1:C:1376:VAL:HA	1:C:1470:LEU:HD13	1.81	0.62
1:C:2117:UNK:O	1:C:2121:UNK:HG3	1.98	0.62
1:A:2092:UNK:O	1:A:2092:UNK:HG2	1.99	0.62
1:B:664:LEU:HD13	1:B:701:ALA:HB1	1.81	0.62
1:B:1002:UNK:O	1:B:1003:UNK:CG	2.47	0.62
1:B:1214:UNK:HB1	1:B:1320:VAL:HB	1.80	0.62
1:C:56:LEU:HD22	1:C:119:LEU:HD13	1.79	0.62
1:C:2176:LEU:HG	1:C:2180:LYS:HE3	1.80	0.62
1:A:2449:UNK:O	1:A:2449:UNK:HG2	1.98	0.62
1:B:892:ILE:HG22	2:B:4000:FMN:HM82	1.80	0.62
1:B:1376:VAL:HA	1:B:1470:LEU:HD13	1.81	0.62
1:C:585:HIS:CD2	1:C:586:SER:H	2.17	0.62
1:C:1095:LEU:HD12	1:C:1096:THR:H	1.64	0.62
1:C:1212:UNK:HG2	1:C:1342:ARG:HE	1.64	0.62
1:A:500:GLN:O	1:A:504:LYS:N	2.24	0.62
1:A:1376:VAL:HA	1:A:1470:LEU:HD13	1.81	0.62
1:C:992:UNK:CG	1:C:994:UNK:HG2	2.29	0.62
1:A:585:HIS:CD2	1:A:586:SER:H	2.17	0.62
1:A:1622:PRO:HD3	1:A:1685:LEU:HD11	1.81	0.62
1:A:1702:GLU:OE2	1:A:1711:VAL:HG13	1.99	0.62
1:B:1702:GLU:OE2	1:B:1711:VAL:HG13	1.99	0.62
1:B:2173:ASP:OD2	1:B:2799:LYS:NZ	2.32	0.62
1:B:2765:GLY:HA2	1:B:2940:VAL:HG21	1.82	0.62
1:C:792:ALA:O	1:C:2433:UNK:HG2	1.96	0.62
1:C:2765:GLY:HA2	1:C:2940:VAL:HG21	1.82	0.62
1:A:992:UNK:CG	1:A:994:UNK:HG2	2.29	0.62
1:B:415:VAL:HG22	1:B:937:UNK:HG1	1.81	0.62
1:B:792:ALA:O	1:B:2433:UNK:HG2	1.96	0.62
1:B:975:UNK:HG3	1:B:993:UNK:CB	2.29	0.62
1:B:1353:PRO:HG3	1:B:1702:GLU:OE2	2.00	0.62
1:B:1725:SER:HB3	1:C:260:LEU:HD13	1.82	0.62
1:B:2237:LEU:HB2	1:B:2287:LEU:HD11	1.82	0.62
1:C:1215:UNK:HG2	1:C:1216:UNK:N	2.14	0.62
1:A:1002:UNK:O	1:A:1003:UNK:CG	2.47	0.62
1:A:1095:LEU:HD12	1:A:1096:THR:H	1.64	0.62
1:B:2092:UNK:HA	1:B:2189:PHE:HB2	1.81	0.62
1:C:164:ALA:HA	1:C:178:LEU:HD13	1.82	0.62
1:C:980:UNK:C	1:C:981:UNK:HG3	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2096:UNK:HG2	1:C:2097:UNK:N	2.14	0.62
1:A:238:SER:OG	1:A:249:THR:OG1	2.16	0.62
1:A:1002:UNK:O	1:A:1002:UNK:HG2	1.99	0.62
1:B:992:UNK:HG3	1:B:996:UNK:HG3	1.66	0.62
1:B:2096:UNK:HG2	1:B:2097:UNK:N	2.14	0.62
1:C:415:VAL:HG22	1:C:937:UNK:HG1	1.81	0.62
1:B:2948:GLN:HG2	1:B:2951:ARG:HH21	1.64	0.61
1:C:203:ASP:O	1:C:205:PRO:HD3	2.00	0.61
1:C:664:LEU:HD13	1:C:701:ALA:HB1	1.81	0.61
1:C:975:UNK:HG3	1:C:993:UNK:CB	2.29	0.61
1:C:1431:ALA:HB3	1:C:1459:THR:HG21	1.82	0.61
1:C:1702:GLU:OE2	1:C:1711:VAL:HG13	1.99	0.61
1:C:2047:THR:OG1	1:C:2205:ASP:OD2	2.17	0.61
1:C:2092:UNK:HA	1:C:2189:PHE:HB2	1.81	0.61
1:C:2297:ARG:H	1:C:2297:ARG:HD3	1.64	0.61
1:C:2948:GLN:HG2	1:C:2951:ARG:HH21	1.64	0.61
1:A:511:ARG:HH11	1:A:543:GLY:HA3	1.65	0.61
1:A:793:ARG:HD3	1:A:2435:UNK:CG	2.27	0.61
1:A:2122:UNK:C	1:A:2125:UNK:HG3	2.30	0.61
1:A:3080:ARG:HG3	1:A:3080:ARG:NH1	2.09	0.61
1:B:409:LYS:HD2	1:B:933:UNK:HA	1.82	0.61
1:B:575:HIS:HD2	1:B:644:LEU:HD22	1.66	0.61
1:B:939:UNK:O	1:B:940:UNK:CG	2.47	0.61
1:B:971:ALA:O	1:B:974:UNK:CG	2.48	0.61
1:C:575:HIS:HD2	1:C:644:LEU:HD22	1.66	0.61
1:C:1622:PRO:HD3	1:C:1685:LEU:HD11	1.81	0.61
1:C:2125:UNK:HA	1:C:2128:UNK:HG3	1.81	0.61
1:A:939:UNK:O	1:A:940:UNK:CG	2.47	0.61
1:B:511:ARG:HH11	1:B:543:GLY:HA3	1.66	0.61
1:B:984:UNK:CG	1:B:987:UNK:CG	2.79	0.61
1:B:2092:UNK:HG2	1:B:2092:UNK:O	1.99	0.61
1:C:34:LEU:H	1:C:393:VAL:HG21	1.65	0.61
1:C:970:ILE:CG1	1:C:996:UNK:HG1	2.31	0.61
1:C:2103:UNK:HG1	1:C:2919:GLY:O	2.00	0.61
1:A:415:VAL:CG2	1:A:937:UNK:HG1	2.31	0.61
1:A:976:UNK:O	1:A:976:UNK:HG2	2.01	0.61
1:A:1725:SER:HB3	1:B:260:LEU:HD13	1.82	0.61
1:B:415:VAL:CG2	1:B:937:UNK:HG1	2.31	0.61
1:C:892:ILE:HG22	2:C:4000:FMN:HM82	1.80	0.61
1:C:1002:UNK:O	1:C:1003:UNK:CG	2.47	0.61
1:C:2112:UNK:N	1:C:2115:UNK:HG1	2.11	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2434:UNK:CG	1:C:2523:GLU:O	2.48	0.61
1:A:164:ALA:HA	1:A:178:LEU:HD13	1.82	0.61
1:B:34:LEU:H	1:B:393:VAL:HG21	1.65	0.61
1:B:106:ALA:HB1	1:B:112:PRO:HB2	1.82	0.61
1:B:929:UNK:O	1:B:930:UNK:CG	2.45	0.61
1:B:1622:PRO:HD3	1:B:1685:LEU:HD11	1.81	0.61
1:A:260:LEU:HD13	1:C:1725:SER:HB3	1.82	0.61
1:A:409:LYS:HD2	1:A:933:UNK:HA	1.82	0.61
1:A:415:VAL:HG22	1:A:937:UNK:HG1	1.81	0.61
1:A:575:HIS:HD2	1:A:644:LEU:HD22	1.66	0.61
1:A:984:UNK:HG2	1:A:987:UNK:CG	2.31	0.61
1:A:1431:ALA:HB3	1:A:1459:THR:HG21	1.82	0.61
1:A:2176:LEU:HG	1:A:2180:LYS:HE3	1.80	0.61
1:A:2469:LEU:HD11	1:A:2653:VAL:HB	1.82	0.61
1:B:2469:LEU:HD11	1:B:2653:VAL:HB	1.82	0.61
1:C:409:LYS:HD2	1:C:933:UNK:HA	1.82	0.61
1:C:971:ALA:O	1:C:974:UNK:CG	2.48	0.61
1:C:984:UNK:HG2	1:C:987:UNK:CG	2.31	0.61
1:C:1227:UNK:O	1:C:1227:UNK:HG2	2.00	0.61
1:A:929:UNK:O	1:A:930:UNK:CG	2.45	0.61
1:A:1126:ILE:HG22	1:A:1196:UNK:HG1	1.81	0.61
1:A:1353:PRO:HG3	1:A:1702:GLU:OE2	2.00	0.61
1:B:2122:UNK:C	1:B:2125:UNK:HG3	2.30	0.61
1:B:2135:UNK:HG3	1:B:2136:ASP:H	1.64	0.61
1:C:34:LEU:O	1:C:38:LEU:N	2.25	0.61
1:C:511:ARG:HH11	1:C:543:GLY:HA3	1.66	0.61
1:C:2469:LEU:HD11	1:C:2653:VAL:HB	1.82	0.61
1:C:3058:ARG:HB2	1:C:3089:LEU:HB2	1.82	0.61
1:A:106:ALA:HB1	1:A:112:PRO:HB2	1.82	0.61
1:A:580:ARG:HG2	1:A:590:LEU:HD21	1.83	0.61
1:A:1212:UNK:HG2	1:A:1342:ARG:HE	1.64	0.61
1:A:2103:UNK:HG1	1:A:2919:GLY:O	2.00	0.61
1:B:70:SER:HG	1:B:142:ARG:HH22	1.49	0.61
1:B:126:VAL:HG12	1:B:182:ALA:HB1	1.83	0.61
1:B:1007:UNK:HB2	1:B:1018:ARG:HE	1.66	0.61
1:B:1227:UNK:HG2	1:B:1227:UNK:O	2.00	0.61
1:B:1431:ALA:HB3	1:B:1459:THR:HG21	1.82	0.61
1:C:415:VAL:CG2	1:C:937:UNK:HG1	2.31	0.61
1:C:750:LEU:HD12	1:C:827:LEU:HD11	1.81	0.61
1:C:1353:PRO:HG3	1:C:1702:GLU:OE2	2.00	0.61
1:B:979:UNK:O	1:B:979:UNK:HG2	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:984:UNK:HG2	1:B:987:UNK:CG	2.31	0.61
1:B:2334:HIS:HD2	1:B:2391:LYS:HG3	1.66	0.61
1:B:2434:UNK:CG	1:B:2523:GLU:O	2.48	0.61
1:C:488:ASN:HA	1:C:521:VAL:HB	1.83	0.61
1:C:1007:UNK:HG2	1:C:1007:UNK:O	2.01	0.61
1:A:680:ALA:HA	1:A:685:ALA:HB2	1.83	0.61
1:A:984:UNK:CG	1:A:987:UNK:CG	2.79	0.61
1:A:1007:UNK:O	1:A:1007:UNK:HG2	2.01	0.61
1:A:1227:UNK:O	1:A:1227:UNK:HG2	2.00	0.61
1:B:970:ILE:CG1	1:B:996:UNK:HG1	2.31	0.61
1:B:3058:ARG:HB2	1:B:3089:LEU:HB2	1.82	0.61
1:C:1315:ARG:HH21	1:C:1323:GLU:HG2	1.64	0.61
1:A:34:LEU:H	1:A:393:VAL:HG21	1.65	0.60
1:A:970:ILE:CG1	1:A:996:UNK:HG1	2.31	0.60
1:A:980:UNK:HB2	1:A:989:UNK:HB2	1.83	0.60
1:A:2765:GLY:HA2	1:A:2940:VAL:HG21	1.82	0.60
1:B:438:THR:HA	1:B:880:HIS:HE1	1.66	0.60
1:B:1095:LEU:HD12	1:B:1096:THR:H	1.64	0.60
1:C:984:UNK:CG	1:C:987:UNK:CG	2.79	0.60
1:C:2173:ASP:OD2	1:C:2799:LYS:NZ	2.32	0.60
1:A:257:ARG:HH12	1:C:1695:LEU:CD2	2.13	0.60
1:A:1007:UNK:HB2	1:A:1018:ARG:HE	1.66	0.60
1:A:2096:UNK:HG2	1:A:2097:UNK:N	2.14	0.60
1:A:2647:VAL:HA	1:A:2650:TRP:HD1	1.66	0.60
1:B:488:ASN:HA	1:B:521:VAL:HB	1.83	0.60
1:B:1315:ARG:HH21	1:B:1323:GLU:HG2	1.64	0.60
1:C:238:SER:OG	1:C:249:THR:OG1	2.15	0.60
1:C:580:ARG:HG2	1:C:590:LEU:HD21	1.83	0.60
1:C:980:UNK:HB2	1:C:989:UNK:HB2	1.83	0.60
1:C:1532:ILE:HA	1:C:1544:ILE:HG12	1.83	0.60
1:C:2237:LEU:HB2	1:C:2287:LEU:HD11	1.82	0.60
1:A:203:ASP:O	1:A:205:PRO:HD3	2.01	0.60
1:A:1989:PHE:HD1	1:A:1992:LYS:HZ3	1.49	0.60
1:A:2112:UNK:CG	1:A:2114:UNK:HG3	2.31	0.60
1:A:2237:LEU:HB2	1:A:2287:LEU:HD11	1.82	0.60
1:A:2372:MET:HB3	1:A:2394:LEU:HD22	1.83	0.60
1:A:2434:UNK:CG	1:A:2523:GLU:O	2.48	0.60
1:B:1098:VAL:HG12	1:B:1100:ASP:H	1.66	0.60
1:C:2800:PHE:HE1	1:C:2812:LEU:HD22	1.67	0.60
1:A:438:THR:HA	1:A:880:HIS:HE1	1.66	0.60
1:A:971:ALA:O	1:A:974:UNK:CG	2.48	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:979:UNK:HG2	1:A:979:UNK:O	2.01	0.60
1:A:1537:LEU:HB2	1:A:1541:GLN:H	1.67	0.60
1:A:2121:UNK:C	1:A:2124:UNK:HG3	2.31	0.60
1:B:164:ALA:HA	1:B:178:LEU:HD13	1.82	0.60
1:B:203:ASP:O	1:B:205:PRO:HD3	2.01	0.60
1:B:680:ALA:HA	1:B:685:ALA:HB2	1.83	0.60
1:B:1002:UNK:O	1:B:1002:UNK:HG2	2.00	0.60
1:B:2121:UNK:C	1:B:2124:UNK:HG3	2.31	0.60
1:C:1537:LEU:HB2	1:C:1541:GLN:H	1.67	0.60
1:C:2112:UNK:CG	1:C:2114:UNK:HG3	2.31	0.60
1:C:2686:MET:HE1	1:C:2935:LYS:HG3	1.83	0.60
1:A:2121:UNK:O	1:A:2124:UNK:CG	2.49	0.60
1:B:1695:LEU:CD2	1:C:257:ARG:HH12	2.13	0.60
1:B:2103:UNK:HG1	1:B:2919:GLY:O	2.00	0.60
1:B:2212:TRP:HA	1:B:2229:LYS:HD3	1.83	0.60
1:C:126:VAL:HG12	1:C:182:ALA:HB1	1.83	0.60
1:C:929:UNK:O	1:C:930:UNK:CG	2.45	0.60
1:C:2212:TRP:HA	1:C:2229:LYS:HD3	1.83	0.60
1:C:2962:ASP:OD1	1:C:2962:ASP:N	2.34	0.60
1:A:488:ASN:HA	1:A:521:VAL:HB	1.83	0.60
1:A:2651:ASN:HD22	1:A:2718:VAL:HG12	1.67	0.60
1:A:3058:ARG:HB2	1:A:3089:LEU:HB2	1.82	0.60
1:B:1012:UNK:C	1:B:1013:UNK:HG3	2.32	0.60
1:A:1309:VAL:HG22	1:A:1331:ILE:HG12	1.84	0.60
1:A:1695:LEU:CD2	1:B:257:ARG:HH12	2.13	0.60
1:A:2334:HIS:HD2	1:A:2391:LYS:HG3	1.66	0.60
1:B:670:GLY:O	1:B:682:ASN:ND2	2.35	0.60
1:B:687:GLY:O	1:B:695:ILE:N	2.34	0.60
1:B:688:ARG:O	1:B:872:ARG:NE	2.34	0.60
1:B:2651:ASN:HD22	1:B:2718:VAL:HG12	1.67	0.60
1:C:976:UNK:HG2	1:C:976:UNK:O	2.01	0.60
1:C:2135:UNK:HG3	1:C:2136:ASP:H	1.64	0.60
1:A:670:GLY:O	1:A:682:ASN:ND2	2.35	0.60
1:A:931:UNK:O	1:A:934:UNK:HG3	2.02	0.60
1:A:975:UNK:HG3	1:A:993:UNK:CB	2.29	0.60
1:B:580:ARG:HG2	1:B:590:LEU:HD21	1.83	0.60
1:B:1435:VAL:HG11	1:B:1463:CYS:HB3	1.84	0.60
1:B:2112:UNK:CG	1:B:2114:UNK:HG3	2.31	0.60
1:B:2647:VAL:HA	1:B:2650:TRP:HD1	1.66	0.60
1:C:1002:UNK:O	1:C:1002:UNK:HG2	1.99	0.60
1:C:1098:VAL:HG12	1:C:1100:ASP:H	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2081:UNK:O	1:C:2085:UNK:HG2	2.02	0.60
1:C:2461:VAL:HG11	1:C:2751:VAL:HG22	1.84	0.60
1:C:2651:ASN:HD22	1:C:2718:VAL:HG12	1.67	0.60
1:A:126:VAL:HG12	1:A:182:ALA:HB1	1.83	0.60
1:A:1532:ILE:HA	1:A:1544:ILE:HG12	1.83	0.60
1:A:2081:UNK:O	1:A:2085:UNK:HG2	2.02	0.60
1:B:931:UNK:O	1:B:934:UNK:HG3	2.02	0.60
1:B:1537:LEU:HB2	1:B:1541:GLN:H	1.67	0.60
1:C:670:GLY:O	1:C:682:ASN:ND2	2.35	0.60
1:C:688:ARG:O	1:C:872:ARG:NE	2.34	0.60
1:C:939:UNK:O	1:C:940:UNK:CG	2.47	0.60
1:C:1007:UNK:HB2	1:C:1018:ARG:HE	1.66	0.60
1:C:2121:UNK:O	1:C:2124:UNK:CG	2.49	0.60
1:C:2122:UNK:C	1:C:2125:UNK:HG3	2.30	0.60
1:C:2334:HIS:HD2	1:C:2391:LYS:HG3	1.66	0.60
1:A:1012:UNK:C	1:A:1013:UNK:HG3	2.32	0.59
1:B:1532:ILE:HA	1:B:1544:ILE:HG12	1.83	0.59
1:C:410:LEU:HB3	1:C:1025:VAL:HG21	1.84	0.59
1:C:1435:VAL:HG11	1:C:1463:CYS:HB3	1.84	0.59
1:C:2121:UNK:C	1:C:2124:UNK:HG3	2.31	0.59
1:A:410:LEU:HB3	1:A:1025:VAL:HG21	1.84	0.59
1:B:1656:LYS:HG2	1:B:1660:LEU:HG	1.85	0.59
1:B:1989:PHE:HD1	1:B:1992:LYS:HZ3	1.50	0.59
1:B:2081:UNK:O	1:B:2085:UNK:HG2	2.02	0.59
1:B:2121:UNK:O	1:B:2124:UNK:CG	2.49	0.59
1:B:2372:MET:HB3	1:B:2394:LEU:HD22	1.83	0.59
1:C:680:ALA:HA	1:C:685:ALA:HB2	1.83	0.59
1:C:2056:PHE:HZ	1:C:2180:LYS:HE2	1.67	0.59
1:C:2429:UNK:O	1:C:2429:UNK:HG2	2.02	0.59
1:A:2431:UNK:O	1:A:2431:UNK:HG2	2.01	0.59
1:B:795:HIS:HB3	1:B:799:PHE:CZ	2.37	0.59
1:C:106:ALA:HB1	1:C:112:PRO:HB2	1.82	0.59
1:C:2431:UNK:HG2	1:C:2431:UNK:O	2.01	0.59
1:C:2712:GLU:HA	1:C:2717:VAL:HG11	1.83	0.59
1:A:795:HIS:HB3	1:A:799:PHE:CZ	2.37	0.59
1:A:1098:VAL:HG12	1:A:1100:ASP:H	1.66	0.59
1:A:2800:PHE:HE1	1:A:2812:LEU:HD22	1.67	0.59
1:A:2820:ILE:HD13	1:A:2943:MET:HG2	1.84	0.59
1:B:1002:UNK:C	1:B:1003:UNK:HG3	2.33	0.59
1:A:688:ARG:O	1:A:872:ARG:NE	2.34	0.59
1:A:2056:PHE:HZ	1:A:2180:LYS:HE2	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2667:THR:HG21	1:B:3058:ARG:NH1	2.17	0.59
1:C:1336:VAL:HG12	1:C:1337:MET:HG3	1.85	0.59
1:C:2372:MET:HB3	1:C:2394:LEU:HD22	1.83	0.59
1:A:2212:TRP:HA	1:A:2229:LYS:HD3	1.83	0.59
1:B:793:ARG:HD3	1:B:2435:UNK:CG	2.27	0.59
1:B:976:UNK:O	1:B:976:UNK:HG2	2.01	0.59
1:B:980:UNK:HB2	1:B:989:UNK:HB2	1.83	0.59
1:C:931:UNK:O	1:C:934:UNK:HG3	2.02	0.59
1:C:2889:ILE:HG12	1:C:2922:LEU:HB3	1.84	0.59
1:B:2431:UNK:O	1:B:2431:UNK:HG2	2.01	0.59
1:A:1656:LYS:HG2	1:A:1660:LEU:HG	1.85	0.59
1:A:2667:THR:HG21	1:A:3058:ARG:NH1	2.17	0.59
1:A:2686:MET:HE1	1:A:2935:LYS:HG3	1.83	0.59
1:A:2693:GLN:O	1:A:2697:HIS:ND1	2.33	0.59
1:A:2712:GLU:HA	1:A:2717:VAL:HG11	1.83	0.59
1:B:992:UNK:CG	1:B:994:UNK:HG2	2.30	0.59
1:B:1007:UNK:HG2	1:B:1007:UNK:O	2.01	0.59
1:C:1701:VAL:HG22	1:C:1732:LEU:HB2	1.84	0.59
1:A:2094:UNK:CG	1:A:2096:UNK:CG	2.75	0.59
1:B:1336:VAL:HG12	1:B:1337:MET:HG3	1.85	0.59
1:B:2056:PHE:HZ	1:B:2180:LYS:HE2	1.67	0.59
1:B:2403:ILE:HG23	1:B:2408:LEU:HD12	1.85	0.59
1:B:2461:VAL:HG11	1:B:2751:VAL:HG22	1.84	0.59
1:C:1616:PRO:HG3	1:C:1668:LEU:HD13	1.85	0.59
1:C:2135:UNK:CG	1:C:2136:ASP:N	2.66	0.59
1:C:2647:VAL:HA	1:C:2650:TRP:HD1	1.66	0.59
1:A:150:THR:O	1:A:152:PRO:HD3	2.03	0.59
1:A:943:UNK:C	1:A:944:UNK:HG3	2.32	0.59
1:B:934:UNK:C	1:B:937:UNK:HG3	2.32	0.59
1:B:2800:PHE:HE1	1:B:2812:LEU:HD22	1.67	0.59
1:C:1309:VAL:HG22	1:C:1331:ILE:HG12	1.84	0.59
1:B:462:GLN:HG3	1:B:468:PHE:HD1	1.68	0.58
1:B:2686:MET:HE1	1:B:2935:LYS:HG3	1.83	0.58
1:C:836:VAL:HG12	1:C:837:VAL:H	1.67	0.58
1:C:979:UNK:HG2	1:C:979:UNK:O	2.01	0.58
1:C:2124:UNK:O	1:C:2127:UNK:CG	2.51	0.58
1:A:1001:UNK:C	1:A:1002:UNK:HG3	2.33	0.58
1:A:1336:VAL:HG12	1:A:1337:MET:HG3	1.85	0.58
1:A:1616:PRO:HG3	1:A:1668:LEU:HD13	1.85	0.58
1:C:438:THR:HA	1:C:880:HIS:HE1	1.66	0.58
1:C:943:UNK:C	1:C:944:UNK:HG3	2.32	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1012:UNK:C	1:C:1013:UNK:HG3	2.32	0.58
1:A:2429:UNK:O	1:A:2429:UNK:HG2	2.02	0.58
1:A:2889:ILE:HG12	1:A:2922:LEU:HB3	1.84	0.58
1:B:1001:UNK:C	1:B:1002:UNK:HG3	2.33	0.58
1:B:1008:UNK:CG	1:B:1019:PHE:HB3	2.33	0.58
1:B:1327:VAL:HB	1:B:1339:ALA:HB3	1.86	0.58
1:B:1701:VAL:HG22	1:B:1732:LEU:HB2	1.84	0.58
1:C:150:THR:O	1:C:152:PRO:HD3	2.03	0.58
1:C:621:SER:OG	1:C:643:ILE:HD13	2.04	0.58
1:C:1001:UNK:C	1:C:1002:UNK:HG3	2.33	0.58
1:A:735:LYS:HD2	1:A:860:VAL:HG23	1.86	0.58
1:A:1008:UNK:O	1:A:1008:UNK:HG2	2.03	0.58
1:B:1253:ARG:HG3	1:B:1253:ARG:NH1	2.18	0.58
1:B:2712:GLU:HA	1:B:2717:VAL:HG11	1.84	0.58
1:C:795:HIS:HB3	1:C:799:PHE:CZ	2.37	0.58
1:C:990:UNK:CG	1:C:998:UNK:HB2	2.34	0.58
1:A:1008:UNK:CG	1:A:1019:PHE:HB3	2.33	0.58
1:A:1327:VAL:HB	1:A:1339:ALA:HB3	1.86	0.58
1:A:2461:VAL:HG11	1:A:2751:VAL:HG22	1.84	0.58
1:C:1253:ARG:HG3	1:C:1253:ARG:NH1	2.18	0.58
1:C:2667:THR:HG21	1:C:3058:ARG:NH1	2.17	0.58
1:A:1701:VAL:HG22	1:A:1732:LEU:HB2	1.84	0.58
1:A:2124:UNK:C	1:A:2127:UNK:HG3	2.34	0.58
1:B:836:VAL:HG12	1:B:837:VAL:H	1.67	0.58
1:C:2521:VAL:HG13	1:C:2529:ARG:HH11	1.68	0.58
1:A:117:LYS:NZ	1:C:1087:PHE:HB3	2.18	0.58
1:A:836:VAL:HG12	1:A:837:VAL:H	1.67	0.58
1:B:1008:UNK:O	1:B:1008:UNK:HG2	2.03	0.58
1:B:1616:PRO:HG3	1:B:1668:LEU:HD13	1.85	0.58
1:B:2487:LEU:HD11	1:B:2495:LEU:HD12	1.86	0.58
1:B:2787:THR:HA	1:B:2790:MET:HG3	1.86	0.58
1:B:2876:LEU:HB3	1:B:2881:VAL:HG12	1.86	0.58
1:C:687:GLY:O	1:C:695:ILE:N	2.34	0.58
1:C:1989:PHE:HD1	1:C:1992:LYS:HZ3	1.51	0.58
1:A:441:ASP:OD2	1:A:443:LYS:HB3	2.04	0.58
1:A:511:ARG:HD2	1:A:517:ILE:O	2.04	0.58
1:A:784:GLU:OE2	1:A:787:LEU:HD12	2.04	0.58
1:A:2101:UNK:O	1:A:2105:UNK:HG3	2.04	0.58
1:B:410:LEU:HB3	1:B:1025:VAL:HG21	1.84	0.58
1:B:970:ILE:CD1	1:B:996:UNK:HG1	2.34	0.58
1:C:970:ILE:CD1	1:C:996:UNK:HG1	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1656:LYS:HG2	1:C:1660:LEU:HG	1.85	0.58
1:A:2487:LEU:HD11	1:A:2495:LEU:HD12	1.86	0.58
1:B:776:ASP:O	1:B:779:TRP:N	2.31	0.58
1:B:990:UNK:CG	1:B:998:UNK:HB2	2.34	0.58
1:B:2339:TRP:HB2	1:B:2398:LEU:HD11	1.86	0.58
1:B:2820:ILE:HD13	1:B:2943:MET:HG2	1.84	0.58
1:A:2521:VAL:HG13	1:A:2529:ARG:HH11	1.68	0.58
1:A:2554:ALA:HB1	1:A:2614:LYS:NZ	2.19	0.58
1:A:2787:THR:HA	1:A:2790:MET:HG3	1.86	0.58
1:B:784:GLU:OE2	1:B:787:LEU:HD12	2.03	0.58
1:B:943:UNK:C	1:B:944:UNK:HG3	2.32	0.58
1:B:1309:VAL:HG22	1:B:1331:ILE:HG12	1.84	0.58
1:A:462:GLN:HG3	1:A:468:PHE:HD1	1.68	0.57
1:A:1091:LEU:HD13	1:A:1281:ALA:HB3	1.86	0.57
1:A:1435:VAL:HG11	1:A:1463:CYS:HB3	1.84	0.57
1:B:1412:HIS:ND1	1:B:1415:GLY:O	2.26	0.57
1:C:441:ASP:OD2	1:C:443:LYS:HB3	2.04	0.57
1:C:1008:UNK:HG2	1:C:1008:UNK:O	2.03	0.57
1:C:2403:ILE:HG23	1:C:2408:LEU:HD12	1.85	0.57
1:A:476:GLU:HA	1:A:479:LEU:HB2	1.86	0.57
1:A:924:LEU:HA	1:A:928:ALA:HB3	1.87	0.57
1:A:999:UNK:CG	1:A:1007:UNK:HG2	2.34	0.57
1:A:1002:UNK:C	1:A:1003:UNK:HG3	2.33	0.57
1:A:1087:PHE:HB3	1:B:117:LYS:NZ	2.18	0.57
1:B:1009:UNK:O	1:B:1009:UNK:HG2	2.04	0.57
1:B:1095:LEU:HD22	1:B:1289:PRO:HA	1.85	0.57
1:B:1226:UNK:HG3	1:B:1313:VAL:CG1	2.35	0.57
1:B:2124:UNK:C	1:B:2127:UNK:HG3	2.34	0.57
1:C:1002:UNK:C	1:C:1003:UNK:HG3	2.33	0.57
1:C:2101:UNK:O	1:C:2105:UNK:HG3	2.04	0.57
1:C:2487:LEU:HD11	1:C:2495:LEU:HD12	1.86	0.57
1:A:1095:LEU:HD22	1:A:1289:PRO:HA	1.85	0.57
1:A:2339:TRP:HB2	1:A:2398:LEU:HD11	1.86	0.57
1:B:621:SER:OG	1:B:643:ILE:HD13	2.04	0.57
1:B:2101:UNK:O	1:B:2105:UNK:HG3	2.04	0.57
1:C:934:UNK:C	1:C:937:UNK:HG3	2.32	0.57
1:C:2339:TRP:HB2	1:C:2398:LEU:HD11	1.86	0.57
1:C:2554:ALA:HB1	1:C:2614:LYS:NZ	2.19	0.57
1:A:621:SER:OG	1:A:643:ILE:HD13	2.04	0.57
1:A:939:UNK:C	1:A:940:UNK:HG3	2.33	0.57
1:A:990:UNK:CG	1:A:998:UNK:HB2	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1405:ALA:HB3	1:A:1408:VAL:HG23	1.86	0.57
1:B:1087:PHE:HB3	1:C:117:LYS:NZ	2.19	0.57
1:C:129:VAL:HG13	1:C:356:PRO:HG2	1.85	0.57
1:C:511:ARG:HD2	1:C:517:ILE:O	2.04	0.57
1:C:1017:ILE:HG23	1:C:1045:VAL:HG21	1.87	0.57
1:A:970:ILE:CD1	1:A:996:UNK:HG1	2.34	0.57
1:A:2124:UNK:O	1:A:2127:UNK:CG	2.51	0.57
1:B:129:VAL:HG13	1:B:356:PRO:HG2	1.85	0.57
1:B:924:LEU:HA	1:B:928:ALA:HB3	1.86	0.57
1:B:2521:VAL:HG13	1:B:2529:ARG:HH11	1.68	0.57
1:B:2889:ILE:HG12	1:B:2922:LEU:HB3	1.84	0.57
1:B:2983:LEU:HB3	1:B:2987:PHE:O	2.05	0.57
1:C:476:GLU:HA	1:C:479:LEU:HB2	1.86	0.57
1:C:490:LEU:HD23	1:C:523:SER:HB2	1.87	0.57
1:C:924:LEU:HA	1:C:928:ALA:HB3	1.87	0.57
1:C:999:UNK:CG	1:C:1007:UNK:HG2	2.34	0.57
1:C:1445:VAL:HG23	1:C:1448:ALA:HB2	1.87	0.57
1:C:2086:UNK:HA	1:C:2089:UNK:HG3	1.86	0.57
1:C:2124:UNK:C	1:C:2127:UNK:HG3	2.34	0.57
1:C:2820:ILE:HD13	1:C:2943:MET:HG2	1.84	0.57
1:C:2846:ALA:HA	1:C:3001:HIS:O	2.05	0.57
1:A:1009:UNK:O	1:A:1009:UNK:HG2	2.03	0.57
1:A:2709:ILE:O	1:A:2713:VAL:HG13	2.05	0.57
1:B:975:UNK:HG2	1:B:976:UNK:N	2.20	0.57
1:B:2429:UNK:HG2	1:B:2429:UNK:O	2.02	0.57
1:C:939:UNK:C	1:C:940:UNK:HG3	2.33	0.57
1:C:1008:UNK:CG	1:C:1019:PHE:HB3	2.33	0.57
1:C:1009:UNK:HG2	1:C:1009:UNK:O	2.04	0.57
1:C:1095:LEU:HD22	1:C:1289:PRO:HA	1.85	0.57
1:C:2622:GLY:HA2	1:C:2812:LEU:HD11	1.87	0.57
1:A:2403:ILE:HG23	1:A:2408:LEU:HD12	1.85	0.57
1:A:2846:ALA:HA	1:A:3001:HIS:O	2.05	0.57
1:B:1445:VAL:HG23	1:B:1448:ALA:HB2	1.87	0.57
1:B:2846:ALA:HA	1:B:3001:HIS:O	2.05	0.57
1:C:784:GLU:OE2	1:C:787:LEU:HD12	2.03	0.57
1:C:2876:LEU:HB3	1:C:2881:VAL:HG12	1.86	0.57
1:A:980:UNK:O	1:A:981:UNK:CG	2.53	0.57
1:A:1537:LEU:HD11	1:A:1714:LEU:HB3	1.87	0.57
1:A:2876:LEU:HB3	1:A:2881:VAL:HG12	1.86	0.57
1:B:441:ASP:OD2	1:B:443:LYS:HB3	2.04	0.57
1:B:735:LYS:HD2	1:B:860:VAL:HG23	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:978:UNK:HB2	1:B:991:UNK:HG2	1.87	0.57
1:B:2084:UNK:O	1:B:2087:UNK:CG	2.52	0.57
1:C:127:PRO:HG3	1:C:183:GLN:HA	1.86	0.57
1:C:929:UNK:C	1:C:930:UNK:HG3	2.35	0.57
1:C:1091:LEU:HD13	1:C:1281:ALA:HB3	1.86	0.57
1:B:127:PRO:HG3	1:B:183:GLN:HA	1.86	0.57
1:B:511:ARG:NH1	1:B:543:GLY:HA3	2.19	0.57
1:B:2100:UNK:CG	1:B:2101:UNK:N	2.68	0.57
1:C:462:GLN:HG3	1:C:468:PHE:HD1	1.68	0.57
1:B:868:ARG:HB3	1:B:872:ARG:HH11	1.70	0.57
1:B:2124:UNK:O	1:B:2127:UNK:CG	2.51	0.57
1:C:980:UNK:O	1:C:981:UNK:CG	2.53	0.57
1:C:2521:VAL:HG13	1:C:2529:ARG:NH1	2.20	0.57
1:C:2787:THR:HA	1:C:2790:MET:HG3	1.86	0.57
1:A:127:PRO:HG3	1:A:183:GLN:HA	1.85	0.56
1:A:129:VAL:HG13	1:A:356:PRO:HG2	1.85	0.56
1:A:511:ARG:NH1	1:A:543:GLY:HA3	2.19	0.56
1:A:868:ARG:HB3	1:A:872:ARG:HH11	1.70	0.56
1:B:1126:ILE:O	1:B:1197:UNK:CG	2.53	0.56
1:B:2961:LEU:HD23	1:B:2978:ARG:HB3	1.87	0.56
1:C:868:ARG:HB3	1:C:872:ARG:HH11	1.70	0.56
1:A:490:LEU:HD23	1:A:523:SER:HB2	1.87	0.56
1:C:735:LYS:HD2	1:C:860:VAL:HG23	1.85	0.56
1:C:793:ARG:HD3	1:C:2435:UNK:CG	2.27	0.56
1:A:37:ARG:O	1:A:41:GLY:N	2.38	0.56
1:A:745:THR:OG1	1:A:834:GLU:O	2.19	0.56
1:A:976:UNK:CG	1:A:993:UNK:HB1	2.29	0.56
1:A:2086:UNK:HA	1:A:2089:UNK:HG3	1.86	0.56
1:B:150:THR:O	1:B:152:PRO:HD3	2.03	0.56
1:B:476:GLU:HA	1:B:479:LEU:HB2	1.86	0.56
1:B:511:ARG:HD2	1:B:517:ILE:O	2.04	0.56
1:B:939:UNK:C	1:B:940:UNK:HG3	2.33	0.56
1:B:999:UNK:CG	1:B:1007:UNK:HG2	2.34	0.56
1:B:1001:UNK:O	1:B:1002:UNK:CG	2.53	0.56
1:B:1637:VAL:HG21	1:B:1671:TRP:CG	2.40	0.56
1:B:2481:MET:O	1:B:2959:ARG:NH2	2.39	0.56
1:B:2521:VAL:HG13	1:B:2529:ARG:NH1	2.20	0.56
1:B:2554:ALA:HB1	1:B:2614:LYS:NZ	2.19	0.56
1:B:2709:ILE:O	1:B:2713:VAL:HG13	2.05	0.56
1:C:177:GLU:HB3	1:C:317:LEU:HD13	1.87	0.56
1:C:1420:THR:OG1	1:C:1485:HIS:NE2	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1537:LEU:HD11	1:C:1714:LEU:HB3	1.86	0.56
1:A:776:ASP:O	1:A:779:TRP:N	2.31	0.56
1:A:978:UNK:HB2	1:A:991:UNK:HG2	1.87	0.56
1:A:1017:ILE:HG23	1:A:1045:VAL:HG21	1.87	0.56
1:A:1253:ARG:HG3	1:A:1253:ARG:NH1	2.18	0.56
1:A:2521:VAL:HG13	1:A:2529:ARG:NH1	2.20	0.56
1:A:2881:VAL:HG13	1:A:2885:ASP:HB2	1.88	0.56
1:B:177:GLU:HB3	1:B:317:LEU:HD13	1.87	0.56
1:B:1091:LEU:HD13	1:B:1281:ALA:HB3	1.86	0.56
1:C:511:ARG:NH1	1:C:543:GLY:HA3	2.19	0.56
1:C:1126:ILE:O	1:C:1197:UNK:CG	2.53	0.56
1:C:2957:PRO:HD3	1:C:2980:PRO:HB3	1.88	0.56
1:A:975:UNK:HG2	1:A:976:UNK:N	2.20	0.56
1:A:990:UNK:HG2	1:A:990:UNK:O	2.05	0.56
1:B:2622:GLY:HA2	1:B:2812:LEU:HD11	1.87	0.56
1:C:2693:GLN:O	1:C:2697:HIS:ND1	2.33	0.56
1:A:2983:LEU:HB3	1:A:2987:PHE:O	2.05	0.56
1:B:1511:ASP:H	1:B:1514:ASP:HB2	1.71	0.56
1:B:2962:ASP:OD1	1:B:2962:ASP:N	2.34	0.56
1:C:475:LEU:O	1:C:479:LEU:N	2.37	0.56
1:C:1327:VAL:HB	1:C:1339:ALA:HB3	1.86	0.56
1:C:1511:ASP:H	1:C:1514:ASP:HB2	1.71	0.56
1:A:1637:VAL:HG21	1:A:1671:TRP:CG	2.40	0.56
1:B:2478:ARG:NH1	1:B:2482:GLU:OE1	2.39	0.56
1:C:1226:UNK:HG3	1:C:1313:VAL:CG1	2.35	0.56
1:C:1637:VAL:HG21	1:C:1671:TRP:CG	2.40	0.56
1:C:2478:ARG:NH1	1:C:2482:GLU:OE1	2.39	0.56
1:A:1126:ILE:O	1:A:1197:UNK:CG	2.53	0.56
1:A:1226:UNK:HG3	1:A:1313:VAL:CG1	2.35	0.56
1:A:1511:ASP:H	1:A:1514:ASP:HB2	1.71	0.56
1:A:2478:ARG:NH1	1:A:2482:GLU:OE1	2.39	0.56
1:A:2961:LEU:HD23	1:A:2978:ARG:HB3	1.87	0.56
1:B:1537:LEU:HD11	1:B:1714:LEU:HB3	1.87	0.56
1:B:2086:UNK:HA	1:B:2089:UNK:HG3	1.86	0.56
1:B:2094:UNK:CG	1:B:2096:UNK:CG	2.75	0.56
1:C:978:UNK:HB2	1:C:991:UNK:HG2	1.87	0.56
1:C:992:UNK:CG	1:C:996:UNK:HG2	2.32	0.56
1:C:2084:UNK:O	1:C:2087:UNK:CG	2.52	0.56
1:C:2709:ILE:O	1:C:2713:VAL:HG13	2.05	0.56
1:C:2961:LEU:HD23	1:C:2978:ARG:HB3	1.87	0.56
1:C:2983:LEU:HB3	1:C:2987:PHE:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:GLY:O	1:A:695:ILE:N	2.34	0.56
1:A:2102:UNK:C	1:A:2105:UNK:HG3	2.36	0.56
1:B:490:LEU:HD23	1:B:523:SER:HB2	1.87	0.56
1:B:1017:ILE:HG23	1:B:1045:VAL:HG21	1.87	0.56
1:B:1618:LEU:HG	1:B:1619:VAL:HG23	1.88	0.56
1:C:1618:LEU:HG	1:C:1619:VAL:HG23	1.88	0.56
1:C:2102:UNK:C	1:C:2105:UNK:HG3	2.36	0.56
1:A:1445:VAL:HG23	1:A:1448:ALA:HB2	1.87	0.56
1:A:2084:UNK:O	1:A:2087:UNK:CG	2.52	0.56
1:B:990:UNK:O	1:B:990:UNK:HG2	2.05	0.56
1:B:1420:THR:OG1	1:B:1485:HIS:NE2	2.38	0.56
1:B:2303:ASP:N	1:B:2303:ASP:OD1	2.39	0.56
1:C:37:ARG:O	1:C:41:GLY:N	2.39	0.56
1:C:975:UNK:HG2	1:C:976:UNK:N	2.20	0.56
1:C:990:UNK:O	1:C:990:UNK:HG2	2.05	0.56
1:C:1405:ALA:HB3	1:C:1408:VAL:HG23	1.86	0.56
1:A:934:UNK:C	1:A:937:UNK:HG3	2.32	0.55
1:B:540:ASN:HD21	1:B:544:ILE:HG13	1.71	0.55
1:B:929:UNK:C	1:B:930:UNK:HG3	2.35	0.55
1:B:2743:ALA:HB3	1:B:2939:ALA:HB3	1.88	0.55
1:A:2481:MET:O	1:A:2959:ARG:NH2	2.39	0.55
1:A:2743:ALA:HB3	1:A:2939:ALA:HB3	1.88	0.55
1:B:1405:ALA:HB3	1:B:1408:VAL:HG23	1.87	0.55
1:A:929:UNK:C	1:A:930:UNK:HG3	2.35	0.55
1:A:1618:LEU:HG	1:A:1619:VAL:HG23	1.88	0.55
1:B:475:LEU:O	1:B:479:LEU:N	2.37	0.55
1:B:737:TYR:HE1	1:B:862:VAL:HA	1.72	0.55
1:B:931:UNK:HG2	1:B:934:UNK:N	2.21	0.55
1:B:2102:UNK:C	1:B:2105:UNK:HG3	2.36	0.55
1:A:2135:UNK:CG	1:A:2136:ASP:N	2.66	0.55
1:A:2622:GLY:HA2	1:A:2812:LEU:HD11	1.87	0.55
1:B:975:UNK:CG	1:B:976:UNK:N	2.70	0.55
1:B:980:UNK:O	1:B:981:UNK:CG	2.53	0.55
1:C:1496:SER:HB3	1:C:1578:ASP:HB3	1.89	0.55
1:C:2442:UNK:HG2	1:C:2442:UNK:O	2.07	0.55
1:C:2481:MET:O	1:C:2959:ARG:NH2	2.39	0.55
1:A:540:ASN:HD21	1:A:544:ILE:HG13	1.71	0.55
1:B:551:PRO:HG3	1:B:560:VAL:HG21	1.89	0.55
1:B:1010:UNK:O	1:B:1017:ILE:N	2.29	0.55
1:C:1010:UNK:O	1:C:1017:ILE:N	2.29	0.55
1:C:2881:VAL:HG13	1:C:2885:ASP:HB2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:HB3	1:A:317:LEU:HD13	1.87	0.55
1:B:2704:ALA:O	1:B:2705:LYS:HD3	2.07	0.55
1:A:931:UNK:HG2	1:A:933:UNK:CG	2.37	0.55
1:A:1690:GLU:O	1:A:1694:GLY:N	2.40	0.55
1:A:1734:SER:HA	1:A:1741:LEU:HD11	1.89	0.55
1:B:2458:ALA:HA	1:B:2824:ARG:HD2	1.89	0.55
1:C:2810:GLY:HA2	1:C:2896:THR:HA	1.89	0.55
1:A:737:TYR:HE1	1:A:862:VAL:HA	1.72	0.55
1:A:931:UNK:HG2	1:A:934:UNK:N	2.21	0.55
1:B:238:SER:OG	1:B:249:THR:OG1	2.15	0.55
1:B:1496:SER:HB3	1:B:1578:ASP:HB3	1.88	0.55
1:B:2135:UNK:CG	1:B:2136:ASP:N	2.66	0.55
1:B:2957:PRO:HD3	1:B:2980:PRO:HB3	1.88	0.55
1:C:737:TYR:HE1	1:C:862:VAL:HA	1.72	0.55
1:C:1690:GLU:O	1:C:1694:GLY:N	2.40	0.55
1:A:2087:UNK:CA	1:A:2090:UNK:HG3	2.37	0.55
1:A:2458:ALA:HA	1:A:2824:ARG:HD2	1.89	0.55
1:A:2704:ALA:O	1:A:2705:LYS:HD3	2.07	0.55
1:B:1724:TYR:OH	1:C:267:GLU:OE2	2.07	0.55
1:B:2418:GLY:O	1:B:2422:UNK:N	2.40	0.55
1:C:144:GLY:O	1:C:148:THR:N	2.34	0.55
1:C:994:UNK:CG	1:C:996:UNK:HG3	2.37	0.55
1:C:1001:UNK:O	1:C:1002:UNK:CG	2.53	0.55
1:A:1001:UNK:O	1:A:1002:UNK:CG	2.53	0.55
1:A:2418:GLY:O	1:A:2422:UNK:N	2.40	0.54
1:B:763:SER:O	1:B:766:ASP:N	2.41	0.54
1:B:1163:ASP:CB	1:B:1199:UNK:HG3	2.37	0.54
1:B:1690:GLU:O	1:B:1694:GLY:N	2.40	0.54
1:B:2442:UNK:O	1:B:2442:UNK:HG2	2.07	0.54
1:A:33:ALA:O	1:A:37:ARG:N	2.35	0.54
1:A:975:UNK:CG	1:A:976:UNK:N	2.70	0.54
1:A:2303:ASP:OD1	1:A:2303:ASP:N	2.39	0.54
1:A:2810:GLY:HA2	1:A:2896:THR:HA	1.89	0.54
1:B:2810:GLY:HA2	1:B:2896:THR:HA	1.89	0.54
1:C:540:ASN:HD21	1:C:544:ILE:HG13	1.71	0.54
1:C:975:UNK:CG	1:C:976:UNK:N	2.70	0.54
1:C:978:UNK:HB2	1:C:991:UNK:CG	2.37	0.54
1:A:2957:PRO:HD3	1:A:2980:PRO:HB3	1.88	0.54
1:C:931:UNK:HG2	1:C:934:UNK:N	2.21	0.54
1:C:2704:ALA:O	1:C:2705:LYS:HD3	2.07	0.54
1:A:1010:UNK:O	1:A:1017:ILE:N	2.29	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2417:SER:O	1:A:2421:ASP:N	2.40	0.54
1:B:2115:UNK:HA	1:B:2118:UNK:HG3	1.90	0.54
1:B:2881:VAL:HG13	1:B:2885:ASP:HB2	1.88	0.54
1:C:763:SER:O	1:C:766:ASP:N	2.41	0.54
1:C:931:UNK:HG2	1:C:933:UNK:CG	2.37	0.54
1:C:2743:ALA:HB3	1:C:2939:ALA:HB3	1.88	0.54
1:A:668:THR:OG1	1:A:698:ILE:HD11	2.08	0.54
1:A:3018:LEU:O	1:A:3022:GLU:HB2	2.08	0.54
1:B:2693:GLN:O	1:B:2697:HIS:ND1	2.33	0.54
1:C:2103:UNK:O	1:C:2106:UNK:HG3	2.08	0.54
1:C:2458:ALA:HA	1:C:2824:ARG:HD2	1.89	0.54
1:C:2860:ALA:HB1	1:C:3005:LEU:HD13	1.90	0.54
1:A:1496:SER:HB3	1:A:1578:ASP:HB3	1.89	0.54
1:B:580:ARG:HH11	1:B:614:GLY:HA3	1.72	0.54
1:C:273:ARG:HD2	1:C:282:VAL:HG12	1.90	0.54
1:C:580:ARG:HH11	1:C:614:GLY:HA3	1.73	0.54
1:C:716:ALA:HA	1:C:719:VAL:HG23	1.90	0.54
1:A:456:GLU:HG2	1:A:486:GLN:HE21	1.73	0.54
1:A:763:SER:O	1:A:766:ASP:N	2.41	0.54
1:A:2122:UNK:CA	1:A:2125:UNK:HG3	2.38	0.54
1:A:2246:ALA:C	1:A:2255:ARG:HH12	2.11	0.54
1:B:37:ARG:O	1:B:41:GLY:N	2.39	0.54
1:B:2768:ASP:OD2	1:B:2936:GLY:N	2.41	0.54
1:C:1003:UNK:CG	1:C:1004:UNK:N	2.53	0.54
1:C:1163:ASP:CB	1:C:1199:UNK:HG3	2.38	0.54
1:C:1357:ILE:HG13	1:C:1710:THR:HG21	1.89	0.54
1:C:2100:UNK:CG	1:C:2101:UNK:N	2.68	0.54
1:C:2115:UNK:HA	1:C:2118:UNK:HG3	1.90	0.54
1:C:2127:UNK:O	1:C:2130:UNK:CG	2.52	0.54
1:C:2418:GLY:O	1:C:2422:UNK:N	2.40	0.54
1:A:978:UNK:HB2	1:A:991:UNK:CG	2.37	0.54
1:A:1357:ILE:HG13	1:A:1710:THR:HG21	1.89	0.54
1:A:2112:UNK:N	1:A:2115:UNK:HG3	2.23	0.54
1:A:2492:VAL:HG21	1:A:2527:VAL:HG22	1.90	0.54
1:B:273:ARG:HD2	1:B:282:VAL:HG12	1.90	0.54
1:B:668:THR:OG1	1:B:698:ILE:HD11	2.08	0.54
1:B:978:UNK:HB2	1:B:991:UNK:CG	2.37	0.54
1:C:456:GLU:HG2	1:C:486:GLN:HE21	1.73	0.54
1:B:2104:UNK:HA	1:B:2107:UNK:HG3	1.90	0.54
1:C:33:ALA:O	1:C:37:ARG:N	2.35	0.54
1:C:3018:LEU:O	1:C:3022:GLU:HB2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:980:UNK:N	1:A:989:UNK:O	2.41	0.54
1:A:994:UNK:CG	1:A:996:UNK:HG3	2.37	0.54
1:A:2012:GLY:C	1:B:2591:ARG:NH1	2.61	0.54
1:B:624:TYR:HA	1:B:629:TRP:CD1	2.43	0.54
1:B:1734:SER:HA	1:B:1741:LEU:HD11	1.89	0.54
1:B:2100:UNK:C	1:B:2103:UNK:HG3	2.31	0.54
1:B:2860:ALA:HB1	1:B:3005:LEU:HD13	1.90	0.54
1:C:624:TYR:HA	1:C:629:TRP:CD1	2.43	0.54
1:C:2087:UNK:CA	1:C:2090:UNK:HG3	2.37	0.54
1:A:267:GLU:OE2	1:C:1724:TYR:OH	2.07	0.53
1:A:368:ILE:HG21	1:A:373:ILE:HG13	1.90	0.53
1:A:475:LEU:O	1:A:479:LEU:N	2.37	0.53
1:A:2100:UNK:CG	1:A:2101:UNK:N	2.68	0.53
1:A:2442:UNK:O	1:A:2442:UNK:HG2	2.07	0.53
1:B:456:GLU:HG2	1:B:486:GLN:HE21	1.73	0.53
1:B:1089:ALA:O	1:B:1091:LEU:N	2.41	0.53
1:B:2417:SER:O	1:B:2421:ASP:N	2.40	0.53
1:C:1323:GLU:N	1:C:1343:LEU:O	2.41	0.53
1:C:2551:PRO:O	1:C:2617:LEU:HB2	2.08	0.53
1:C:2653:VAL:HA	1:C:3051:MET:HE3	1.90	0.53
1:A:624:TYR:HA	1:A:629:TRP:CD1	2.43	0.53
1:A:1089:ALA:O	1:A:1091:LEU:N	2.42	0.53
1:B:2103:UNK:O	1:B:2106:UNK:HG3	2.08	0.53
1:B:2425:UNK:O	1:B:2425:UNK:HG2	2.09	0.53
1:B:2492:VAL:HG21	1:B:2527:VAL:HG22	1.90	0.53
1:C:33:ALA:O	1:C:37:ARG:HG2	2.08	0.53
1:C:551:PRO:HG3	1:C:560:VAL:HG21	1.89	0.53
1:C:992:UNK:HG2	1:C:994:UNK:HG2	1.87	0.53
1:C:999:UNK:HG3	1:C:1007:UNK:HG2	1.90	0.53
1:C:1734:SER:HA	1:C:1741:LEU:HD11	1.89	0.53
1:C:2104:UNK:HA	1:C:2107:UNK:HG3	1.90	0.53
1:C:2303:ASP:OD1	1:C:2303:ASP:N	2.39	0.53
1:A:580:ARG:HH11	1:A:614:GLY:HA3	1.72	0.53
1:A:1163:ASP:CB	1:A:1199:UNK:HG3	2.38	0.53
1:B:992:UNK:HG2	1:B:994:UNK:HG2	1.87	0.53
1:B:994:UNK:CG	1:B:996:UNK:HG3	2.37	0.53
1:B:2088:UNK:HG2	1:B:2188:ARG:HH12	1.73	0.53
1:C:2768:ASP:OD2	1:C:2936:GLY:N	2.41	0.53
1:A:526:ILE:HD12	1:A:549:PHE:HB3	1.90	0.53
1:A:1323:GLU:N	1:A:1343:LEU:O	2.41	0.53
1:A:2088:UNK:HG2	1:A:2188:ARG:HH12	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2425:UNK:HG2	1:A:2425:UNK:O	2.09	0.53
1:A:2768:ASP:OD2	1:A:2936:GLY:N	2.41	0.53
1:C:668:THR:OG1	1:C:698:ILE:HD11	2.08	0.53
1:C:836:VAL:HG21	1:C:2437:UNK:HB2	1.90	0.53
1:C:970:ILE:HD13	1:C:996:UNK:HG1	1.91	0.53
1:C:2122:UNK:CA	1:C:2125:UNK:HG3	2.38	0.53
1:A:792:ALA:HA	1:A:799:PHE:CE2	2.43	0.53
1:A:992:UNK:CG	1:A:996:UNK:HG2	2.32	0.53
1:A:1425:VAL:HG13	1:A:1474:LEU:HD13	1.91	0.53
1:A:2085:UNK:C	1:A:2088:UNK:HG3	2.38	0.53
1:A:2104:UNK:HA	1:A:2107:UNK:HG3	1.90	0.53
1:B:2551:PRO:O	1:B:2617:LEU:HB2	2.08	0.53
1:B:3018:LEU:O	1:B:3022:GLU:HB2	2.08	0.53
1:C:500:GLN:O	1:C:504:LYS:N	2.24	0.53
1:C:980:UNK:N	1:C:989:UNK:O	2.41	0.53
1:C:1089:ALA:O	1:C:1091:LEU:N	2.42	0.53
1:C:2492:VAL:HG21	1:C:2527:VAL:HG22	1.90	0.53
1:A:551:PRO:HG3	1:A:560:VAL:HG21	1.89	0.53
1:A:716:ALA:HA	1:A:719:VAL:HG23	1.90	0.53
1:A:2081:UNK:C	1:A:2084:UNK:HG3	2.39	0.53
1:A:2591:ARG:NH1	1:C:2012:GLY:C	2.61	0.53
1:B:411:PRO:HD2	1:B:1025:VAL:HG11	1.91	0.53
1:B:980:UNK:N	1:B:989:UNK:O	2.41	0.53
1:B:1148:GLU:O	1:B:1150:ALA:N	2.42	0.53
1:B:1538:ARG:NH1	1:B:1722:PRO:HB3	2.18	0.53
1:B:2086:UNK:O	1:B:2089:UNK:CG	2.52	0.53
1:C:745:THR:HG23	1:C:834:GLU:HA	1.90	0.53
1:C:1425:VAL:HG13	1:C:1474:LEU:HD13	1.91	0.53
1:C:2123:UNK:O	1:C:2126:UNK:CG	2.55	0.53
1:C:2631:PRO:HG3	1:C:2649:LEU:HD13	1.90	0.53
1:A:836:VAL:HG21	1:A:2437:UNK:HB2	1.90	0.53
1:A:970:ILE:HD13	1:A:996:UNK:HG1	1.91	0.53
1:A:999:UNK:HG3	1:A:1007:UNK:HG2	1.90	0.53
1:A:1087:PHE:HB3	1:B:117:LYS:HZ1	1.74	0.53
1:B:33:ALA:O	1:B:37:ARG:HG2	2.08	0.53
1:B:526:ILE:HD12	1:B:549:PHE:HB3	1.90	0.53
1:B:992:UNK:HG1	1:B:994:UNK:HG3	1.81	0.53
1:C:1226:UNK:HB1	1:C:1282:THR:HG21	1.90	0.53
1:C:2082:UNK:O	1:C:2086:UNK:HG3	2.09	0.53
1:A:588:GLU:HB3	1:A:593:LEU:HD11	1.91	0.53
1:A:961:ARG:NH2	1:A:1196:UNK:O	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1420:THR:OG1	1:A:1485:HIS:NE2	2.38	0.53
1:A:2088:UNK:C	1:A:2188:ARG:NH1	2.72	0.53
1:A:2135:UNK:CG	1:A:2136:ASP:H	2.22	0.53
1:B:836:VAL:HG21	1:B:2437:UNK:HB2	1.90	0.53
1:B:931:UNK:HG2	1:B:933:UNK:CG	2.37	0.53
1:B:1151:GLU:HB2	1:B:1179:ALA:HB3	1.90	0.53
1:B:1488:VAL:HG12	1:B:1490:ARG:HH11	1.73	0.53
1:B:2012:GLY:C	1:C:2591:ARG:NH1	2.61	0.53
1:B:2135:UNK:CG	1:B:2136:ASP:H	2.22	0.53
1:B:2246:ALA:C	1:B:2255:ARG:HH12	2.11	0.53
1:C:1174:VAL:HB	1:C:1188:LEU:HB3	1.91	0.53
1:C:1634:ARG:HD2	1:C:1638:PRO:HA	1.91	0.53
1:A:1148:GLU:O	1:A:1150:ALA:N	2.42	0.53
1:A:1151:GLU:HB2	1:A:1179:ALA:HB3	1.90	0.53
1:B:970:ILE:HD13	1:B:996:UNK:HG1	1.91	0.53
1:B:2631:PRO:HG3	1:B:2649:LEU:HD13	1.90	0.53
1:B:2740:CYS:HB2	1:B:2998:GLY:HA2	1.91	0.53
1:C:2246:ALA:C	1:C:2255:ARG:HH12	2.11	0.53
1:C:2425:UNK:O	1:C:2425:UNK:HG2	2.09	0.53
1:A:33:ALA:O	1:A:37:ARG:HG2	2.08	0.53
1:A:992:UNK:HG2	1:A:994:UNK:HG2	1.87	0.53
1:A:2860:ALA:HB1	1:A:3005:LEU:HD13	1.90	0.53
1:B:33:ALA:O	1:B:37:ARG:N	2.35	0.53
1:B:1323:GLU:N	1:B:1343:LEU:O	2.42	0.53
1:B:2087:UNK:CA	1:B:2090:UNK:HG3	2.37	0.53
1:C:2088:UNK:C	1:C:2188:ARG:NH1	2.72	0.53
1:C:2094:UNK:H	1:C:2097:UNK:HG3	1.74	0.53
1:C:2112:UNK:N	1:C:2115:UNK:HG3	2.23	0.53
1:A:1634:ARG:HD2	1:A:1638:PRO:HA	1.91	0.52
1:A:2103:UNK:O	1:A:2106:UNK:HG3	2.08	0.52
1:A:2115:UNK:HA	1:A:2118:UNK:HG3	1.90	0.52
1:A:2551:PRO:O	1:A:2617:LEU:HB2	2.08	0.52
1:B:961:ARG:NH2	1:B:1196:UNK:O	2.42	0.52
1:B:2081:UNK:C	1:B:2084:UNK:HG3	2.39	0.52
1:C:368:ILE:HG21	1:C:373:ILE:HG13	1.90	0.52
1:C:1530:LEU:HD21	1:C:1554:LEU:HD22	1.91	0.52
1:C:2215:THR:HG22	1:C:2216:GLU:HG3	1.91	0.52
1:C:2740:CYS:HB2	1:C:2998:GLY:HA2	1.92	0.52
1:A:208:VAL:HG12	1:A:248:ILE:HG12	1.92	0.52
1:B:2085:UNK:C	1:B:2088:UNK:HG3	2.38	0.52
1:B:2112:UNK:N	1:B:2115:UNK:HG3	2.23	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:PRO:HD2	1:C:1025:VAL:HG11	1.91	0.52
1:C:2085:UNK:C	1:C:2088:UNK:HG3	2.38	0.52
1:C:2554:ALA:HB1	1:C:2614:LYS:HZ2	1.74	0.52
1:A:1174:VAL:HB	1:A:1188:LEU:HB3	1.91	0.52
1:B:716:ALA:HA	1:B:719:VAL:HG23	1.90	0.52
1:B:1001:UNK:HG1	1:B:1018:ARG:HH22	1.74	0.52
1:C:71:GLU:HG2	1:C:142:ARG:NH2	2.24	0.52
1:A:71:GLU:HG2	1:A:142:ARG:NH2	2.24	0.52
1:A:745:THR:HG23	1:A:834:GLU:HA	1.90	0.52
1:A:931:UNK:HG2	1:A:933:UNK:HG2	1.91	0.52
1:A:1530:LEU:HD21	1:A:1554:LEU:HD22	1.91	0.52
1:A:1733:ASN:HD22	1:A:1736:ARG:HD2	1.74	0.52
1:A:2089:UNK:HA	1:A:2188:ARG:HH11	1.74	0.52
1:A:2808:ARG:HB2	1:A:2895:SER:O	2.10	0.52
1:B:71:GLU:HG2	1:B:142:ARG:NH2	2.24	0.52
1:B:2094:UNK:HG2	1:B:2096:UNK:CG	2.23	0.52
1:C:1151:GLU:HB2	1:C:1179:ALA:HB3	1.90	0.52
1:C:1538:ARG:NH1	1:C:1722:PRO:HB3	2.18	0.52
1:A:400:TRP:CZ3	1:A:636:PRO:HB2	2.45	0.52
1:B:368:ILE:HG21	1:B:373:ILE:HG13	1.90	0.52
1:B:1287:VAL:O	1:B:1291:LYS:HG3	2.10	0.52
1:B:1357:ILE:HG13	1:B:1710:THR:HG21	1.89	0.52
1:B:2089:UNK:HA	1:B:2188:ARG:HH11	1.74	0.52
1:B:2094:UNK:H	1:B:2097:UNK:HG3	1.75	0.52
1:B:2236:LEU:HD23	1:B:2288:HIS:HB2	1.92	0.52
1:C:1148:GLU:O	1:C:1150:ALA:N	2.42	0.52
1:C:2135:UNK:CG	1:C:2136:ASP:H	2.22	0.52
1:A:411:PRO:HD2	1:A:1025:VAL:HG11	1.91	0.52
1:A:1110:VAL:HG13	1:A:1172:VAL:HG11	1.92	0.52
1:A:1287:VAL:O	1:A:1291:LYS:HG3	2.10	0.52
1:A:2631:PRO:HG3	1:A:2649:LEU:HD13	1.90	0.52
1:B:745:THR:HG23	1:B:834:GLU:HA	1.90	0.52
1:B:999:UNK:HG3	1:B:1007:UNK:HG2	1.90	0.52
1:B:1093:PRO:HB3	1:B:1277:HIS:HE1	1.75	0.52
1:B:2087:UNK:HA	1:B:2090:UNK:CG	2.39	0.52
1:B:2808:ARG:HB2	1:B:2895:SER:O	2.10	0.52
1:C:526:ILE:HD12	1:C:549:PHE:HB3	1.90	0.52
1:C:2081:UNK:C	1:C:2084:UNK:HG3	2.39	0.52
1:A:273:ARG:HD2	1:A:282:VAL:HG12	1.90	0.52
1:A:1093:PRO:HB3	1:A:1277:HIS:HE1	1.75	0.52
1:A:1164:THR:HA	1:A:1204:UNK:O	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2094:UNK:H	1:A:2097:UNK:HG3	1.75	0.52
1:B:1110:VAL:HG13	1:B:1172:VAL:HG11	1.92	0.52
1:B:1226:UNK:HB1	1:B:1282:THR:HG21	1.90	0.52
1:C:208:VAL:HB	1:C:255:LEU:HD13	1.92	0.52
1:C:961:ARG:NH2	1:C:1196:UNK:O	2.42	0.52
1:C:1110:VAL:HG13	1:C:1172:VAL:HG11	1.92	0.52
1:C:1287:VAL:O	1:C:1291:LYS:HG3	2.10	0.52
1:C:2122:UNK:HA	1:C:2125:UNK:CG	2.40	0.52
1:B:2122:UNK:CA	1:B:2125:UNK:HG3	2.38	0.52
1:C:577:GLU:OE2	2:C:4000:FMN:O3'	2.28	0.52
1:A:577:GLU:OE2	2:A:4000:FMN:O3'	2.28	0.52
1:A:2215:THR:HG22	1:A:2216:GLU:HG3	1.92	0.52
1:A:2740:CYS:HB2	1:A:2998:GLY:HA2	1.92	0.52
1:B:1425:VAL:HG13	1:B:1474:LEU:HD13	1.91	0.52
1:B:1622:PRO:HD3	1:B:1685:LEU:HD21	1.92	0.52
1:C:208:VAL:HG12	1:C:248:ILE:HG12	1.92	0.52
1:C:400:TRP:CZ3	1:C:636:PRO:HB2	2.45	0.52
1:C:2087:UNK:C	1:C:2090:UNK:HG3	2.40	0.52
1:C:2088:UNK:HG2	1:C:2188:ARG:HH12	1.73	0.52
1:A:542:VAL:HG11	1:A:964:VAL:HB	1.92	0.52
1:B:106:ALA:O	1:B:112:PRO:HD2	2.10	0.52
1:B:144:GLY:O	1:B:148:THR:N	2.34	0.52
1:B:588:GLU:HB3	1:B:593:LEU:HD11	1.91	0.52
1:B:1174:VAL:HB	1:B:1188:LEU:HB3	1.91	0.52
1:B:2087:UNK:C	1:B:2090:UNK:HG3	2.40	0.52
1:B:2122:UNK:HA	1:B:2125:UNK:CG	2.40	0.52
1:B:2698:GLY:HA3	1:B:2705:LYS:HG3	1.92	0.52
1:C:106:ALA:O	1:C:112:PRO:HD2	2.10	0.52
1:C:1119:THR:O	1:C:1123:PHE:HB2	2.10	0.52
1:C:2094:UNK:HG2	1:C:2096:UNK:CG	2.23	0.52
1:C:2236:LEU:HD23	1:C:2288:HIS:HB2	1.92	0.52
1:A:336:TRP:CE2	1:A:360:LEU:HD11	2.45	0.51
1:A:2094:UNK:HG2	1:A:2096:UNK:CG	2.23	0.51
1:A:2552:ASP:OD1	1:A:2552:ASP:N	2.43	0.51
1:B:176:VAL:O	1:B:180:ALA:N	2.36	0.51
1:B:336:TRP:CE2	1:B:360:LEU:HD11	2.45	0.51
1:B:405:PRO:HG3	1:B:625:LEU:HG	1.92	0.51
1:B:1530:LEU:HD21	1:B:1554:LEU:HD22	1.91	0.51
1:B:2088:UNK:C	1:B:2188:ARG:NH1	2.72	0.51
1:C:420:LYS:HB3	1:C:641:ASP:OD2	2.10	0.51
1:C:932:UNK:O	1:C:936:UNK:CG	2.48	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:984:UNK:HG2	1:C:987:UNK:HG2	1.92	0.51
1:A:1226:UNK:HB1	1:A:1282:THR:HG21	1.90	0.51
1:A:1488:VAL:HG12	1:A:1490:ARG:HH11	1.73	0.51
1:B:1598:GLU:HG2	1:B:1666:ILE:HD13	1.93	0.51
1:B:2082:UNK:O	1:B:2086:UNK:HG3	2.09	0.51
1:C:1164:THR:HA	1:C:1204:UNK:O	2.10	0.51
1:A:2082:UNK:O	1:A:2086:UNK:HG3	2.09	0.51
1:A:2087:UNK:HA	1:A:2090:UNK:CG	2.39	0.51
1:B:2215:THR:HG22	1:B:2216:GLU:HG3	1.91	0.51
1:C:588:GLU:HB3	1:C:593:LEU:HD11	1.91	0.51
1:C:2790:MET:HG2	1:C:2809:LEU:HD11	1.93	0.51
1:A:1119:THR:O	1:A:1123:PHE:HB2	2.10	0.51
1:A:2086:UNK:O	1:A:2089:UNK:CG	2.52	0.51
1:A:2087:UNK:C	1:A:2090:UNK:HG3	2.40	0.51
1:A:2401:ILE:HG23	1:A:2403:ILE:H	1.75	0.51
1:A:2690:THR:O	1:A:2693:GLN:HG2	2.11	0.51
1:B:400:TRP:CZ3	1:B:636:PRO:HB2	2.45	0.51
1:B:420:LYS:HB3	1:B:641:ASP:OD2	2.10	0.51
1:B:542:VAL:HG11	1:B:964:VAL:HB	1.92	0.51
1:B:1733:ASN:HD22	1:B:1736:ARG:HD2	1.74	0.51
1:B:2123:UNK:O	1:B:2126:UNK:CG	2.56	0.51
1:B:2434:UNK:O	1:B:2434:UNK:HG2	2.11	0.51
1:C:508:GLN:HA	1:C:540:ASN:HB3	1.92	0.51
1:A:206:PRO:HG2	1:A:294:VAL:HA	1.92	0.51
1:A:1622:PRO:HD3	1:A:1685:LEU:HD21	1.92	0.51
1:B:745:THR:OG1	1:B:834:GLU:O	2.19	0.51
1:B:1634:ARG:HD2	1:B:1638:PRO:HA	1.91	0.51
1:C:2417:SER:O	1:C:2421:ASP:N	2.40	0.51
1:A:2122:UNK:HA	1:A:2125:UNK:CG	2.40	0.51
1:B:984:UNK:HG2	1:B:987:UNK:HG2	1.93	0.51
1:B:2690:THR:O	1:B:2693:GLN:HG2	2.11	0.51
1:A:420:LYS:HB3	1:A:641:ASP:OD2	2.10	0.51
1:A:937:UNK:HG2	1:A:938:UNK:N	2.26	0.51
1:A:2790:MET:HG2	1:A:2809:LEU:HD11	1.93	0.51
1:B:206:PRO:HG2	1:B:294:VAL:HA	1.92	0.51
1:C:746:TYR:HA	1:C:749:TRP:HD1	1.76	0.51
1:C:2089:UNK:HA	1:C:2188:ARG:HH11	1.74	0.51
1:C:2401:ILE:HG23	1:C:2403:ILE:H	1.76	0.51
1:A:2434:UNK:HG2	1:A:2434:UNK:O	2.11	0.51
1:B:208:VAL:HB	1:B:255:LEU:HD13	1.92	0.51
1:B:1164:THR:HA	1:B:1204:UNK:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2401:ILE:HG23	1:B:2403:ILE:H	1.76	0.51
1:C:792:ALA:HA	1:C:799:PHE:CE2	2.43	0.51
1:C:1488:VAL:HG12	1:C:1490:ARG:HH11	1.73	0.51
1:C:1598:GLU:HG2	1:C:1666:ILE:HD13	1.92	0.51
1:C:1733:ASN:HD22	1:C:1736:ARG:HD2	1.74	0.51
1:A:106:ALA:O	1:A:112:PRO:HD2	2.10	0.51
1:A:2105:UNK:HG2	1:A:2106:UNK:N	2.26	0.51
1:A:2123:UNK:O	1:A:2126:UNK:CG	2.56	0.51
1:A:2653:VAL:HA	1:A:3051:MET:HE3	1.92	0.51
1:A:2667:THR:HG21	1:A:3058:ARG:HH11	1.76	0.51
1:B:937:UNK:HG2	1:B:938:UNK:N	2.25	0.51
1:B:981:UNK:HG1	1:B:987:UNK:C	2.41	0.51
1:B:1119:THR:O	1:B:1123:PHE:HB2	2.10	0.51
1:C:2754:ILE:HA	1:C:2759:ALA:O	2.11	0.51
1:C:936:UNK:O	1:C:941:UNK:N	2.44	0.51
1:C:937:UNK:HG2	1:C:938:UNK:N	2.25	0.51
1:C:1001:UNK:HG1	1:C:1018:ARG:HH22	1.74	0.51
1:C:2086:UNK:O	1:C:2089:UNK:CG	2.52	0.51
1:C:2698:GLY:HA3	1:C:2705:LYS:HG3	1.92	0.51
1:A:42:GLU:H	1:A:42:GLU:CD	2.14	0.50
1:A:272:GLU:HB3	1:A:280:GLY:O	2.11	0.50
1:A:2236:LEU:HD23	1:A:2288:HIS:HB2	1.92	0.50
1:A:2554:ALA:HB1	1:A:2614:LYS:HZ2	1.74	0.50
1:B:42:GLU:CD	1:B:42:GLU:H	2.14	0.50
1:B:1317:GLY:H	1:B:1324:VAL:HG12	1.76	0.50
1:C:1986:LEU:HA	1:C:1989:PHE:HD2	1.76	0.50
1:C:2056:PHE:CZ	1:C:2180:LYS:HE2	2.47	0.50
1:C:2452:UNK:CG	1:C:2453:UNK:N	2.73	0.50
1:A:1331:ILE:HG13	1:A:1336:VAL:HG21	1.94	0.50
1:A:1634:ARG:HH11	1:A:1639:ALA:N	2.08	0.50
1:B:746:TYR:HA	1:B:749:TRP:HD1	1.76	0.50
1:C:42:GLU:H	1:C:42:GLU:CD	2.14	0.50
1:C:336:TRP:CE2	1:C:360:LEU:HD11	2.45	0.50
1:C:1622:PRO:HD3	1:C:1685:LEU:HD21	1.92	0.50
1:C:2104:UNK:C	1:C:2107:UNK:HG3	2.42	0.50
1:C:2361:VAL:HG11	1:C:2398:LEU:HD23	1.93	0.50
1:C:2434:UNK:O	1:C:2434:UNK:HG2	2.11	0.50
1:A:780:ARG:HD2	1:A:816:LEU:HB3	1.93	0.50
1:A:1598:GLU:HG2	1:A:1666:ILE:HD13	1.93	0.50
1:A:2180:LYS:HZ1	1:A:2962:ASP:HB3	1.75	0.50
1:A:2245:VAL:HG13	1:A:2255:ARG:CZ	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2662:SER:HB2	1:A:2833:LEU:HD22	1.93	0.50
1:B:1590:VAL:HG11	1:B:1671:TRP:CD2	2.47	0.50
1:B:2104:UNK:C	1:B:2107:UNK:HG3	2.42	0.50
1:B:2653:VAL:HA	1:B:3051:MET:HE3	1.93	0.50
1:C:1093:PRO:HB3	1:C:1277:HIS:HE1	1.75	0.50
1:C:1212:UNK:HG1	1:C:1342:ARG:HE	1.76	0.50
1:C:2245:VAL:HG13	1:C:2255:ARG:CZ	2.41	0.50
1:C:2808:ARG:HB2	1:C:2895:SER:O	2.10	0.50
1:A:257:ARG:NH1	1:C:1695:LEU:HD23	2.23	0.50
1:A:1317:GLY:H	1:A:1324:VAL:HG12	1.76	0.50
1:A:1380:ALA:HB1	1:A:1474:LEU:HD12	1.93	0.50
1:A:2261:LYS:HA	1:A:2265:TRP:HB2	1.94	0.50
1:C:272:GLU:HB3	1:C:280:GLY:O	2.11	0.50
1:C:780:ARG:HD2	1:C:816:LEU:HB3	1.93	0.50
1:C:1590:VAL:HG11	1:C:1671:TRP:CD2	2.47	0.50
1:A:1538:ARG:NH1	1:A:1722:PRO:HB3	2.18	0.50
1:A:2698:GLY:HA3	1:A:2705:LYS:HG3	1.92	0.50
1:B:2127:UNK:O	1:B:2130:UNK:CG	2.52	0.50
1:C:2140:VAL:HG22	1:C:2165:ILE:HD12	1.93	0.50
1:A:1590:VAL:HG11	1:A:1671:TRP:CD2	2.47	0.50
1:B:1331:ILE:HG13	1:B:1336:VAL:HG21	1.94	0.50
1:C:1010:UNK:CG	1:C:1017:ILE:HB	2.42	0.50
1:A:208:VAL:HB	1:A:255:LEU:HD13	1.92	0.50
1:A:932:UNK:O	1:A:936:UNK:CG	2.48	0.50
1:A:936:UNK:O	1:A:941:UNK:N	2.45	0.50
1:A:2754:ILE:HA	1:A:2759:ALA:O	2.11	0.50
1:B:133:GLN:HG2	1:B:355:GLY:HA2	1.94	0.50
1:B:207:MET:HA	1:B:249:THR:HG22	1.94	0.50
1:B:208:VAL:HG12	1:B:248:ILE:HG12	1.92	0.50
1:B:272:GLU:HB3	1:B:280:GLY:O	2.11	0.50
1:B:936:UNK:O	1:B:941:UNK:N	2.44	0.50
1:B:1711:VAL:HA	1:B:1714:LEU:HG	1.93	0.50
1:C:405:PRO:HG3	1:C:625:LEU:HG	1.93	0.50
1:C:1207:UNK:O	1:C:1207:UNK:HG2	2.12	0.50
1:C:2552:ASP:OD1	1:C:2552:ASP:N	2.43	0.50
1:A:405:PRO:HG3	1:A:625:LEU:HG	1.93	0.50
1:A:505:ARG:HA	1:A:508:GLN:HB2	1.94	0.50
1:A:981:UNK:HG1	1:A:987:UNK:C	2.41	0.50
1:A:1212:UNK:O	1:A:1342:ARG:NH2	2.45	0.50
1:A:1212:UNK:HG1	1:A:1342:ARG:HE	1.75	0.50
1:A:1986:LEU:HA	1:A:1989:PHE:HD2	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2623:ALA:HB2	1:A:2812:LEU:HD21	1.94	0.50
1:A:2811:PHE:HB3	1:A:2894:THR:HG22	1.94	0.50
1:C:206:PRO:HG2	1:C:294:VAL:HA	1.92	0.50
1:C:542:VAL:HG11	1:C:964:VAL:HB	1.92	0.50
1:C:981:UNK:HG1	1:C:987:UNK:C	2.41	0.50
1:C:2274:LEU:HD23	1:C:2277:ILE:HD12	1.94	0.50
1:C:2690:THR:O	1:C:2693:GLN:HG2	2.11	0.50
1:A:133:GLN:HG2	1:A:355:GLY:HA2	1.94	0.50
1:A:1212:UNK:HG2	1:A:1342:ARG:NE	2.26	0.50
1:B:2334:HIS:HB3	1:B:2391:LYS:HA	1.94	0.50
1:C:981:UNK:HG1	1:C:987:UNK:O	2.12	0.50
1:C:981:UNK:CG	1:C:987:UNK:O	2.60	0.50
1:A:990:UNK:HG3	1:A:998:UNK:HB2	1.94	0.49
1:A:2334:HIS:HB3	1:A:2391:LYS:HA	1.94	0.49
1:B:990:UNK:HG3	1:B:998:UNK:HB2	1.94	0.49
1:B:2557:LEU:HD22	1:B:2613:ARG:HB2	1.94	0.49
1:B:2667:THR:HG21	1:B:3058:ARG:HH11	1.76	0.49
1:B:2829:LEU:HD21	1:B:3014:PHE:HE2	1.76	0.49
1:C:1331:ILE:HG13	1:C:1336:VAL:HG21	1.94	0.49
1:C:1711:VAL:HA	1:C:1714:LEU:HG	1.94	0.49
1:C:2261:LYS:HA	1:C:2265:TRP:HB2	1.94	0.49
1:C:2557:LEU:HD22	1:C:2613:ARG:HB2	1.94	0.49
1:A:984:UNK:HG2	1:A:987:UNK:HG2	1.93	0.49
1:A:1001:UNK:HG1	1:A:1018:ARG:HH22	1.74	0.49
1:A:2104:UNK:C	1:A:2107:UNK:HG3	2.42	0.49
1:A:2127:UNK:O	1:A:2130:UNK:CG	2.52	0.49
1:B:1986:LEU:HA	1:B:1989:PHE:HD2	1.76	0.49
1:B:2056:PHE:CZ	1:B:2180:LYS:HE2	2.47	0.49
1:B:2140:VAL:HG22	1:B:2165:ILE:HD12	1.93	0.49
1:B:2361:VAL:HG11	1:B:2398:LEU:HD23	1.93	0.49
1:B:2754:ILE:HA	1:B:2759:ALA:O	2.11	0.49
1:C:1317:GLY:H	1:C:1324:VAL:HG12	1.76	0.49
1:C:2811:PHE:HB3	1:C:2894:THR:HG22	1.94	0.49
1:A:508:GLN:HA	1:A:540:ASN:HB3	1.92	0.49
1:A:647:THR:OG1	2:A:4000:FMN:O3P	2.27	0.49
1:A:981:UNK:CG	1:A:987:UNK:O	2.60	0.49
1:A:1207:UNK:O	1:A:1207:UNK:HG2	2.12	0.49
1:A:2056:PHE:CZ	1:A:2180:LYS:HE2	2.47	0.49
1:A:2140:VAL:HG22	1:A:2165:ILE:HD12	1.93	0.49
1:B:1212:UNK:O	1:B:1342:ARG:NH2	2.45	0.49
1:B:1212:UNK:HG1	1:B:1342:ARG:HE	1.75	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1178:ASN:HB2	1:C:1185:LEU:HD11	1.94	0.49
1:C:1212:UNK:O	1:C:1342:ARG:NH2	2.45	0.49
1:A:2361:VAL:HG11	1:A:2398:LEU:HD23	1.93	0.49
1:B:577:GLU:OE2	2:B:4000:FMN:O3'	2.28	0.49
1:B:1119:THR:HA	1:B:1123:PHE:CD1	2.47	0.49
1:C:776:ASP:O	1:C:779:TRP:N	2.31	0.49
1:C:1119:THR:HA	1:C:1123:PHE:CD1	2.48	0.49
1:C:1637:VAL:HG21	1:C:1671:TRP:CD2	2.48	0.49
1:C:2662:SER:HB2	1:C:2833:LEU:HD22	1.93	0.49
1:A:2274:LEU:HD23	1:A:2277:ILE:HD12	1.94	0.49
1:A:2557:LEU:HD22	1:A:2613:ARG:HB2	1.94	0.49
1:A:3080:ARG:CG	1:A:3080:ARG:NH1	2.72	0.49
1:B:981:UNK:HG1	1:B:987:UNK:O	2.12	0.49
1:B:1637:VAL:HG21	1:B:1671:TRP:CD2	2.48	0.49
1:B:2105:UNK:HG2	1:B:2106:UNK:N	2.26	0.49
1:B:2245:VAL:HG13	1:B:2255:ARG:CZ	2.41	0.49
1:C:184:LEU:HB3	1:C:311:TRP:HE3	1.78	0.49
1:C:1380:ALA:HB1	1:C:1474:LEU:HD12	1.94	0.49
1:A:981:UNK:HG1	1:A:987:UNK:O	2.12	0.49
1:B:505:ARG:HA	1:B:508:GLN:HB2	1.94	0.49
1:B:508:GLN:HA	1:B:540:ASN:HB3	1.92	0.49
1:B:976:UNK:CG	1:B:993:UNK:HB1	2.29	0.49
1:B:1212:UNK:HG2	1:B:1342:ARG:NE	2.26	0.49
1:B:2662:SER:HB2	1:B:2833:LEU:HD22	1.94	0.49
1:C:207:MET:HA	1:C:249:THR:HG22	1.94	0.49
1:A:184:LEU:HB3	1:A:311:TRP:HE3	1.78	0.49
1:A:1119:THR:HA	1:A:1123:PHE:CD1	2.47	0.49
1:A:2503:LYS:HE3	1:A:2505:GLU:OE2	2.13	0.49
1:B:932:UNK:HA	1:B:935:UNK:HG3	1.94	0.49
1:B:2790:MET:HG2	1:B:2809:LEU:HD11	1.93	0.49
1:C:2087:UNK:HA	1:C:2090:UNK:CG	2.39	0.49
1:C:2105:UNK:HG2	1:C:2106:UNK:N	2.26	0.49
1:C:3080:ARG:HG3	1:C:3080:ARG:NH1	2.09	0.49
1:A:117:LYS:HZ1	1:C:1087:PHE:HB3	1.78	0.49
1:A:207:MET:HA	1:A:249:THR:HG22	1.94	0.49
1:A:1010:UNK:CG	1:A:1017:ILE:HB	2.42	0.49
1:A:2829:LEU:HD21	1:A:3014:PHE:HE2	1.77	0.49
1:B:981:UNK:CG	1:B:987:UNK:O	2.60	0.49
1:B:1010:UNK:CG	1:B:1017:ILE:HB	2.42	0.49
1:B:1291:LYS:HA	1:B:1344:ALA:HB3	1.95	0.49
1:B:2261:LYS:HA	1:B:2265:TRP:HB2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:ILE:HD13	1:C:327:GLU:HG2	1.95	0.49
1:C:1362:MET:HG3	1:C:1430:VAL:HG21	1.95	0.49
1:A:444:ILE:HD12	1:A:655:ALA:HA	1.95	0.49
1:A:790:ALA:HB3	1:A:826:LEU:HD21	1.95	0.49
1:A:1695:LEU:HD23	1:B:257:ARG:NH1	2.23	0.49
1:A:2291:LEU:HD21	1:A:2332:LEU:HD22	1.95	0.49
1:A:2962:ASP:OD1	1:A:2962:ASP:N	2.34	0.49
1:B:184:LEU:HB3	1:B:311:TRP:HE3	1.78	0.49
1:B:780:ARG:HD2	1:B:816:LEU:HB3	1.93	0.49
1:B:792:ALA:HA	1:B:799:PHE:CE2	2.43	0.49
1:B:1380:ALA:HB1	1:B:1474:LEU:HD12	1.93	0.49
1:B:2087:UNK:O	1:B:2090:UNK:HG3	2.13	0.49
1:B:2274:LEU:HD23	1:B:2277:ILE:HD12	1.94	0.49
1:C:932:UNK:HA	1:C:935:UNK:HG3	1.94	0.49
1:C:992:UNK:HG1	1:C:994:UNK:HG3	1.81	0.49
1:C:999:UNK:O	1:C:1007:UNK:N	2.46	0.49
1:C:2094:UNK:O	1:C:2098:UNK:HG3	2.13	0.49
1:A:746:TYR:HA	1:A:749:TRP:HD1	1.76	0.49
1:B:999:UNK:O	1:B:1007:UNK:N	2.46	0.49
1:C:997:UNK:HB1	1:C:1009:UNK:HG2	1.95	0.49
1:C:2334:HIS:HB3	1:C:2391:LYS:HA	1.94	0.49
1:A:868:ARG:HB3	1:A:872:ARG:NH1	2.28	0.48
1:A:1012:UNK:O	1:A:1012:UNK:HG2	2.13	0.48
1:A:1111:PHE:HE1	1:A:1129:LEU:HD11	1.78	0.48
1:A:1637:VAL:HG21	1:A:1671:TRP:CD2	2.48	0.48
1:A:2087:UNK:O	1:A:2090:UNK:HG3	2.13	0.48
1:B:361:THR:HG21	1:B:377:PRO:HG3	1.95	0.48
1:B:444:ILE:HD12	1:B:655:ALA:HA	1.95	0.48
1:B:1207:UNK:HG2	1:B:1207:UNK:O	2.12	0.48
1:B:2094:UNK:O	1:B:2098:UNK:HG3	2.13	0.48
1:B:2120:UNK:HG2	1:B:2121:UNK:N	2.28	0.48
1:C:2100:UNK:C	1:C:2103:UNK:HG3	2.31	0.48
1:C:2118:UNK:HG2	1:C:2119:UNK:N	2.28	0.48
1:C:2667:THR:HG21	1:C:3058:ARG:HH11	1.76	0.48
1:C:2829:LEU:HD21	1:C:3014:PHE:HE2	1.76	0.48
1:A:999:UNK:O	1:A:1007:UNK:N	2.46	0.48
1:A:1225:UNK:HG1	1:A:1283:ASP:CG	2.34	0.48
1:A:1651:THR:HB	1:A:1656:LYS:HD2	1.95	0.48
1:A:2926:SER:HB3	1:A:2976:TRP:HH2	1.79	0.48
1:B:2086:UNK:CA	1:B:2089:UNK:HG3	2.43	0.48
1:C:1533:VAL:HG13	1:C:1582:HIS:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:932:UNK:HA	1:A:935:UNK:HG3	1.94	0.48
1:A:2086:UNK:CA	1:A:2089:UNK:HG3	2.43	0.48
1:B:501:VAL:HA	1:B:504:LYS:HE2	1.96	0.48
1:B:790:ALA:HB3	1:B:826:LEU:HD21	1.95	0.48
1:B:1003:UNK:CG	1:B:1004:UNK:N	2.53	0.48
1:B:1533:VAL:HG13	1:B:1582:HIS:HB2	1.95	0.48
1:B:2115:UNK:O	1:B:2119:UNK:HG3	2.13	0.48
1:B:2291:LEU:HD21	1:B:2332:LEU:HD22	1.95	0.48
1:B:2820:ILE:HD12	1:B:2822:LEU:HD21	1.95	0.48
1:C:133:GLN:HG2	1:C:355:GLY:HA2	1.94	0.48
1:C:361:THR:HG21	1:C:377:PRO:HG3	1.95	0.48
1:C:996:UNK:HG2	1:C:996:UNK:O	2.13	0.48
1:C:2503:LYS:HE3	1:C:2505:GLU:OE2	2.13	0.48
1:C:2623:ALA:HB2	1:C:2812:LEU:HD21	1.94	0.48
1:A:1435:VAL:HG22	1:A:1703:ILE:HD12	1.95	0.48
1:A:2103:UNK:CG	1:A:2919:GLY:O	2.62	0.48
1:A:2167:THR:HB	1:A:2198:ALA:HB3	1.96	0.48
1:B:2623:ALA:HB2	1:B:2812:LEU:HD21	1.94	0.48
1:C:2667:THR:HB	1:C:3081:LEU:HD11	1.95	0.48
1:C:2848:GLY:H	1:C:3001:HIS:CD2	2.31	0.48
1:A:1711:VAL:HA	1:A:1714:LEU:HG	1.93	0.48
1:A:1996:PRO:O	1:A:2000:LEU:N	2.41	0.48
1:A:2060:TRP:HZ2	1:A:2966:ASP:HA	1.79	0.48
1:A:2170:ARG:HB2	1:A:2175:ARG:HG3	1.95	0.48
1:B:1087:PHE:HB3	1:C:117:LYS:HZ3	1.77	0.48
1:B:1103:VAL:HG21	1:B:1269:MET:SD	2.54	0.48
1:B:1435:VAL:HG22	1:B:1703:ILE:HD12	1.95	0.48
1:B:2167:THR:HB	1:B:2198:ALA:HB3	1.96	0.48
1:B:2667:THR:HB	1:B:3081:LEU:HD11	1.96	0.48
1:C:505:ARG:HA	1:C:508:GLN:HB2	1.94	0.48
1:C:976:UNK:CG	1:C:993:UNK:HB1	2.29	0.48
1:C:1381:ASP:OD1	1:C:1391:SER:OG	2.22	0.48
1:C:2736:PRO:HG2	1:C:2746:SER:HA	1.96	0.48
1:A:184:LEU:HD13	1:A:311:TRP:HB3	1.96	0.48
1:A:2848:GLY:H	1:A:3001:HIS:CD2	2.31	0.48
1:B:982:UNK:CG	1:B:983:UNK:N	2.76	0.48
1:B:1133:VAL:O	1:B:1193:ALA:N	2.42	0.48
1:B:1695:LEU:HD23	1:C:257:ARG:NH1	2.23	0.48
1:B:2060:TRP:HZ2	1:B:2966:ASP:HA	1.79	0.48
1:B:2645:ASP:OD1	1:B:2647:VAL:HG23	2.14	0.48
1:B:2811:PHE:HB3	1:B:2894:THR:HG22	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:ILE:HD12	1:C:655:ALA:HA	1.95	0.48
1:C:1012:UNK:O	1:C:1012:UNK:HG2	2.13	0.48
1:C:1103:VAL:HG21	1:C:1269:MET:SD	2.54	0.48
1:C:1291:LYS:HA	1:C:1344:ALA:HB3	1.95	0.48
1:C:2087:UNK:O	1:C:2090:UNK:HG3	2.13	0.48
1:C:2088:UNK:O	1:C:2188:ARG:NH1	2.47	0.48
1:C:2645:ASP:OD1	1:C:2647:VAL:HG23	2.13	0.48
1:C:2648:ALA:HA	1:C:2718:VAL:HG13	1.96	0.48
1:C:2820:ILE:HD12	1:C:2822:LEU:HD21	1.95	0.48
1:A:1178:ASN:HB2	1:A:1185:LEU:HD11	1.94	0.48
1:A:2115:UNK:O	1:A:2119:UNK:HG3	2.13	0.48
1:B:803:GLU:OE1	1:B:2431:UNK:CG	2.62	0.48
1:B:931:UNK:CG	1:B:934:UNK:HG3	2.44	0.48
1:B:1362:MET:HG3	1:B:1430:VAL:HG21	1.95	0.48
1:B:1508:ILE:HB	1:B:1562:ARG:HD3	1.96	0.48
1:B:2103:UNK:CG	1:B:2919:GLY:O	2.62	0.48
1:C:1634:ARG:HH11	1:C:1639:ALA:N	2.08	0.48
1:C:2060:TRP:HZ2	1:C:2966:ASP:HA	1.79	0.48
1:A:144:GLY:O	1:A:148:THR:N	2.34	0.48
1:A:931:UNK:CG	1:A:934:UNK:HG3	2.44	0.48
1:A:985:UNK:HG2	1:A:986:UNK:N	2.29	0.48
1:A:1103:VAL:HG21	1:A:1269:MET:SD	2.54	0.48
1:A:1163:ASP:CG	1:A:1199:UNK:HG3	2.34	0.48
1:A:1291:LYS:HA	1:A:1344:ALA:HB3	1.95	0.48
1:A:1362:MET:HG3	1:A:1430:VAL:HG21	1.95	0.48
1:A:2088:UNK:O	1:A:2188:ARG:NH1	2.47	0.48
1:A:2180:LYS:NZ	1:A:2962:ASP:HB3	2.29	0.48
1:A:2592:PRO:HA	1:A:2599:TRP:CD1	2.49	0.48
1:A:2666:PRO:CB	1:A:2727:VAL:HA	2.44	0.48
1:B:305:ILE:HD13	1:B:327:GLU:HG2	1.95	0.48
1:C:868:ARG:HB3	1:C:872:ARG:NH1	2.28	0.48
1:C:990:UNK:HG3	1:C:998:UNK:HB2	1.94	0.48
1:C:1212:UNK:HG2	1:C:1342:ARG:NE	2.26	0.48
1:C:2094:UNK:HG1	1:C:2096:UNK:HG3	1.90	0.48
1:C:2115:UNK:O	1:C:2119:UNK:HG3	2.13	0.48
1:C:2167:THR:HB	1:C:2198:ALA:HB3	1.96	0.48
1:C:2666:PRO:CB	1:C:2727:VAL:HA	2.44	0.48
1:A:305:ILE:HD13	1:A:327:GLU:HG2	1.95	0.48
1:A:997:UNK:N	1:A:1009:UNK:O	2.47	0.48
1:A:2094:UNK:O	1:A:2098:UNK:HG3	2.13	0.48
1:A:2120:UNK:HG2	1:A:2121:UNK:N	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2645:ASP:OD1	1:A:2647:VAL:HG23	2.14	0.48
1:A:2667:THR:HB	1:A:3081:LEU:HD11	1.96	0.48
1:B:171:LYS:HE3	1:B:173:ALA:HB3	1.96	0.48
1:B:647:THR:HG22	1:B:901:ILE:HD11	1.96	0.48
1:B:2088:UNK:O	1:B:2188:ARG:NH1	2.47	0.48
1:C:997:UNK:N	1:C:1009:UNK:O	2.47	0.48
1:C:1467:VAL:HA	1:C:1605:LYS:HD2	1.96	0.48
1:C:2592:PRO:HA	1:C:2599:TRP:CD1	2.49	0.48
1:C:2926:SER:HB3	1:C:2976:TRP:HH2	1.78	0.48
1:A:2762:VAL:HG22	1:A:2822:LEU:HB2	1.96	0.48
1:A:2820:ILE:HD12	1:A:2822:LEU:HD21	1.95	0.48
1:B:575:HIS:CD2	1:B:644:LEU:HD22	2.49	0.48
1:B:808:ALA:HB3	1:B:811:ASP:HB2	1.96	0.48
1:B:997:UNK:N	1:B:1009:UNK:O	2.47	0.48
1:B:2352:ILE:HG12	1:B:2412:ALA:HB1	1.96	0.48
1:C:171:LYS:HE3	1:C:173:ALA:HB3	1.96	0.48
1:C:301:LEU:HD13	1:C:330:LEU:HD22	1.96	0.48
1:C:575:HIS:CD2	1:C:644:LEU:HD22	2.48	0.48
1:C:641:ASP:N	1:C:641:ASP:OD1	2.47	0.48
1:C:1651:THR:HB	1:C:1656:LYS:HD2	1.95	0.48
1:C:2448:UNK:O	1:C:2448:UNK:HG2	2.13	0.48
1:A:176:VAL:O	1:A:180:ALA:N	2.36	0.47
1:A:996:UNK:HG2	1:A:996:UNK:O	2.13	0.47
1:A:2736:PRO:HG2	1:A:2746:SER:HA	1.96	0.47
1:B:670:GLY:HA3	1:B:899:ALA:HB2	1.96	0.47
1:B:674:TRP:CD1	1:B:895:THR:HG21	2.49	0.47
1:B:2180:LYS:NZ	1:B:2962:ASP:HB3	2.29	0.47
1:B:2448:UNK:HG2	1:B:2448:UNK:O	2.13	0.47
1:B:2666:PRO:CB	1:B:2727:VAL:HA	2.44	0.47
1:C:1013:UNK:CG	1:C:1014:UNK:N	2.58	0.47
1:C:1435:VAL:HG22	1:C:1703:ILE:HD12	1.95	0.47
1:C:2843:GLN:HG2	1:C:2845:PHE:CZ	2.49	0.47
1:A:2348:GLN:O	1:A:2416:MET:HG3	2.15	0.47
1:A:2554:ALA:HB1	1:A:2614:LYS:HD2	1.95	0.47
1:B:1012:UNK:O	1:B:1012:UNK:HG2	2.14	0.47
1:B:1111:PHE:HE1	1:B:1129:LEU:HD11	1.78	0.47
1:B:1651:THR:HB	1:B:1656:LYS:HD2	1.95	0.47
1:B:2101:UNK:HG2	1:B:2102:UNK:N	2.29	0.47
1:B:2434:UNK:HG3	1:B:2523:GLU:O	2.14	0.47
1:B:2503:LYS:HE3	1:B:2505:GLU:OE2	2.13	0.47
1:B:2592:PRO:HA	1:B:2599:TRP:CD1	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2848:GLY:H	1:B:3001:HIS:CD2	2.31	0.47
1:B:2884:ASP:HA	1:B:2916:ARG:NH1	2.30	0.47
1:C:184:LEU:HD13	1:C:311:TRP:HB3	1.96	0.47
1:C:606:ASN:HD22	1:C:606:ASN:H	1.62	0.47
1:C:647:THR:HG22	1:C:901:ILE:HD11	1.96	0.47
1:C:1010:UNK:HG2	1:C:1017:ILE:HB	1.96	0.47
1:C:2180:LYS:NZ	1:C:2962:ASP:HB3	2.29	0.47
1:C:2554:ALA:HB1	1:C:2614:LYS:HD2	1.95	0.47
1:A:1533:VAL:HG13	1:A:1582:HIS:HB2	1.95	0.47
1:A:2434:UNK:HG3	1:A:2523:GLU:O	2.14	0.47
1:B:365:ALA:O	1:B:369:ARG:N	2.42	0.47
1:B:1072:TRP:HE1	1:B:1077:VAL:HG22	1.80	0.47
1:B:1178:ASN:HB2	1:B:1185:LEU:HD11	1.94	0.47
1:B:1625:LEU:HD11	1:B:1660:LEU:HB3	1.95	0.47
1:B:2927:GLN:HE22	1:B:2941:PHE:C	2.17	0.47
1:C:176:VAL:O	1:C:180:ALA:N	2.36	0.47
1:C:790:ALA:HB3	1:C:826:LEU:HD21	1.95	0.47
1:C:1163:ASP:CG	1:C:1199:UNK:HG3	2.34	0.47
1:C:1225:UNK:HG1	1:C:1283:ASP:CG	2.34	0.47
1:C:1450:ALA:N	1:C:1613:ARG:O	2.48	0.47
1:A:365:ALA:HB3	1:A:366:PRO:HD3	1.96	0.47
1:A:674:TRP:CD1	1:A:895:THR:HG21	2.50	0.47
1:B:2093:UNK:HG1	1:B:2132:UNK:HB1	1.95	0.47
1:B:2123:UNK:HA	1:B:2126:UNK:HG3	1.97	0.47
1:B:2252:VAL:HG22	1:B:2255:ARG:NH2	2.30	0.47
1:B:2461:VAL:HG21	1:B:2751:VAL:HG13	1.96	0.47
1:B:2648:ALA:HA	1:B:2718:VAL:HG13	1.96	0.47
1:C:365:ALA:HB3	1:C:366:PRO:HD3	1.96	0.47
1:C:674:TRP:CD1	1:C:895:THR:HG21	2.49	0.47
1:C:808:ALA:HB3	1:C:811:ASP:HB2	1.96	0.47
1:C:985:UNK:HG2	1:C:986:UNK:N	2.29	0.47
1:C:2170:ARG:HB2	1:C:2175:ARG:HG3	1.95	0.47
1:A:997:UNK:HB1	1:A:1009:UNK:CG	2.44	0.47
1:A:1508:ILE:HB	1:A:1562:ARG:HD3	1.97	0.47
1:A:2118:UNK:HG2	1:A:2119:UNK:N	2.28	0.47
1:A:2648:ALA:HA	1:A:2718:VAL:HG13	1.96	0.47
1:A:2843:GLN:HG2	1:A:2845:PHE:CZ	2.49	0.47
1:A:2927:GLN:HE22	1:A:2941:PHE:C	2.17	0.47
1:B:832:ASP:O	1:B:836:VAL:HG23	2.14	0.47
1:B:985:UNK:HG2	1:B:986:UNK:N	2.29	0.47
1:B:997:UNK:HB1	1:B:1009:UNK:HG2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2170:ARG:HB2	1:B:2175:ARG:HG3	1.96	0.47
1:C:1455:VAL:HB	1:C:1480:ARG:HH12	1.80	0.47
1:C:2103:UNK:CG	1:C:2919:GLY:O	2.62	0.47
1:C:2123:UNK:HA	1:C:2126:UNK:HG3	1.97	0.47
1:C:2461:VAL:HG21	1:C:2751:VAL:HG13	1.96	0.47
1:A:606:ASN:H	1:A:606:ASN:HD22	1.63	0.47
1:A:997:UNK:HB1	1:A:1009:UNK:HG2	1.95	0.47
1:A:2093:UNK:HG1	1:A:2132:UNK:HB1	1.95	0.47
1:A:2448:UNK:HG2	1:A:2448:UNK:O	2.13	0.47
1:B:641:ASP:OD1	1:B:641:ASP:N	2.47	0.47
1:B:683:GLY:CA	1:B:700:ASN:HB2	2.44	0.47
1:B:932:UNK:O	1:B:936:UNK:CG	2.47	0.47
1:B:996:UNK:HG2	1:B:996:UNK:O	2.13	0.47
1:B:1590:VAL:HG11	1:B:1671:TRP:CE2	2.50	0.47
1:B:2376:LEU:HD22	1:B:2392:VAL:HG21	1.97	0.47
1:B:2681:THR:O	1:B:2764:ALA:HA	2.15	0.47
1:C:966:PRO:O	1:C:970:ILE:N	2.48	0.47
1:C:997:UNK:HB1	1:C:1009:UNK:CG	2.45	0.47
1:C:1723:GLU:C	1:C:1725:SER:H	2.18	0.47
1:C:2927:GLN:HE22	1:C:2941:PHE:C	2.17	0.47
1:A:713:ALA:O	1:A:868:ARG:NH2	2.48	0.47
1:A:782:ARG:HD3	1:A:853:LEU:HD22	1.97	0.47
1:A:1381:ASP:OD1	1:A:1391:SER:OG	2.22	0.47
1:A:1625:LEU:HD11	1:A:1660:LEU:HB3	1.96	0.47
1:A:1672:GLN:HE21	1:A:1672:GLN:HB3	1.58	0.47
1:A:1723:GLU:C	1:A:1725:SER:H	2.18	0.47
1:A:2101:UNK:HG2	1:A:2102:UNK:N	2.29	0.47
1:A:2800:PHE:CE1	1:A:2812:LEU:HD22	2.50	0.47
1:A:2884:ASP:HA	1:A:2916:ARG:NH1	2.29	0.47
1:B:184:LEU:HD13	1:B:311:TRP:HB3	1.96	0.47
1:B:365:ALA:HB3	1:B:366:PRO:HD3	1.96	0.47
1:B:745:THR:HG22	1:B:747:LEU:H	1.80	0.47
1:B:1163:ASP:CG	1:B:1199:UNK:HG3	2.34	0.47
1:B:1455:VAL:HB	1:B:1480:ARG:HH12	1.80	0.47
1:B:1672:GLN:HE21	1:B:1672:GLN:HB3	1.58	0.47
1:B:2630:ASP:HB3	1:B:2633:VAL:HG23	1.97	0.47
1:B:2926:SER:HB3	1:B:2976:TRP:HH2	1.79	0.47
1:C:210:VAL:HG22	1:C:287:PHE:CD1	2.50	0.47
1:C:670:GLY:HA3	1:C:899:ALA:HB2	1.96	0.47
1:C:832:ASP:O	1:C:836:VAL:HG23	2.14	0.47
1:C:941:UNK:HG3	1:C:942:UNK:N	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1625:LEU:HD11	1:C:1660:LEU:HB3	1.96	0.47
1:C:2120:UNK:HG2	1:C:2121:UNK:N	2.28	0.47
1:C:2762:VAL:HG22	1:C:2822:LEU:HB2	1.96	0.47
1:C:2773:GLU:HA	1:C:2776:ILE:HG22	1.97	0.47
1:A:301:LEU:HD13	1:A:330:LEU:HD22	1.96	0.47
1:A:966:PRO:O	1:A:970:ILE:N	2.48	0.47
1:A:1010:UNK:HG2	1:A:1017:ILE:HB	1.96	0.47
1:A:1467:VAL:HA	1:A:1605:LYS:HD2	1.96	0.47
1:A:2210:VAL:HB	1:A:2277:ILE:HD11	1.96	0.47
1:B:778:THR:HG21	1:B:854:GLY:HA3	1.97	0.47
1:B:868:ARG:HB3	1:B:872:ARG:NH1	2.28	0.47
1:B:931:UNK:HG2	1:B:933:UNK:HG2	1.92	0.47
1:B:2125:UNK:HA	1:B:2128:UNK:CG	2.45	0.47
1:B:2450:UNK:HG1	1:B:3016:ALA:CB	2.17	0.47
1:B:2762:VAL:HG22	1:B:2822:LEU:HB2	1.96	0.47
1:C:803:GLU:OE1	1:C:2431:UNK:CG	2.62	0.47
1:C:931:UNK:CG	1:C:934:UNK:HG3	2.44	0.47
1:C:1276:GLN:HE21	1:C:1292:LEU:HD13	1.79	0.47
1:C:2086:UNK:CA	1:C:2089:UNK:HG3	2.43	0.47
1:C:2376:LEU:HD22	1:C:2392:VAL:HG21	1.97	0.47
1:C:2681:THR:O	1:C:2764:ALA:HA	2.15	0.47
1:A:198:ILE:HG12	1:C:1087:PHE:CE1	2.50	0.47
1:A:803:GLU:OE1	1:A:2431:UNK:CG	2.62	0.47
1:A:808:ALA:HB3	1:A:811:ASP:HB2	1.96	0.47
1:A:832:ASP:O	1:A:836:VAL:HG23	2.14	0.47
1:A:2785:ALA:HB1	1:A:2809:LEU:HG	1.97	0.47
1:B:210:VAL:HG22	1:B:287:PHE:CD1	2.50	0.47
1:B:585:HIS:HD2	1:B:586:SER:H	1.62	0.47
1:B:713:ALA:O	1:B:868:ARG:NH2	2.48	0.47
1:B:782:ARG:HD3	1:B:853:LEU:HD22	1.97	0.47
1:B:941:UNK:HG3	1:B:942:UNK:N	2.30	0.47
1:B:1010:UNK:HG2	1:B:1017:ILE:HB	1.96	0.47
1:B:1457:GLU:OE2	1:B:1614:TYR:OH	2.30	0.47
1:B:2554:ALA:HB1	1:B:2614:LYS:HD2	1.96	0.47
1:C:2291:LEU:HD21	1:C:2332:LEU:HD22	1.95	0.47
1:A:141:ALA:O	1:A:145:MET:HB2	2.15	0.47
1:A:2482:GLU:HG2	1:A:2956:PRO:HB3	1.97	0.47
1:B:301:LEU:HD13	1:B:330:LEU:HD22	1.96	0.47
1:B:992:UNK:CG	1:B:996:UNK:HG2	2.32	0.47
1:B:1723:GLU:C	1:B:1725:SER:H	2.18	0.47
1:B:2843:GLN:HG2	1:B:2845:PHE:CZ	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:836:VAL:HG12	1:C:837:VAL:N	2.29	0.47
1:C:1111:PHE:HE1	1:C:1129:LEU:HD11	1.78	0.47
1:C:2101:UNK:HG2	1:C:2102:UNK:N	2.29	0.47
1:C:2125:UNK:HA	1:C:2128:UNK:CG	2.44	0.47
1:C:2427:UNK:O	1:C:2427:UNK:HG2	2.15	0.47
1:C:3080:ARG:CG	1:C:3080:ARG:NH1	2.72	0.47
1:A:836:VAL:HG12	1:A:837:VAL:N	2.29	0.46
1:A:1237:ARG:CZ	1:B:95:PRO:HB2	2.46	0.46
1:A:2058:ASP:OD1	1:A:2058:ASP:N	2.46	0.46
1:B:94:ARG:HG3	1:B:95:PRO:HD3	1.98	0.46
1:B:836:VAL:HG12	1:B:837:VAL:N	2.29	0.46
1:B:966:PRO:O	1:B:970:ILE:N	2.48	0.46
1:B:997:UNK:HB1	1:B:1009:UNK:CG	2.44	0.46
1:B:1467:VAL:HA	1:B:1605:LYS:HD2	1.96	0.46
1:C:222:LEU:HD21	1:C:236:VAL:HA	1.97	0.46
1:C:1590:VAL:HG11	1:C:1671:TRP:CE2	2.50	0.46
1:C:2104:UNK:HA	1:C:2107:UNK:CG	2.46	0.46
1:C:2210:VAL:HB	1:C:2277:ILE:HD11	1.97	0.46
1:C:2252:VAL:HG13	1:C:2255:ARG:HH21	1.81	0.46
1:A:670:GLY:HA3	1:A:899:ALA:HB2	1.96	0.46
1:A:778:THR:HG21	1:A:854:GLY:HA3	1.97	0.46
1:A:941:UNK:HG3	1:A:942:UNK:N	2.30	0.46
1:A:2077:UNK:CG	1:A:2079:UNK:HG3	2.41	0.46
1:A:2096:UNK:C	1:A:2099:UNK:HG3	2.43	0.46
1:B:518:ASP:HA	1:B:543:GLY:O	2.15	0.46
1:B:2961:LEU:HD22	1:B:2976:TRP:CD1	2.51	0.46
1:C:84:GLU:HB2	1:C:85:PRO:HD3	1.97	0.46
1:C:501:VAL:HA	1:C:504:LYS:HE2	1.96	0.46
1:C:656:THR:HG1	1:C:880:HIS:CE1	2.30	0.46
1:C:713:ALA:O	1:C:868:ARG:NH2	2.48	0.46
1:C:931:UNK:HG2	1:C:933:UNK:HG2	1.92	0.46
1:C:1508:ILE:HB	1:C:1562:ARG:HD3	1.97	0.46
1:C:2096:UNK:C	1:C:2099:UNK:HG3	2.43	0.46
1:C:2352:ILE:HG12	1:C:2412:ALA:HB1	1.96	0.46
1:A:171:LYS:HE3	1:A:173:ALA:HB3	1.96	0.46
1:A:210:VAL:HG22	1:A:287:PHE:CD1	2.50	0.46
1:A:361:THR:HG21	1:A:377:PRO:HG3	1.95	0.46
1:A:365:ALA:O	1:A:369:ARG:N	2.42	0.46
1:A:2252:VAL:HG13	1:A:2255:ARG:HH21	1.80	0.46
1:A:2352:ILE:HG12	1:A:2412:ALA:HB1	1.96	0.46
1:A:2681:THR:O	1:A:2764:ALA:HA	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2978:ARG:NH1	1:A:2979:GLU:OE2	2.49	0.46
1:B:205:PRO:CD	1:B:289:PRO:HB3	2.46	0.46
1:B:996:UNK:HA	1:B:1010:UNK:HA	1.97	0.46
1:B:1001:UNK:O	1:B:1005:UNK:HB2	2.16	0.46
1:B:1319:ASP:HB2	1:B:1342:ARG:NH1	2.31	0.46
1:B:2118:UNK:HG2	1:B:2119:UNK:N	2.28	0.46
1:C:982:UNK:CG	1:C:983:UNK:N	2.76	0.46
1:C:2434:UNK:HG3	1:C:2523:GLU:O	2.14	0.46
1:C:2884:ASP:HA	1:C:2916:ARG:NH1	2.29	0.46
1:A:84:GLU:HB2	1:A:85:PRO:HD3	1.98	0.46
1:A:518:ASP:HA	1:A:543:GLY:O	2.15	0.46
1:A:683:GLY:CA	1:A:700:ASN:HB2	2.44	0.46
1:A:1612:GLY:N	1:A:1623:PHE:O	2.48	0.46
1:A:1699:ARG:HG3	1:A:1730:GLU:HB3	1.97	0.46
1:A:2461:VAL:HG21	1:A:2751:VAL:HG13	1.96	0.46
1:B:1634:ARG:HH11	1:B:1639:ALA:N	2.08	0.46
1:B:2252:VAL:HG13	1:B:2255:ARG:HH21	1.81	0.46
1:B:2736:PRO:HG2	1:B:2746:SER:HA	1.95	0.46
1:C:518:ASP:HA	1:C:543:GLY:O	2.15	0.46
1:C:2348:GLN:O	1:C:2416:MET:HG3	2.15	0.46
1:A:1325:LEU:HD11	1:A:1343:LEU:HD22	1.98	0.46
1:A:1346:PRO:HG2	1:A:1699:ARG:HD3	1.98	0.46
1:A:2961:LEU:HD22	1:A:2976:TRP:CD1	2.51	0.46
1:B:768:LYS:HA	1:B:775:LEU:HD11	1.97	0.46
1:B:1237:ARG:CZ	1:C:95:PRO:HB2	2.46	0.46
1:B:1276:GLN:HE21	1:B:1292:LEU:HD13	1.79	0.46
1:B:1699:ARG:HG3	1:B:1730:GLU:HB3	1.97	0.46
1:B:2543:PHE:HA	1:B:2624:GLN:HE22	1.81	0.46
1:B:2554:ALA:HB1	1:B:2614:LYS:HZ2	1.78	0.46
1:C:745:THR:HG22	1:C:747:LEU:H	1.80	0.46
1:C:782:ARG:HD3	1:C:853:LEU:HD22	1.97	0.46
1:C:2252:VAL:HG22	1:C:2255:ARG:NH2	2.30	0.46
1:B:2104:UNK:HA	1:B:2107:UNK:CG	2.46	0.46
1:C:141:ALA:O	1:C:145:MET:HB2	2.15	0.46
1:C:406:THR:OG1	1:C:418:GLU:OE1	2.34	0.46
1:C:534:ASP:O	1:C:538:GLU:HG3	2.16	0.46
1:C:778:THR:HG21	1:C:854:GLY:HA3	1.97	0.46
1:C:1325:LEU:HD11	1:C:1343:LEU:HD22	1.98	0.46
1:C:1699:ARG:HG3	1:C:1730:GLU:HB3	1.97	0.46
1:C:2361:VAL:HG21	1:C:2401:ILE:HD11	1.98	0.46
1:A:575:HIS:CD2	1:A:644:LEU:HD22	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1072:TRP:CD1	1:A:1097:VAL:HG22	2.51	0.46
1:A:1590:VAL:HG11	1:A:1671:TRP:CE2	2.50	0.46
1:A:3065:PRO:O	1:A:3069:GLN:N	2.42	0.46
1:B:84:GLU:HB2	1:B:85:PRO:HD3	1.97	0.46
1:B:141:ALA:O	1:B:145:MET:HB2	2.15	0.46
1:B:406:THR:OG1	1:B:418:GLU:OE1	2.34	0.46
1:B:540:ASN:ND2	1:B:544:ILE:HG13	2.30	0.46
1:B:606:ASN:HD22	1:B:606:ASN:H	1.62	0.46
1:B:1072:TRP:CD1	1:B:1097:VAL:HG22	2.51	0.46
1:B:2210:VAL:HB	1:B:2277:ILE:HD11	1.96	0.46
1:B:2348:GLN:O	1:B:2416:MET:HG3	2.15	0.46
1:C:1001:UNK:O	1:C:1005:UNK:HB2	2.16	0.46
1:C:1094:THR:O	1:C:1288:PRO:HG2	2.15	0.46
1:C:1319:ASP:HB2	1:C:1342:ARG:NH1	2.31	0.46
1:C:1346:PRO:HG2	1:C:1699:ARG:HD3	1.98	0.46
1:C:2482:GLU:HG2	1:C:2956:PRO:HB3	1.97	0.46
1:C:2957:PRO:HB3	1:C:2979:GLU:C	2.36	0.46
1:A:167:ALA:HB3	1:A:178:LEU:HD21	1.98	0.46
1:A:277:LEU:HD22	1:A:676:GLY:O	2.16	0.46
1:A:501:VAL:HA	1:A:504:LYS:HE2	1.96	0.46
1:A:1205:UNK:HG2	1:A:1206:UNK:N	2.30	0.46
1:A:1212:UNK:CG	1:A:1342:ARG:HH21	2.17	0.46
1:A:1276:GLN:HE21	1:A:1292:LEU:HD13	1.79	0.46
1:A:2104:UNK:HA	1:A:2107:UNK:CG	2.46	0.46
1:A:2376:LEU:HD22	1:A:2392:VAL:HG21	1.97	0.46
1:A:2630:ASP:HB3	1:A:2633:VAL:HG23	1.97	0.46
1:A:2957:PRO:HB3	1:A:2979:GLU:C	2.36	0.46
1:B:2957:PRO:HB3	1:B:2979:GLU:C	2.36	0.46
1:B:2978:ARG:NH1	1:B:2979:GLU:OE2	2.49	0.46
1:C:94:ARG:HG3	1:C:95:PRO:HD3	1.98	0.46
1:C:996:UNK:HA	1:C:1010:UNK:HA	1.97	0.46
1:A:95:PRO:HB2	1:C:1237:ARG:CZ	2.45	0.46
1:A:647:THR:HG22	1:A:901:ILE:HD11	1.96	0.46
1:A:1455:VAL:HB	1:A:1480:ARG:HH12	1.80	0.46
1:A:2212:TRP:HA	1:A:2229:LYS:HB3	1.98	0.46
1:A:2252:VAL:HG22	1:A:2255:ARG:NH2	2.30	0.46
1:A:2610:ARG:NH1	1:A:2700:LEU:HD21	2.31	0.46
1:A:2773:GLU:HA	1:A:2776:ILE:HG22	1.97	0.46
1:A:2790:MET:SD	1:A:2800:PHE:HB2	2.56	0.46
1:B:111:GLU:HB2	1:B:112:PRO:HD3	1.98	0.46
1:B:984:UNK:HG1	1:B:987:UNK:CG	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1205:UNK:HG2	1:B:1206:UNK:N	2.31	0.46
1:B:1304:LYS:O	1:B:1307:ASP:HB2	2.16	0.46
1:B:2619:ARG:NH1	1:B:2779:GLY:HA2	2.31	0.46
1:C:111:GLU:HB2	1:C:112:PRO:HD3	1.98	0.46
1:C:1205:UNK:HG2	1:C:1206:UNK:N	2.30	0.46
1:C:2619:ARG:NH1	1:C:2779:GLY:HA2	2.31	0.46
1:C:2946:LEU:HD22	1:C:2994:VAL:HG23	1.98	0.46
1:A:205:PRO:CD	1:A:289:PRO:HB3	2.46	0.46
1:A:745:THR:HG22	1:A:747:LEU:H	1.80	0.46
1:A:868:ARG:HD3	1:A:872:ARG:HH12	1.81	0.46
1:A:1087:PHE:CE1	1:B:198:ILE:HG12	2.51	0.46
1:A:2123:UNK:HA	1:A:2126:UNK:HG3	1.97	0.46
1:A:2125:UNK:HA	1:A:2128:UNK:CG	2.45	0.46
1:A:2879:LEU:HD13	1:A:3009:VAL:HG11	1.98	0.46
1:B:1087:PHE:CE1	1:C:198:ILE:HG12	2.51	0.46
1:B:2770:LEU:HB3	1:B:2815:GLN:HB3	1.97	0.46
1:C:408:VAL:CG1	1:C:943:UNK:HG1	2.46	0.46
1:C:1072:TRP:CD1	1:C:1097:VAL:HG22	2.51	0.46
1:C:1304:LYS:O	1:C:1307:ASP:HB2	2.16	0.46
1:C:2234:PRO:HB2	1:C:2287:LEU:HD13	1.98	0.46
1:C:2879:LEU:HD13	1:C:3009:VAL:HG11	1.98	0.46
1:A:111:GLU:HB2	1:A:112:PRO:HD3	1.98	0.45
1:A:2100:UNK:C	1:A:2103:UNK:HG3	2.31	0.45
1:A:2137:GLU:O	1:A:2163:THR:N	2.30	0.45
1:A:2891:LYS:HG3	1:A:2924:ILE:HD13	1.98	0.45
1:B:793:ARG:HA	1:B:2435:UNK:HG1	1.97	0.45
1:B:1094:THR:O	1:B:1288:PRO:HG2	2.15	0.45
1:B:1325:LEU:HD11	1:B:1343:LEU:HD22	1.98	0.45
1:B:2094:UNK:HG1	1:B:2096:UNK:HG3	1.90	0.45
1:B:2672:TRP:CD1	1:B:2831:MET:HG2	2.52	0.45
1:B:2773:GLU:HA	1:B:2776:ILE:HG22	1.97	0.45
1:B:2889:ILE:HD11	1:B:2922:LEU:HD22	1.98	0.45
1:A:793:ARG:HA	1:A:2435:UNK:HG1	1.98	0.45
1:A:996:UNK:HA	1:A:1010:UNK:HA	1.97	0.45
1:A:1003:UNK:CG	1:A:1004:UNK:N	2.53	0.45
1:A:1094:THR:O	1:A:1288:PRO:HG2	2.15	0.45
1:A:1319:ASP:HB2	1:A:1342:ARG:NH1	2.31	0.45
1:A:1450:ALA:N	1:A:1613:ARG:O	2.48	0.45
1:A:2543:PHE:HA	1:A:2624:GLN:HE22	1.81	0.45
1:B:1702:GLU:OE1	1:B:1712:ALA:N	2.49	0.45
1:B:2234:PRO:HB2	1:B:2287:LEU:HD13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2482:GLU:HG2	1:B:2956:PRO:HB3	1.97	0.45
1:B:2946:LEU:HD22	1:B:2994:VAL:HG23	1.98	0.45
1:C:47:ALA:O	1:C:353:ASP:HA	2.17	0.45
1:C:277:LEU:HD22	1:C:676:GLY:O	2.16	0.45
1:C:540:ASN:ND2	1:C:544:ILE:HG13	2.30	0.45
1:C:683:GLY:CA	1:C:700:ASN:HB2	2.44	0.45
1:C:1462:ALA:HB2	1:C:1468:TYR:HE1	1.81	0.45
1:C:2212:TRP:HA	1:C:2229:LYS:HB3	1.98	0.45
1:C:2961:LEU:HD22	1:C:2976:TRP:CD1	2.51	0.45
1:A:94:ARG:HG3	1:A:95:PRO:HD3	1.98	0.45
1:A:944:UNK:O	1:A:944:UNK:CG	2.59	0.45
1:A:1133:VAL:O	1:A:1193:ALA:N	2.42	0.45
1:A:1462:ALA:HB2	1:A:1468:TYR:HE1	1.81	0.45
1:A:1483:LYS:O	1:A:1487:ILE:HG23	2.17	0.45
1:A:2619:ARG:NH1	1:A:2779:GLY:HA2	2.31	0.45
1:B:351:ILE:HB	1:B:375:ILE:HG12	1.99	0.45
1:B:1352:PHE:HA	1:B:1353:PRO:HD3	1.72	0.45
1:B:1462:ALA:HB2	1:B:1468:TYR:HE1	1.81	0.45
1:B:2891:LYS:HG3	1:B:2924:ILE:HD13	1.99	0.45
1:C:205:PRO:CD	1:C:289:PRO:HB3	2.46	0.45
1:C:381:ARG:O	1:C:384:GLN:HG2	2.17	0.45
1:C:746:TYR:HB2	1:C:833:ALA:HB1	1.99	0.45
1:C:984:UNK:HG1	1:C:987:UNK:CG	2.46	0.45
1:C:2070:LEU:O	1:C:2074:GLU:HG3	2.16	0.45
1:C:2472:TYR:CZ	1:C:2930:LEU:HD22	2.52	0.45
1:A:222:LEU:HD21	1:A:236:VAL:HA	1.97	0.45
1:A:747:LEU:HD22	1:A:751:ARG:CZ	2.47	0.45
1:A:784:GLU:OE2	1:A:816:LEU:HD21	2.16	0.45
1:A:2246:ALA:N	1:A:2255:ARG:NH1	2.64	0.45
1:A:2672:TRP:CD1	1:A:2831:MET:HG2	2.52	0.45
1:A:2845:PHE:HD2	1:A:2860:ALA:HA	1.82	0.45
1:A:2889:ILE:HD11	1:A:2922:LEU:HD22	1.98	0.45
1:B:47:ALA:O	1:B:353:ASP:HA	2.17	0.45
1:B:1001:UNK:HG1	1:B:1018:ARG:HH21	1.80	0.45
1:B:1346:PRO:HG2	1:B:1699:ARG:HD3	1.98	0.45
1:B:2096:UNK:C	1:B:2099:UNK:HG3	2.43	0.45
1:B:2769:ASP:OD1	1:B:2770:LEU:N	2.49	0.45
1:B:2785:ALA:HB1	1:B:2809:LEU:HG	1.97	0.45
1:B:2879:LEU:HD13	1:B:3009:VAL:HG11	1.98	0.45
1:C:585:HIS:CB	1:C:694:ASP:HB2	2.47	0.45
1:C:684:MET:HG3	1:C:895:THR:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1212:UNK:HG2	1:C:1342:ARG:CZ	2.47	0.45
1:C:1483:LYS:O	1:C:1487:ILE:HG23	2.17	0.45
1:A:222:LEU:HD13	1:A:248:ILE:HD12	1.99	0.45
1:A:381:ARG:O	1:A:384:GLN:HG2	2.17	0.45
1:A:544:ILE:O	1:A:546:HIS:N	2.41	0.45
1:A:684:MET:HG3	1:A:895:THR:HA	1.98	0.45
1:A:2427:UNK:O	1:A:2427:UNK:HG2	2.15	0.45
1:A:2770:LEU:HB3	1:A:2815:GLN:HB3	1.97	0.45
1:B:207:MET:HG3	1:B:292:VAL:HB	1.98	0.45
1:B:746:TYR:HB2	1:B:833:ALA:HB1	1.99	0.45
1:B:868:ARG:HD3	1:B:872:ARG:HH12	1.81	0.45
1:B:2246:ALA:N	1:B:2255:ARG:NH1	2.64	0.45
1:C:351:ILE:HB	1:C:375:ILE:HG12	1.99	0.45
1:C:511:ARG:CB	1:C:540:ASN:HB2	2.46	0.45
1:C:768:LYS:HA	1:C:775:LEU:HD11	1.97	0.45
1:C:2785:ALA:HB1	1:C:2809:LEU:HG	1.97	0.45
1:C:2790:MET:SD	1:C:2800:PHE:HB2	2.56	0.45
1:A:408:VAL:CG1	1:A:943:UNK:HG1	2.46	0.45
1:A:534:ASP:O	1:A:538:GLU:HG3	2.16	0.45
1:A:540:ASN:ND2	1:A:544:ILE:HG13	2.30	0.45
1:A:1001:UNK:O	1:A:1005:UNK:HB2	2.15	0.45
1:A:1702:GLU:OE1	1:A:1712:ALA:N	2.49	0.45
1:A:2070:LEU:O	1:A:2074:GLU:HG3	2.16	0.45
1:B:195:ARG:NH1	1:B:198:ILE:HD12	2.31	0.45
1:B:585:HIS:CB	1:B:694:ASP:HB2	2.47	0.45
1:B:1450:ALA:N	1:B:1613:ARG:O	2.48	0.45
1:B:1519:VAL:HG13	1:B:1530:LEU:HD23	1.98	0.45
1:C:167:ALA:HB3	1:C:178:LEU:HD21	1.98	0.45
1:C:1488:VAL:HB	1:C:1579:VAL:HG22	1.99	0.45
1:C:1553:ALA:O	1:C:1557:GLU:HG2	2.17	0.45
1:C:2630:ASP:HB3	1:C:2633:VAL:HG23	1.97	0.45
1:A:406:THR:OG1	1:A:418:GLU:OE1	2.34	0.45
1:A:768:LYS:HA	1:A:775:LEU:HD11	1.98	0.45
1:A:1072:TRP:HE1	1:A:1077:VAL:HG22	1.80	0.45
1:A:2080:UNK:HG2	1:A:2083:UNK:CG	2.45	0.45
1:A:2361:VAL:HG21	1:A:2401:ILE:HD11	1.98	0.45
1:B:534:ASP:O	1:B:538:GLU:HG3	2.16	0.45
1:B:1488:VAL:HB	1:B:1579:VAL:HG22	1.99	0.45
1:B:1605:LYS:H	1:B:1658:LYS:HE2	1.82	0.45
1:B:1996:PRO:O	1:B:2000:LEU:N	2.41	0.45
1:B:2137:GLU:O	1:B:2163:THR:N	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2212:TRP:HA	1:B:2229:LYS:HB3	1.98	0.45
1:B:2452:UNK:CG	1:B:2453:UNK:N	2.73	0.45
1:B:2452:UNK:HA	1:B:3017:ALA:HA	1.99	0.45
1:B:2790:MET:SD	1:B:2800:PHE:HB2	2.56	0.45
1:B:3080:ARG:CG	1:B:3080:ARG:NH1	2.72	0.45
1:C:747:LEU:HD22	1:C:751:ARG:CZ	2.47	0.45
1:C:763:SER:HB3	1:C:766:ASP:HB2	1.99	0.45
1:C:1684:ASP:HA	1:C:1687:PHE:HD2	1.82	0.45
1:A:195:ARG:NH1	1:A:198:ILE:HD12	2.31	0.45
1:B:763:SER:HB3	1:B:766:ASP:HB2	1.99	0.45
1:B:1212:UNK:HG2	1:B:1342:ARG:CZ	2.47	0.45
1:B:2361:VAL:HG21	1:B:2401:ILE:HD11	1.98	0.45
1:B:2845:PHE:HD2	1:B:2860:ALA:HA	1.81	0.45
1:C:195:ARG:NH1	1:C:198:ILE:HD12	2.31	0.45
1:C:222:LEU:HD13	1:C:248:ILE:HD12	1.99	0.45
1:C:784:GLU:OE2	1:C:816:LEU:HD21	2.16	0.45
1:C:1996:PRO:O	1:C:2000:LEU:N	2.41	0.45
1:C:2093:UNK:HG1	1:C:2132:UNK:HB1	1.95	0.45
1:C:2114:UNK:HA	1:C:2117:UNK:HG3	1.99	0.45
1:C:2610:ARG:NH1	1:C:2700:LEU:HD21	2.31	0.45
1:C:2769:ASP:OD1	1:C:2770:LEU:N	2.49	0.45
1:C:2770:LEU:HB3	1:C:2815:GLN:HB3	1.97	0.45
1:C:2845:PHE:HD2	1:C:2860:ALA:HA	1.81	0.45
1:A:351:ILE:HB	1:A:375:ILE:HG12	1.99	0.45
1:A:1605:LYS:H	1:A:1658:LYS:HE2	1.82	0.45
1:A:2591:ARG:HH12	1:C:2014:SER:H	1.65	0.45
1:B:167:ALA:HB3	1:B:178:LEU:HD21	1.98	0.45
1:B:222:LEU:HD21	1:B:236:VAL:HA	1.97	0.45
1:B:336:TRP:CH2	1:B:360:LEU:HD21	2.52	0.45
1:B:784:GLU:OE2	1:B:816:LEU:HD21	2.16	0.45
1:B:997:UNK:O	1:B:1009:UNK:HG3	2.17	0.45
1:B:1171:PRO:HA	1:B:1191:ARG:HG2	1.99	0.45
1:B:1284:GLY:HA2	1:B:1343:LEU:HD11	1.99	0.45
1:B:2610:ARG:NH1	1:B:2700:LEU:HD21	2.31	0.45
1:C:544:ILE:O	1:C:546:HIS:N	2.40	0.45
1:C:1072:TRP:HE1	1:C:1077:VAL:HG22	1.80	0.45
1:C:1634:ARG:NH1	1:C:1639:ALA:N	2.65	0.45
1:C:2296:ASN:HB3	1:C:2299:MET:SD	2.57	0.45
1:C:2672:TRP:CD1	1:C:2831:MET:HG2	2.52	0.45
1:C:2845:PHE:CD2	1:C:2860:ALA:HA	2.52	0.45
1:A:746:TYR:HB2	1:A:833:ALA:HB1	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:PHE:CZ	1:A:2433:UNK:CG	2.99	0.45
1:A:997:UNK:O	1:A:1009:UNK:HG3	2.17	0.45
1:A:1488:VAL:HB	1:A:1579:VAL:HG22	1.99	0.45
1:A:2014:SER:H	1:B:2591:ARG:HH12	1.65	0.45
1:A:2946:LEU:HD22	1:A:2994:VAL:HG23	1.98	0.45
1:B:381:ARG:O	1:B:384:GLN:HG2	2.17	0.45
1:B:544:ILE:O	1:B:546:HIS:N	2.41	0.45
1:B:2619:ARG:HH12	1:B:2779:GLY:HA2	1.81	0.45
1:C:868:ARG:HD3	1:C:872:ARG:HH12	1.81	0.45
1:C:1001:UNK:HG1	1:C:1018:ARG:HH21	1.80	0.45
1:C:1581:PHE:HB2	1:C:1586:LEU:HD22	1.99	0.45
1:C:2246:ALA:N	1:C:2255:ARG:HH12	2.15	0.45
1:C:2246:ALA:N	1:C:2255:ARG:NH1	2.64	0.45
1:C:2800:PHE:CE1	1:C:2812:LEU:HD22	2.50	0.45
1:C:2978:ARG:NH1	1:C:2979:GLU:OE2	2.49	0.45
1:A:210:VAL:HG22	1:A:287:PHE:HD1	1.83	0.44
1:A:984:UNK:HG1	1:A:987:UNK:CG	2.46	0.44
1:A:999:UNK:C	1:A:1007:UNK:HG3	2.46	0.44
1:A:1212:UNK:HG2	1:A:1342:ARG:CZ	2.47	0.44
1:A:2845:PHE:CD2	1:A:2860:ALA:HA	2.52	0.44
1:B:664:LEU:HB3	1:B:701:ALA:HB1	1.99	0.44
1:B:799:PHE:CZ	1:B:2433:UNK:CG	2.99	0.44
1:B:1285:LYS:HB3	1:B:1286:PRO:HD2	1.99	0.44
1:B:2300:PHE:CZ	1:B:2398:LEU:HB3	2.52	0.44
1:B:2427:UNK:O	1:B:2427:UNK:HG2	2.15	0.44
1:B:2891:LYS:HZ2	1:B:2903:GLU:HG2	1.82	0.44
1:C:365:ALA:O	1:C:369:ARG:N	2.42	0.44
1:C:664:LEU:HB3	1:C:701:ALA:HB1	1.99	0.44
1:C:997:UNK:O	1:C:1009:UNK:HG3	2.18	0.44
1:C:1702:GLU:OE1	1:C:1712:ALA:N	2.49	0.44
1:C:2891:LYS:HG3	1:C:2924:ILE:HD13	1.98	0.44
1:A:207:MET:HG3	1:A:292:VAL:HB	1.98	0.44
1:A:1304:LYS:O	1:A:1307:ASP:HB2	2.16	0.44
1:A:1634:ARG:NH1	1:A:1639:ALA:N	2.65	0.44
1:B:210:VAL:HG22	1:B:287:PHE:HD1	1.82	0.44
1:B:277:LEU:HD22	1:B:676:GLY:O	2.16	0.44
1:B:550:LYS:HD3	1:B:577:GLU:OE2	2.17	0.44
1:B:999:UNK:HG2	1:B:1007:UNK:HG1	1.96	0.44
1:B:1612:GLY:N	1:B:1623:PHE:O	2.48	0.44
1:B:2299:MET:H	1:B:2299:MET:HG2	1.68	0.44
1:C:207:MET:HG3	1:C:292:VAL:HB	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:VAL:HG22	1:C:287:PHE:HD1	1.83	0.44
1:C:671:THR:HB	1:C:682:ASN:CG	2.38	0.44
1:C:2300:PHE:CZ	1:C:2398:LEU:HB3	2.52	0.44
1:C:2452:UNK:HA	1:C:3017:ALA:HA	1.98	0.44
1:C:2543:PHE:HA	1:C:2624:GLN:HE22	1.81	0.44
1:C:2619:ARG:HH12	1:C:2779:GLY:HA2	1.81	0.44
1:C:2831:MET:HB3	1:C:2831:MET:HE2	1.88	0.44
1:A:47:ALA:O	1:A:353:ASP:HA	2.17	0.44
1:A:511:ARG:CB	1:A:540:ASN:HB2	2.46	0.44
1:A:664:LEU:HB3	1:A:701:ALA:HB1	1.99	0.44
1:A:2120:UNK:O	1:A:2123:UNK:CG	2.66	0.44
1:A:2246:ALA:N	1:A:2255:ARG:HH12	2.15	0.44
1:A:2300:PHE:CZ	1:A:2398:LEU:HB3	2.52	0.44
1:A:2452:UNK:CG	1:A:2453:UNK:N	2.73	0.44
1:A:2555:SER:HA	1:A:2556:PRO:HD2	1.84	0.44
1:B:684:MET:HG3	1:B:895:THR:HA	1.98	0.44
1:B:747:LEU:HD22	1:B:751:ARG:CZ	2.47	0.44
1:B:1350:TYR:CD1	1:B:1703:ILE:HD11	2.53	0.44
1:B:2080:UNK:HG2	1:B:2083:UNK:CG	2.45	0.44
1:B:2472:TYR:CZ	1:B:2930:LEU:HD22	2.52	0.44
1:C:336:TRP:CH2	1:C:360:LEU:HD21	2.52	0.44
1:C:1171:PRO:HA	1:C:1191:ARG:HG2	1.99	0.44
1:C:2209:LEU:O	1:C:2213:VAL:HG23	2.18	0.44
1:C:2891:LYS:HZ2	1:C:2903:GLU:HG2	1.83	0.44
1:A:583:GLY:HA2	1:A:892:ILE:HD13	2.00	0.44
1:A:1519:VAL:HG13	1:A:1530:LEU:HD23	1.99	0.44
1:B:44:TYR:O	1:B:153:VAL:N	2.44	0.44
1:B:222:LEU:HD13	1:B:248:ILE:HD12	1.99	0.44
1:B:999:UNK:C	1:B:1007:UNK:HG3	2.47	0.44
1:B:1553:ALA:O	1:B:1557:GLU:HG2	2.17	0.44
1:B:2083:UNK:HA	1:B:2086:UNK:HG3	2.00	0.44
1:C:583:GLY:HA2	1:C:892:ILE:HD13	2.00	0.44
1:C:1605:LYS:H	1:C:1658:LYS:HE2	1.82	0.44
1:C:2080:UNK:HG2	1:C:2083:UNK:CG	2.45	0.44
1:C:2889:ILE:HD11	1:C:2922:LEU:HD22	1.98	0.44
1:A:475:LEU:HD23	1:A:475:LEU:HA	1.79	0.44
1:A:671:THR:HB	1:A:682:ASN:CG	2.38	0.44
1:A:1284:GLY:HA2	1:A:1343:LEU:HD11	1.99	0.44
1:A:1350:TYR:CD1	1:A:1703:ILE:HD11	2.53	0.44
1:A:2014:SER:N	1:B:2591:ARG:NH1	2.66	0.44
1:A:2452:UNK:HA	1:A:3017:ALA:HA	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2472:TYR:CZ	1:A:2930:LEU:HD22	2.52	0.44
1:A:2591:ARG:NH1	1:C:2014:SER:N	2.66	0.44
1:A:2619:ARG:HH12	1:A:2779:GLY:HA2	1.81	0.44
1:B:515:ALA:HA	1:B:516:PRO:HD3	1.84	0.44
1:B:1225:UNK:HG1	1:B:1283:ASP:CG	2.34	0.44
1:B:1503:ILE:HB	1:B:1542:TYR:HB2	2.00	0.44
1:B:2296:ASN:HB3	1:B:2299:MET:SD	2.57	0.44
1:B:2334:HIS:CD2	1:B:2391:LYS:HG3	2.50	0.44
1:C:970:ILE:HG23	1:C:992:UNK:HG1	2.00	0.44
1:C:1093:PRO:HB3	1:C:1277:HIS:CE1	2.52	0.44
1:A:2234:PRO:HB2	1:A:2287:LEU:HD13	1.98	0.44
1:A:2769:ASP:OD1	1:A:2770:LEU:N	2.49	0.44
1:B:1634:ARG:NH1	1:B:1639:ALA:N	2.65	0.44
1:B:1684:ASP:HA	1:B:1687:PHE:HD2	1.82	0.44
1:B:1723:GLU:O	1:B:1725:SER:N	2.51	0.44
1:B:2114:UNK:HA	1:B:2117:UNK:HG3	1.99	0.44
1:B:2246:ALA:N	1:B:2255:ARG:HH12	2.15	0.44
1:C:793:ARG:HA	1:C:2435:UNK:HG1	1.97	0.44
1:C:1350:TYR:CD1	1:C:1703:ILE:HD11	2.53	0.44
1:C:1723:GLU:O	1:C:1725:SER:N	2.51	0.44
1:C:2119:UNK:HG2	1:C:2120:UNK:N	2.33	0.44
1:C:2471:PRO:HA	1:C:2625:ILE:HA	2.00	0.44
1:C:2580:PHE:HE1	1:C:2603:ARG:HH21	1.66	0.44
1:A:88:SER:HB3	1:A:314:THR:OG1	2.18	0.44
1:A:412:ASP:H	1:A:1025:VAL:CG2	2.31	0.44
1:A:550:LYS:HD3	1:A:577:GLU:OE2	2.17	0.44
1:A:585:HIS:CB	1:A:694:ASP:HB2	2.47	0.44
1:A:657:THR:HB	1:A:662:LYS:HE3	2.00	0.44
1:A:1705:VAL:O	1:A:1735:GLU:HB2	2.18	0.44
1:A:2296:ASN:HB3	1:A:2299:MET:SD	2.57	0.44
1:B:671:THR:HB	1:B:682:ASN:CG	2.38	0.44
1:B:782:ARG:NH1	1:B:857:VAL:HG22	2.33	0.44
1:B:944:UNK:O	1:B:944:UNK:CG	2.59	0.44
1:B:1537:LEU:HD13	1:B:1541:GLN:HB2	2.00	0.44
1:B:2014:SER:H	1:C:2591:ARG:HH12	1.65	0.44
1:B:2209:LEU:O	1:B:2213:VAL:HG23	2.18	0.44
1:B:2297:ARG:HH22	1:B:2391:LYS:HZ3	1.65	0.44
1:C:745:THR:OG1	1:C:834:GLU:O	2.19	0.44
1:C:782:ARG:NH1	1:C:857:VAL:HG22	2.33	0.44
1:C:1284:GLY:HA2	1:C:1343:LEU:HD11	1.99	0.44
1:C:1537:LEU:HD13	1:C:1541:GLN:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1582:HIS:HA	1:C:1674:ALA:O	2.18	0.44
1:A:163:LEU:HD13	1:A:181:LEU:HD23	2.00	0.44
1:A:763:SER:HB3	1:A:766:ASP:HB2	1.99	0.44
1:A:1171:PRO:HA	1:A:1191:ARG:HG2	1.99	0.44
1:A:1581:PHE:HB2	1:A:1586:LEU:HD22	1.99	0.44
1:A:2013:LEU:HD23	1:A:2013:LEU:HA	1.87	0.44
1:A:2252:VAL:HG22	1:A:2255:ARG:HH21	1.82	0.44
1:B:408:VAL:CG1	1:B:943:UNK:HG1	2.46	0.44
1:B:2845:PHE:CD2	1:B:2860:ALA:HA	2.52	0.44
1:C:393:VAL:HG12	1:C:394:PRO:N	2.32	0.44
1:C:2122:UNK:O	1:C:2125:UNK:CG	2.63	0.44
1:C:2334:HIS:CD2	1:C:2391:LYS:HG3	2.50	0.44
1:C:2958:ASN:HD22	1:C:2976:TRP:HE1	1.65	0.44
1:A:1553:ALA:O	1:A:1557:GLU:HG2	2.17	0.44
1:A:1684:ASP:HA	1:A:1687:PHE:HD2	1.82	0.44
1:A:2094:UNK:HG1	1:A:2096:UNK:HG3	1.90	0.44
1:B:647:THR:OG1	2:B:4000:FMN:O3P	2.27	0.44
1:B:995:UNK:HB1	1:B:1011:UNK:HG2	1.99	0.44
1:B:1483:LYS:O	1:B:1487:ILE:HG23	2.17	0.44
1:B:2119:UNK:HG2	1:B:2120:UNK:N	2.33	0.44
1:B:2462:VAL:HG13	1:B:2835:VAL:HG13	2.00	0.44
1:B:2753:LYS:HA	1:B:2753:LYS:HD3	1.83	0.44
1:B:2958:ASN:HD22	1:B:2976:TRP:HE1	1.65	0.44
1:C:550:LYS:HD3	1:C:577:GLU:OE2	2.17	0.44
1:C:857:VAL:HG13	1:C:859:PHE:H	1.83	0.44
1:C:1285:LYS:HB3	1:C:1286:PRO:HD2	1.99	0.44
1:C:1733:ASN:H	1:C:1737:ASP:HB2	1.83	0.44
1:A:782:ARG:NH1	1:A:857:VAL:HG22	2.33	0.43
1:A:981:UNK:CG	1:A:987:UNK:C	2.96	0.43
1:A:1093:PRO:HB3	1:A:1277:HIS:CE1	2.52	0.43
1:A:1133:VAL:N	1:A:1193:ALA:O	2.48	0.43
1:A:1268:GLY:HA2	1:A:1271:LEU:HD12	1.99	0.43
1:A:1285:LYS:HB3	1:A:1286:PRO:HD2	1.99	0.43
1:A:1733:ASN:H	1:A:1737:ASP:HB2	1.83	0.43
1:A:2083:UNK:HA	1:A:2086:UNK:HG3	2.00	0.43
1:A:2297:ARG:HH22	1:A:2391:LYS:HZ3	1.66	0.43
1:A:2989:LEU:HD12	1:A:2989:LEU:HA	1.77	0.43
1:B:344:HIS:CD2	1:B:373:ILE:HG13	2.53	0.43
1:B:583:GLY:HA2	1:B:892:ILE:HD13	2.00	0.43
1:B:602:ARG:NH2	1:B:641:ASP:OD1	2.27	0.43
1:B:657:THR:HB	1:B:662:LYS:HE3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1093:PRO:HB3	1:B:1277:HIS:CE1	2.52	0.43
1:B:2903:GLU:OE2	1:B:2995:THR:OG1	2.36	0.43
1:C:931:UNK:HG3	1:C:934:UNK:HG3	2.00	0.43
1:C:2120:UNK:O	1:C:2123:UNK:CG	2.65	0.43
1:C:2710:LEU:O	1:C:2713:VAL:HG22	2.18	0.43
1:A:336:TRP:CH2	1:A:360:LEU:HD21	2.52	0.43
1:A:602:ARG:NH2	1:A:641:ASP:OD1	2.27	0.43
1:A:695:ILE:HG22	1:A:697:GLU:HG3	2.01	0.43
1:A:982:UNK:CG	1:A:983:UNK:N	2.76	0.43
1:A:999:UNK:HG2	1:A:1007:UNK:HG1	1.96	0.43
1:A:3044:ALA:HB1	1:A:3050:PRO:HB3	2.00	0.43
1:B:340:ILE:HD11	1:B:351:ILE:HD13	2.01	0.43
1:B:2070:LEU:O	1:B:2074:GLU:HG3	2.16	0.43
1:B:2120:UNK:O	1:B:2123:UNK:CG	2.66	0.43
1:C:34:LEU:O	1:C:38:LEU:HG	2.18	0.43
1:C:874:ASP:OD2	1:C:877:TRP:CD1	2.72	0.43
1:C:1133:VAL:O	1:C:1193:ALA:N	2.42	0.43
1:C:1163:ASP:HA	1:C:1168:ARG:HA	2.01	0.43
1:A:393:VAL:HG12	1:A:394:PRO:N	2.32	0.43
1:A:641:ASP:OD1	1:A:641:ASP:N	2.48	0.43
1:A:2114:UNK:HA	1:A:2117:UNK:HG3	1.99	0.43
1:B:970:ILE:HG23	1:B:992:UNK:HG1	2.00	0.43
1:B:1705:VAL:O	1:B:1735:GLU:HB2	2.18	0.43
1:C:981:UNK:HG2	1:C:988:UNK:HA	2.01	0.43
1:C:1268:GLY:HA2	1:C:1271:LEU:HD12	2.00	0.43
1:C:1612:GLY:N	1:C:1623:PHE:O	2.48	0.43
1:C:2180:LYS:HZ1	1:C:2962:ASP:HB3	1.82	0.43
1:C:2462:VAL:HG13	1:C:2835:VAL:HG13	2.00	0.43
1:A:341:THR:HG23	1:A:344:HIS:ND1	2.34	0.43
1:A:580:ARG:HD3	1:A:896:ALA:HB3	2.01	0.43
1:A:1582:HIS:HA	1:A:1674:ALA:O	2.18	0.43
1:A:2541:ARG:O	1:A:2621:VAL:HG13	2.18	0.43
1:B:393:VAL:HG12	1:B:394:PRO:N	2.32	0.43
1:B:857:VAL:HG13	1:B:859:PHE:H	1.83	0.43
1:B:981:UNK:CG	1:B:987:UNK:C	2.96	0.43
1:B:2541:ARG:O	1:B:2621:VAL:HG13	2.18	0.43
1:B:2580:PHE:HE1	1:B:2603:ARG:HH21	1.66	0.43
1:B:2710:LEU:O	1:B:2713:VAL:HG22	2.18	0.43
1:C:657:THR:HB	1:C:662:LYS:HE3	2.00	0.43
1:C:2115:UNK:HA	1:C:2118:UNK:CG	2.49	0.43
1:A:344:HIS:CD2	1:A:373:ILE:HG13	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1163:ASP:HA	1:A:1168:ARG:HA	2.01	0.43
1:A:1723:GLU:O	1:A:1725:SER:N	2.51	0.43
1:A:2209:LEU:O	1:A:2213:VAL:HG23	2.18	0.43
1:B:516:PRO:HA	1:B:962:MET:SD	2.58	0.43
1:B:1268:GLY:HA2	1:B:1271:LEU:HD12	1.99	0.43
1:B:2092:UNK:O	1:B:2092:UNK:CG	2.64	0.43
1:B:2471:PRO:HA	1:B:2625:ILE:HA	2.00	0.43
1:B:2512:TRP:O	1:B:2520:LEU:HD12	2.19	0.43
1:C:276:LYS:HB3	1:C:587:TRP:CH2	2.53	0.43
1:C:647:THR:N	2:C:4000:FMN:O3P	2.51	0.43
1:C:1519:VAL:HG13	1:C:1530:LEU:HD23	1.99	0.43
1:C:2095:UNK:C	1:C:2098:UNK:HG3	2.49	0.43
1:C:2706:PRO:O	1:C:2709:ILE:HG12	2.19	0.43
1:C:3044:ALA:HB1	1:C:3050:PRO:HB3	2.00	0.43
1:A:315:VAL:C	1:A:317:LEU:H	2.22	0.43
1:A:874:ASP:OD2	1:A:877:TRP:CD1	2.71	0.43
1:A:2297:ARG:HH12	1:A:2391:LYS:NZ	2.17	0.43
1:A:2462:VAL:HG13	1:A:2835:VAL:HG13	2.00	0.43
1:A:2591:ARG:HH12	1:C:2014:SER:N	2.16	0.43
1:B:276:LYS:HB3	1:B:587:TRP:CH2	2.53	0.43
1:B:315:VAL:C	1:B:317:LEU:H	2.22	0.43
1:B:412:ASP:H	1:B:1025:VAL:CG2	2.31	0.43
1:B:1581:PHE:HB2	1:B:1586:LEU:HD22	1.99	0.43
1:B:2426:UNK:O	1:B:2426:UNK:HG2	2.18	0.43
1:B:2610:ARG:NH1	1:B:2700:LEU:HD11	2.25	0.43
1:C:163:LEU:HD13	1:C:181:LEU:HD23	2.00	0.43
1:C:340:ILE:HD11	1:C:351:ILE:HD13	2.01	0.43
1:C:344:HIS:CD2	1:C:373:ILE:HG13	2.53	0.43
1:C:580:ARG:HD3	1:C:896:ALA:HB3	2.01	0.43
1:C:695:ILE:HG22	1:C:697:GLU:HG3	2.00	0.43
1:C:782:ARG:HH11	1:C:857:VAL:HG22	1.83	0.43
1:C:999:UNK:C	1:C:1007:UNK:HG3	2.47	0.43
1:C:2083:UNK:HA	1:C:2086:UNK:HG3	2.00	0.43
1:A:857:VAL:HG13	1:A:859:PHE:H	1.83	0.43
1:A:931:UNK:HG3	1:A:934:UNK:HG3	2.01	0.43
1:A:2471:PRO:HA	1:A:2625:ILE:HA	2.00	0.43
1:A:2891:LYS:HZ2	1:A:2903:GLU:HG2	1.83	0.43
1:B:658:SER:HB2	1:B:661:VAL:HG23	2.01	0.43
1:B:940:UNK:O	1:B:940:UNK:CG	2.60	0.43
1:B:1582:HIS:HA	1:B:1674:ALA:O	2.18	0.43
1:B:2786:ASP:OD2	1:B:2789:MET:HG2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:SER:HB3	1:C:314:THR:OG1	2.18	0.43
1:C:1705:VAL:O	1:C:1735:GLU:HB2	2.18	0.43
1:C:2903:GLU:OE2	1:C:2995:THR:OG1	2.36	0.43
1:A:276:LYS:HB3	1:A:587:TRP:CH2	2.53	0.43
1:A:408:VAL:HG13	1:A:943:UNK:CG	2.48	0.43
1:A:1070:VAL:N	1:A:1152:PHE:O	2.52	0.43
1:A:2710:LEU:O	1:A:2713:VAL:HG22	2.18	0.43
1:A:2903:GLU:OE2	1:A:2995:THR:OG1	2.36	0.43
1:A:2958:ASN:HD22	1:A:2976:TRP:HE1	1.65	0.43
1:B:34:LEU:O	1:B:38:LEU:HG	2.18	0.43
1:B:88:SER:HB3	1:B:314:THR:OG1	2.18	0.43
1:B:488:ASN:OD1	1:B:523:SER:OG	2.34	0.43
1:B:647:THR:N	2:B:4000:FMN:O3P	2.51	0.43
1:B:856:PRO:HG2	1:B:874:ASP:HB2	2.00	0.43
1:B:931:UNK:HG3	1:B:934:UNK:HG3	2.01	0.43
1:B:981:UNK:HG2	1:B:988:UNK:HA	2.00	0.43
1:B:1021:LEU:HB3	1:B:1034:GLU:HG2	2.01	0.43
1:B:1619:VAL:HA	1:B:1620:PRO:HD2	1.80	0.43
1:B:2014:SER:N	1:C:2591:ARG:NH1	2.66	0.43
1:C:613:GLY:HA2	2:C:4000:FMN:O5'	2.19	0.43
1:C:2064:ARG:HG2	1:C:2100:UNK:HG1	2.01	0.43
1:C:2810:GLY:HA2	1:C:2896:THR:HG22	2.01	0.43
1:A:34:LEU:O	1:A:38:LEU:HG	2.19	0.43
1:A:340:ILE:HD11	1:A:351:ILE:HD13	2.01	0.43
1:A:709:LEU:HD21	1:A:872:ARG:NE	2.34	0.43
1:A:981:UNK:HG2	1:A:988:UNK:HA	2.01	0.43
1:A:1352:PHE:HA	1:A:1353:PRO:HD3	1.72	0.43
1:A:1503:ILE:HB	1:A:1542:TYR:HB2	2.00	0.43
1:A:2119:UNK:HG2	1:A:2120:UNK:N	2.34	0.43
1:A:2122:UNK:O	1:A:2125:UNK:CG	2.63	0.43
1:A:2299:MET:H	1:A:2299:MET:HG2	1.68	0.43
1:A:2530:TYR:O	1:A:2533:ALA:N	2.52	0.43
1:A:2706:PRO:O	1:A:2709:ILE:HG12	2.19	0.43
1:A:2786:ASP:OD2	1:A:2789:MET:HG2	2.19	0.43
1:B:163:LEU:HD13	1:B:181:LEU:HD23	2.00	0.43
1:B:307:ILE:HG22	1:B:311:TRP:CE2	2.54	0.43
1:B:511:ARG:CB	1:B:540:ASN:HB2	2.46	0.43
1:B:780:ARG:NH1	1:B:817:GLU:OE2	2.52	0.43
1:B:782:ARG:HH11	1:B:857:VAL:HG22	1.83	0.43
1:B:1133:VAL:N	1:B:1193:ALA:O	2.48	0.43
1:B:1317:GLY:O	1:B:1324:VAL:HG12	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2665:THR:HA	1:B:2666:PRO:HD3	1.86	0.43
1:B:3044:ALA:HB1	1:B:3050:PRO:HB3	2.00	0.43
1:C:475:LEU:HD23	1:C:475:LEU:HA	1.79	0.43
1:C:856:PRO:HG2	1:C:874:ASP:HB2	2.00	0.43
1:C:2530:TYR:O	1:C:2533:ALA:N	2.52	0.43
1:A:780:ARG:NH1	1:A:817:GLU:OE2	2.52	0.43
1:A:885:GLU:HG2	1:A:887:ASP:H	1.84	0.43
1:A:999:UNK:HG2	1:A:1007:UNK:HG3	1.96	0.43
1:A:1084:THR:CG2	1:A:1274:ALA:HA	2.48	0.43
1:A:2092:UNK:O	1:A:2092:UNK:CG	2.64	0.43
1:A:2244:ARG:HG2	1:A:2245:VAL:N	2.34	0.43
1:A:2580:PHE:HE1	1:A:2603:ARG:HH21	1.66	0.43
1:A:2695:MET:HG3	1:A:2696:TYR:N	2.34	0.43
1:B:393:VAL:O	1:B:395:GLU:N	2.52	0.43
1:B:695:ILE:HG22	1:B:697:GLU:HG3	2.00	0.43
1:B:2810:GLY:HA2	1:B:2896:THR:HG22	2.01	0.43
1:C:1117:ALA:HA	1:C:1120:GLU:HB2	2.01	0.43
1:C:2058:ASP:OD1	1:C:2058:ASP:N	2.46	0.43
1:C:2096:UNK:CG	1:C:2097:UNK:N	2.82	0.43
1:C:2137:GLU:O	1:C:2163:THR:N	2.30	0.43
1:C:2557:LEU:HB3	1:C:2613:ARG:HB2	2.01	0.43
1:A:782:ARG:HH11	1:A:857:VAL:HG22	1.83	0.42
1:A:1087:PHE:HD2	1:B:117:LYS:HZ1	1.67	0.42
1:A:2426:UNK:O	1:A:2426:UNK:HG2	2.18	0.42
1:B:874:ASP:OD2	1:B:877:TRP:CD1	2.72	0.42
1:B:1087:PHE:CZ	1:C:203:ASP:OD2	2.72	0.42
1:B:1733:ASN:H	1:B:1737:ASP:HB2	1.83	0.42
1:B:2014:SER:N	1:C:2591:ARG:HH12	2.16	0.42
1:B:2244:ARG:HG2	1:B:2245:VAL:N	2.34	0.42
1:B:2957:PRO:HB3	1:B:2980:PRO:N	2.34	0.42
1:C:78:GLU:HB2	1:C:176:VAL:HG21	2.01	0.42
1:C:1084:THR:CG2	1:C:1274:ALA:HA	2.49	0.42
1:C:1317:GLY:O	1:C:1324:VAL:HG12	2.19	0.42
1:C:1660:LEU:HD23	1:C:1660:LEU:HA	1.86	0.42
1:C:2426:UNK:O	1:C:2426:UNK:HG2	2.18	0.42
1:C:2541:ARG:O	1:C:2621:VAL:HG13	2.18	0.42
1:C:2889:ILE:HB	1:C:2924:ILE:HG12	2.01	0.42
1:A:1662:ARG:HG3	1:A:1663:LYS:N	2.34	0.42
1:A:2810:GLY:HA2	1:A:2896:THR:HG22	2.01	0.42
1:B:355:GLY:HA2	1:B:356:PRO:HD3	1.86	0.42
1:B:1117:ALA:HA	1:B:1120:GLU:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1551:LEU:HD13	1:B:1551:LEU:HA	1.80	0.42
1:B:2115:UNK:HA	1:B:2118:UNK:CG	2.48	0.42
1:B:2180:LYS:HZ1	1:B:2962:ASP:HB3	1.82	0.42
1:B:2296:ASN:ND2	1:B:2395:THR:HG21	2.34	0.42
1:B:2706:PRO:O	1:B:2709:ILE:HG12	2.19	0.42
1:B:2800:PHE:CE1	1:B:2812:LEU:HD22	2.50	0.42
1:B:2891:LYS:HZ1	1:B:2904:THR:N	2.17	0.42
1:C:341:THR:HG23	1:C:344:HIS:ND1	2.34	0.42
1:C:516:PRO:HA	1:C:962:MET:SD	2.58	0.42
1:C:709:LEU:HD21	1:C:872:ARG:NE	2.34	0.42
1:C:1533:VAL:N	1:C:1543:ALA:O	2.52	0.42
1:C:1662:ARG:HG3	1:C:1663:LYS:N	2.34	0.42
1:C:2077:UNK:CG	1:C:2079:UNK:HG3	2.41	0.42
1:C:2141:VAL:HG22	1:C:2238:PHE:HD2	1.85	0.42
1:A:211:THR:HB	1:A:286:VAL:HB	2.02	0.42
1:A:613:GLY:HA2	2:A:4000:FMN:O5'	2.19	0.42
1:A:1504:ARG:HA	1:A:1540:SER:O	2.19	0.42
1:A:2095:UNK:C	1:A:2098:UNK:HG3	2.49	0.42
1:A:2141:VAL:HG22	1:A:2238:PHE:HD2	1.85	0.42
1:A:2808:ARG:HH21	1:A:2901:PRO:HD3	1.85	0.42
1:A:2957:PRO:HB3	1:A:2980:PRO:N	2.34	0.42
1:B:45:ALA:O	1:B:351:ILE:HA	2.20	0.42
1:B:2122:UNK:O	1:B:2125:UNK:CG	2.63	0.42
1:B:2252:VAL:HG22	1:B:2255:ARG:HH21	1.82	0.42
1:B:2911:ALA:O	1:B:2916:ARG:HB2	2.19	0.42
1:C:307:ILE:HG22	1:C:311:TRP:CE2	2.54	0.42
1:C:438:THR:HA	1:C:880:HIS:CE1	2.51	0.42
1:C:999:UNK:HG2	1:C:1007:UNK:HG1	1.96	0.42
1:C:1275:ALA:HB2	1:C:1311:PHE:CE2	2.55	0.42
1:A:516:PRO:HA	1:A:962:MET:SD	2.58	0.42
1:A:970:ILE:HG23	1:A:992:UNK:HG1	2.00	0.42
1:A:1106:CYS:SG	1:A:1174:VAL:HG11	2.60	0.42
1:A:1317:GLY:O	1:A:1324:VAL:HG12	2.19	0.42
1:A:2105:UNK:C	1:A:2108:UNK:HG3	2.34	0.42
1:B:53:SER:HA	1:B:359:ILE:HG13	2.01	0.42
1:B:1163:ASP:HA	1:B:1168:ARG:HA	2.01	0.42
1:B:2095:UNK:C	1:B:2098:UNK:HG3	2.49	0.42
1:C:2252:VAL:HG22	1:C:2255:ARG:HH21	1.82	0.42
1:C:2584:ASP:O	1:C:2586:GLU:N	2.53	0.42
1:A:107:LEU:HD13	1:A:113:VAL:HB	2.02	0.42
1:A:1021:LEU:HB3	1:A:1034:GLU:HG2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1087:PHE:CZ	1:B:203:ASP:OD2	2.72	0.42
1:A:1280:THR:O	1:A:1288:PRO:HB3	2.20	0.42
1:A:1399:ASN:HA	1:A:1400:PRO:HD3	1.86	0.42
1:A:1537:LEU:HD13	1:A:1541:GLN:HB2	2.00	0.42
1:A:2512:TRP:O	1:A:2520:LEU:HD12	2.19	0.42
1:B:211:THR:HB	1:B:286:VAL:HB	2.01	0.42
1:B:341:THR:HG23	1:B:344:HIS:ND1	2.34	0.42
1:B:1280:THR:O	1:B:1288:PRO:HB3	2.20	0.42
1:B:1660:LEU:HD23	1:B:1660:LEU:HA	1.85	0.42
1:B:2444:UNK:HB2	1:B:2988:PRO:HB3	2.01	0.42
1:B:2695:MET:HG3	1:B:2696:TYR:N	2.34	0.42
1:B:2836:LEU:HD23	1:B:2836:LEU:HA	1.87	0.42
1:C:981:UNK:CG	1:C:987:UNK:C	2.96	0.42
1:C:999:UNK:HG2	1:C:1007:UNK:HG3	1.96	0.42
1:C:1106:CYS:SG	1:C:1174:VAL:HG11	2.60	0.42
1:C:2244:ARG:HG2	1:C:2245:VAL:N	2.34	0.42
1:C:2444:UNK:HB2	1:C:2988:PRO:HB3	2.01	0.42
1:C:2512:TRP:O	1:C:2520:LEU:HD12	2.19	0.42
1:C:2620:THR:OG1	1:C:2791:ARG:NH2	2.53	0.42
1:C:2911:ALA:O	1:C:2916:ARG:HB2	2.19	0.42
1:C:2961:LEU:HD22	1:C:2976:TRP:HD1	1.85	0.42
1:A:2610:ARG:NH1	1:A:2700:LEU:HD11	2.25	0.42
1:A:2805:ASP:OD2	1:A:2807:ARG:HB2	2.20	0.42
1:B:42:GLU:HA	1:B:43:PRO:HD3	1.91	0.42
1:B:107:LEU:HD13	1:B:113:VAL:HB	2.01	0.42
1:B:613:GLY:HA2	2:B:4000:FMN:O5'	2.19	0.42
1:B:2294:SER:HB3	1:B:2310:LYS:HB2	2.02	0.42
1:B:2297:ARG:HH12	1:B:2391:LYS:NZ	2.17	0.42
1:B:2889:ILE:HB	1:B:2924:ILE:HG12	2.01	0.42
1:C:45:ALA:O	1:C:351:ILE:HA	2.20	0.42
1:C:970:ILE:O	1:C:974:UNK:HG3	2.20	0.42
1:C:1504:ARG:HA	1:C:1540:SER:O	2.19	0.42
1:C:1637:VAL:HA	1:C:1638:PRO:HD2	1.91	0.42
1:C:2297:ARG:HH12	1:C:2391:LYS:NZ	2.17	0.42
1:C:2846:ALA:O	1:C:2859:GLY:HA3	2.19	0.42
1:C:3065:PRO:O	1:C:3069:GLN:N	2.42	0.42
1:A:307:ILE:HG22	1:A:311:TRP:CE2	2.54	0.42
1:A:647:THR:N	2:A:4000:FMN:O3P	2.51	0.42
1:A:856:PRO:HG2	1:A:874:ASP:HB2	2.00	0.42
1:A:1275:ALA:O	1:A:1279:VAL:HG23	2.20	0.42
1:A:2115:UNK:HA	1:A:2118:UNK:CG	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2889:ILE:HG13	1:A:2922:LEU:HD13	2.02	0.42
1:A:2911:ALA:O	1:A:2916:ARG:HB2	2.19	0.42
1:B:479:LEU:HD21	1:B:485:ILE:HD11	2.02	0.42
1:B:668:THR:HG23	1:B:683:GLY:HA3	2.02	0.42
1:B:885:GLU:HG2	1:B:887:ASP:H	1.84	0.42
1:B:1275:ALA:HB2	1:B:1311:PHE:CE2	2.55	0.42
1:B:1504:ARG:HA	1:B:1540:SER:O	2.19	0.42
1:B:1656:LYS:N	1:B:1657:PRO:HD2	2.35	0.42
1:B:1703:ILE:HG22	1:B:1704:GLY:H	1.85	0.42
1:C:50:GLY:O	1:C:53:SER:OG	2.36	0.42
1:C:658:SER:HB2	1:C:661:VAL:HG23	2.01	0.42
1:C:780:ARG:NH1	1:C:817:GLU:OE2	2.52	0.42
1:C:795:HIS:NE2	1:C:797:GLN:HB2	2.35	0.42
1:C:1120:GLU:HA	1:C:1125:VAL:CG2	2.50	0.42
1:C:2120:UNK:C	1:C:2123:UNK:HG3	2.50	0.42
1:C:2125:UNK:CA	1:C:2128:UNK:HG3	2.49	0.42
1:C:2297:ARG:HH22	1:C:2391:LYS:HZ3	1.67	0.42
1:C:2891:LYS:NZ	1:C:2903:GLU:HB3	2.35	0.42
1:A:336:TRP:HE3	1:A:339:GLU:OE2	2.03	0.42
1:A:488:ASN:OD1	1:A:523:SER:OG	2.34	0.42
1:A:1687:PHE:CE1	1:A:1723:GLU:HG2	2.55	0.42
1:A:2296:ASN:ND2	1:A:2395:THR:HG21	2.34	0.42
1:B:436:THR:OG1	1:B:437:PRO:HD3	2.19	0.42
1:B:999:UNK:O	1:B:1007:UNK:CG	2.61	0.42
1:B:2300:PHE:HZ	1:B:2398:LEU:HB3	1.85	0.42
1:B:2620:THR:OG1	1:B:2791:ARG:NH2	2.53	0.42
1:B:2846:ALA:O	1:B:2859:GLY:HA3	2.19	0.42
1:B:2961:LEU:HD22	1:B:2976:TRP:HD1	1.85	0.42
1:C:315:VAL:C	1:C:317:LEU:H	2.22	0.42
1:C:336:TRP:HE3	1:C:339:GLU:OE2	2.03	0.42
1:C:412:ASP:H	1:C:1025:VAL:CG2	2.31	0.42
1:C:479:LEU:HD21	1:C:485:ILE:HD11	2.02	0.42
1:C:957:LEU:O	1:C:1034:GLU:HB2	2.20	0.42
1:C:1021:LEU:HB3	1:C:1034:GLU:HG2	2.01	0.42
1:C:1503:ILE:HB	1:C:1542:TYR:HB2	2.00	0.42
1:C:1656:LYS:N	1:C:1657:PRO:HD2	2.35	0.42
1:C:2113:UNK:HG2	1:C:2114:UNK:N	2.35	0.42
1:A:78:GLU:HB2	1:A:176:VAL:HG21	2.01	0.42
1:A:658:SER:HB2	1:A:661:VAL:HG23	2.01	0.42
1:A:1228:VAL:HB	1:A:1311:PHE:HB2	2.02	0.42
1:A:1380:ALA:HB1	1:A:1474:LEU:CD1	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2055:VAL:HG22	1:A:2194:TRP:CD1	2.55	0.42
1:A:2064:ARG:HG2	1:A:2100:UNK:HG1	2.01	0.42
1:A:2584:ASP:O	1:A:2586:GLU:N	2.53	0.42
1:A:2620:THR:OG1	1:A:2791:ARG:NH2	2.53	0.42
1:A:2753:LYS:HD3	1:A:2753:LYS:HA	1.83	0.42
1:A:2846:ALA:O	1:A:2859:GLY:HA3	2.20	0.42
1:B:408:VAL:HG13	1:B:943:UNK:CG	2.48	0.42
1:B:2530:TYR:O	1:B:2533:ALA:N	2.52	0.42
1:B:2557:LEU:HB3	1:B:2613:ARG:HB2	2.01	0.42
1:B:2800:PHE:CZ	1:B:2812:LEU:HD13	2.55	0.42
1:C:53:SER:HA	1:C:359:ILE:HG13	2.01	0.42
1:C:436:THR:OG1	1:C:437:PRO:HD3	2.19	0.42
1:C:1275:ALA:O	1:C:1279:VAL:HG23	2.20	0.42
1:C:1280:THR:O	1:C:1288:PRO:HB3	2.20	0.42
1:C:2294:SER:HB3	1:C:2310:LYS:HB2	2.02	0.42
1:A:436:THR:OG1	1:A:437:PRO:HD3	2.19	0.42
1:A:668:THR:HG23	1:A:683:GLY:HA3	2.02	0.42
1:A:1008:UNK:O	1:A:1008:UNK:CG	2.67	0.42
1:A:1275:ALA:HB2	1:A:1311:PHE:CE2	2.55	0.42
1:A:1460:ALA:O	1:A:1464:VAL:HG22	2.20	0.42
1:A:2123:UNK:CA	1:A:2126:UNK:HG3	2.50	0.42
1:A:2125:UNK:CA	1:A:2128:UNK:HG3	2.49	0.42
1:A:2800:PHE:CZ	1:A:2812:LEU:HD13	2.55	0.42
1:B:970:ILE:O	1:B:974:UNK:HG3	2.20	0.42
1:B:2055:VAL:HG22	1:B:2194:TRP:CD1	2.55	0.42
1:B:2584:ASP:O	1:B:2586:GLU:N	2.53	0.42
1:B:2892:HIS:HA	1:B:2942:GLN:HE22	1.85	0.42
1:C:668:THR:HG23	1:C:683:GLY:HA3	2.02	0.42
1:C:1228:VAL:HB	1:C:1311:PHE:HB2	2.02	0.42
1:C:2354:SER:O	1:C:2358:GLU:HG3	2.20	0.42
1:C:2957:PRO:HB3	1:C:2980:PRO:N	2.34	0.42
1:A:53:SER:HA	1:A:359:ILE:HG13	2.01	0.41
1:A:203:ASP:OD2	1:C:1087:PHE:CZ	2.72	0.41
1:A:976:UNK:O	1:A:976:UNK:CG	2.68	0.41
1:A:1117:ALA:HA	1:A:1120:GLU:HB2	2.01	0.41
1:A:1656:LYS:N	1:A:1657:PRO:HD2	2.35	0.41
1:A:2014:SER:N	1:B:2591:ARG:HH12	2.16	0.41
1:A:2096:UNK:CG	1:A:2097:UNK:N	2.82	0.41
1:A:2300:PHE:HZ	1:A:2398:LEU:HB3	1.85	0.41
1:A:2891:LYS:NZ	1:A:2903:GLU:HB3	2.35	0.41
1:B:709:LEU:HD21	1:B:872:ARG:NE	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1120:GLU:HA	1:B:1125:VAL:CG2	2.50	0.41
1:B:1611:ILE:HG23	1:B:1624:THR:HA	2.02	0.41
1:B:2077:UNK:CG	1:B:2079:UNK:HG3	2.41	0.41
1:B:2125:UNK:CA	1:B:2128:UNK:HG3	2.49	0.41
1:B:2141:VAL:HG22	1:B:2238:PHE:HD2	1.85	0.41
1:B:2354:SER:O	1:B:2358:GLU:HG3	2.20	0.41
1:B:2405:MET:HE2	1:B:2405:MET:HA	2.02	0.41
1:B:2808:ARG:HH21	1:B:2901:PRO:HD3	1.85	0.41
1:B:2889:ILE:HG13	1:B:2922:LEU:HD13	2.02	0.41
1:C:160:GLN:HA	1:C:329:ILE:HD13	2.02	0.41
1:C:1352:PHE:HA	1:C:1353:PRO:HD3	1.72	0.41
1:C:1703:ILE:HG22	1:C:1704:GLY:H	1.85	0.41
1:C:2299:MET:H	1:C:2299:MET:HG2	1.68	0.41
1:C:2450:UNK:HG1	1:C:3016:ALA:CB	2.17	0.41
1:A:266:ALA:O	1:A:270:GLU:HG3	2.20	0.41
1:A:438:THR:HA	1:A:880:HIS:CE1	2.51	0.41
1:A:669:LYS:O	1:A:682:ASN:HB3	2.20	0.41
1:A:970:ILE:O	1:A:974:UNK:HG3	2.20	0.41
1:A:984:UNK:HG2	1:A:984:UNK:O	2.20	0.41
1:A:2294:SER:HB3	1:A:2310:LYS:HB2	2.02	0.41
1:A:2591:ARG:NH1	1:C:2014:SER:H	2.19	0.41
1:B:50:GLY:O	1:B:53:SER:OG	2.36	0.41
1:B:78:GLU:HB2	1:B:176:VAL:HG21	2.01	0.41
1:B:266:ALA:O	1:B:270:GLU:HG3	2.20	0.41
1:C:360:LEU:HA	1:C:363:LEU:HB3	2.02	0.41
1:C:559:SER:O	1:C:563:ILE:HG12	2.20	0.41
1:C:618:PRO:HB3	1:C:915:PHE:HA	2.02	0.41
1:C:756:LEU:HD13	1:C:859:PHE:CD2	2.55	0.41
1:C:1611:ILE:HG23	1:C:1624:THR:HA	2.02	0.41
1:C:2200:MET:HB3	1:C:2200:MET:HE3	1.95	0.41
1:C:2503:LYS:HG3	1:C:2513:TYR:HB2	2.02	0.41
1:C:2786:ASP:OD2	1:C:2789:MET:HG2	2.19	0.41
1:C:2800:PHE:CZ	1:C:2812:LEU:HD13	2.55	0.41
1:C:2808:ARG:HH21	1:C:2901:PRO:HD3	1.85	0.41
1:A:70:SER:HG	1:A:142:ARG:HH22	1.65	0.41
1:A:360:LEU:HA	1:A:363:LEU:HB3	2.02	0.41
1:A:559:SER:O	1:A:563:ILE:HG12	2.20	0.41
1:A:795:HIS:NE2	1:A:797:GLN:HB2	2.35	0.41
1:A:1611:ILE:HG23	1:A:1624:THR:HA	2.02	0.41
1:A:2444:UNK:HB2	1:A:2988:PRO:HB3	2.01	0.41
1:A:2563:LEU:HD21	1:A:2567:PHE:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2919:GLY:O	1:A:2921:PRO:HD3	2.21	0.41
1:B:336:TRP:HE3	1:B:339:GLU:OE2	2.03	0.41
1:B:487:PHE:O	1:B:521:VAL:N	2.51	0.41
1:B:1228:VAL:HB	1:B:1311:PHE:HB2	2.02	0.41
1:B:1706:LYS:HA	1:B:1735:GLU:HG3	2.02	0.41
1:B:2064:ARG:HG2	1:B:2100:UNK:HG1	2.01	0.41
1:B:2805:ASP:OD2	1:B:2807:ARG:HB2	2.20	0.41
1:C:211:THR:HB	1:C:286:VAL:HB	2.01	0.41
1:C:369:ARG:HA	1:C:369:ARG:HD2	1.85	0.41
1:C:1095:LEU:HD23	1:C:1098:VAL:HA	2.03	0.41
1:C:2123:UNK:CA	1:C:2126:UNK:HG3	2.50	0.41
1:C:2695:MET:HG3	1:C:2696:TYR:N	2.34	0.41
1:A:2557:LEU:HB3	1:A:2613:ARG:HB2	2.01	0.41
1:A:2892:HIS:HA	1:A:2942:GLN:HE22	1.85	0.41
1:B:436:THR:HG22	1:B:460:GLY:HA3	2.03	0.41
1:B:580:ARG:HD3	1:B:896:ALA:HB3	2.01	0.41
1:B:980:UNK:C	1:B:981:UNK:CG	2.96	0.41
1:B:1095:LEU:HD23	1:B:1098:VAL:HA	2.02	0.41
1:B:1106:CYS:SG	1:B:1174:VAL:HG11	2.60	0.41
1:B:1224:UNK:O	1:B:1224:UNK:HG2	2.20	0.41
1:B:1662:ARG:HG3	1:B:1663:LYS:N	2.34	0.41
1:B:2891:LYS:NZ	1:B:2903:GLU:HB3	2.35	0.41
1:C:266:ALA:O	1:C:270:GLU:HG3	2.20	0.41
1:C:669:LYS:O	1:C:682:ASN:HB3	2.20	0.41
1:C:2055:VAL:HG22	1:C:2194:TRP:CD1	2.55	0.41
1:C:2296:ASN:ND2	1:C:2395:THR:HG21	2.34	0.41
1:A:117:LYS:HZ1	1:C:1087:PHE:HD2	1.68	0.41
1:A:233:LEU:HB3	1:A:251:THR:OG1	2.21	0.41
1:A:1703:ILE:HG22	1:A:1704:GLY:H	1.85	0.41
1:A:2134:UNK:HB1	1:A:2189:PHE:HD2	1.85	0.41
1:A:2354:SER:O	1:A:2358:GLU:HG3	2.20	0.41
1:A:2492:VAL:HG12	1:A:2526:ILE:HG22	2.02	0.41
1:A:2889:ILE:HB	1:A:2924:ILE:HG12	2.01	0.41
1:B:669:LYS:O	1:B:682:ASN:HB3	2.20	0.41
1:B:793:ARG:HH12	1:B:2523:GLU:CD	2.24	0.41
1:B:1460:ALA:O	1:B:1464:VAL:HG22	2.20	0.41
1:B:2096:UNK:CG	1:B:2097:UNK:N	2.82	0.41
1:B:2123:UNK:CA	1:B:2126:UNK:HG3	2.50	0.41
1:B:2205:ASP:O	1:B:2209:LEU:HB2	2.21	0.41
1:B:2503:LYS:HG3	1:B:2513:TYR:HB2	2.02	0.41
1:B:2563:LEU:HD21	1:B:2567:PHE:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:GLY:C	1:C:375:ILE:HG13	2.41	0.41
1:C:417:LEU:HD21	1:C:625:LEU:HD21	2.02	0.41
1:C:885:GLU:HG2	1:C:887:ASP:H	1.84	0.41
1:C:1399:ASN:HA	1:C:1400:PRO:HD3	1.86	0.41
1:C:1672:GLN:HE21	1:C:1672:GLN:HB3	1.58	0.41
1:C:1687:PHE:CE1	1:C:1723:GLU:HG2	2.55	0.41
1:C:2092:UNK:O	1:C:2092:UNK:CG	2.64	0.41
1:C:2104:UNK:CA	1:C:2107:UNK:HG3	2.50	0.41
1:C:2889:ILE:HG13	1:C:2922:LEU:HD13	2.02	0.41
1:A:202:GLY:O	1:A:289:PRO:HD2	2.21	0.41
1:A:587:TRP:CZ2	1:A:694:ASP:OD2	2.74	0.41
1:A:756:LEU:HD13	1:A:859:PHE:CD2	2.55	0.41
1:A:1491:ASP:HB2	1:A:1495:ARG:HB2	2.02	0.41
1:A:2014:SER:H	1:B:2591:ARG:NH1	2.18	0.41
1:A:2113:UNK:HA	1:A:2116:UNK:HG3	2.03	0.41
1:A:2113:UNK:HG2	1:A:2114:UNK:N	2.35	0.41
1:B:936:UNK:HA	1:B:939:UNK:CG	2.51	0.41
1:B:2058:ASP:OD1	1:B:2058:ASP:N	2.46	0.41
1:B:2483:VAL:HG13	1:B:2954:VAL:HG11	2.03	0.41
1:C:585:HIS:HB3	1:C:694:ASP:HB2	2.03	0.41
1:C:1634:ARG:NH1	1:C:1639:ALA:H	2.11	0.41
1:C:1706:LYS:HA	1:C:1735:GLU:HG3	2.03	0.41
1:C:2113:UNK:HA	1:C:2116:UNK:HG3	2.03	0.41
1:C:2468:GLU:OE2	1:C:2478:ARG:NH2	2.48	0.41
1:A:160:GLN:HA	1:A:329:ILE:HD13	2.02	0.41
1:A:393:VAL:O	1:A:395:GLU:N	2.52	0.41
1:A:957:LEU:O	1:A:1034:GLU:HB2	2.20	0.41
1:A:1400:PRO:O	1:A:1415:GLY:HA2	2.21	0.41
1:A:1535:PHE:O	1:A:1679:TRP:N	2.48	0.41
1:A:2141:VAL:HG22	1:A:2238:PHE:CD2	2.56	0.41
1:A:2770:LEU:CB	1:A:2815:GLN:HB3	2.51	0.41
1:B:202:GLY:O	1:B:289:PRO:HD2	2.21	0.41
1:B:233:LEU:HB3	1:B:251:THR:OG1	2.21	0.41
1:B:709:LEU:HD11	1:B:872:ARG:CZ	2.51	0.41
1:B:1275:ALA:O	1:B:1279:VAL:HG23	2.20	0.41
1:B:1400:PRO:O	1:B:1415:GLY:HA2	2.21	0.41
1:B:1491:ASP:HB2	1:B:1495:ARG:HB2	2.02	0.41
1:B:2120:UNK:C	1:B:2123:UNK:HG3	2.50	0.41
1:B:2286:ARG:HD3	1:B:2331:SER:OG	2.20	0.41
1:B:2770:LEU:CB	1:B:2815:GLN:HB3	2.51	0.41
1:C:515:ALA:HA	1:C:516:PRO:HD3	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1460:ALA:O	1:C:1464:VAL:HG22	2.20	0.41
1:C:2286:ARG:HD3	1:C:2331:SER:OG	2.20	0.41
1:C:2710:LEU:HD12	1:C:2713:VAL:HG21	2.03	0.41
1:C:2805:ASP:OD2	1:C:2807:ARG:HB2	2.20	0.41
1:C:2919:GLY:O	1:C:2921:PRO:HD3	2.21	0.41
1:A:479:LEU:HD21	1:A:485:ILE:HD11	2.02	0.41
1:A:1099:PRO:HB2	1:A:1295:TRP:HE1	1.86	0.41
1:A:2831:MET:HE2	1:A:2831:MET:HB3	1.87	0.41
1:B:160:GLN:HA	1:B:329:ILE:HD13	2.02	0.41
1:B:374:GLY:C	1:B:375:ILE:HG13	2.41	0.41
1:B:559:SER:O	1:B:563:ILE:HG12	2.20	0.41
1:B:957:LEU:O	1:B:1034:GLU:HB2	2.20	0.41
1:B:1164:THR:HG22	1:B:1204:UNK:HB2	2.03	0.41
1:B:1695:LEU:HD12	1:B:1695:LEU:HA	1.71	0.41
1:B:2113:UNK:HA	1:B:2116:UNK:HG3	2.03	0.41
1:B:2891:LYS:HZ2	1:B:2903:GLU:CG	2.34	0.41
1:B:3065:PRO:O	1:B:3069:GLN:N	2.42	0.41
1:C:107:LEU:HD13	1:C:113:VAL:HB	2.01	0.41
1:C:2114:UNK:O	1:C:2118:UNK:HG3	2.21	0.41
1:C:2428:UNK:O	1:C:2428:UNK:CG	2.67	0.41
1:C:3062:HIS:H	1:C:3066:GLU:HG3	1.86	0.41
1:A:45:ALA:O	1:A:351:ILE:HA	2.20	0.41
1:A:133:GLN:O	1:A:137:VAL:HG23	2.21	0.41
1:A:278:ARG:HD2	1:A:674:TRP:CE3	2.56	0.41
1:A:585:HIS:HB3	1:A:694:ASP:HB2	2.03	0.41
1:A:594:LEU:O	1:A:598:TYR:HB2	2.21	0.41
1:A:795:HIS:HE2	1:A:797:GLN:HB2	1.86	0.41
1:A:936:UNK:HA	1:A:939:UNK:CG	2.51	0.41
1:A:985:UNK:O	1:A:988:UNK:HG3	2.21	0.41
1:A:1224:UNK:O	1:A:1224:UNK:HG2	2.20	0.41
1:A:1634:ARG:NH1	1:A:1639:ALA:H	2.11	0.41
1:A:2104:UNK:CA	1:A:2107:UNK:HG3	2.50	0.41
1:A:2114:UNK:O	1:A:2118:UNK:HG3	2.21	0.41
1:A:2961:LEU:HD22	1:A:2976:TRP:HD1	1.85	0.41
1:A:3057:ASP:OD1	1:A:3057:ASP:N	2.54	0.41
1:B:360:LEU:HA	1:B:363:LEU:HB3	2.03	0.41
1:B:369:ARG:HA	1:B:369:ARG:HD2	1.85	0.41
1:B:618:PRO:HB3	1:B:915:PHE:HA	2.02	0.41
1:B:795:HIS:NE2	1:B:797:GLN:HB2	2.35	0.41
1:B:1017:ILE:HG12	1:B:1045:VAL:HG11	2.03	0.41
1:B:1637:VAL:HA	1:B:1638:PRO:HD2	1.90	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1687:PHE:CE1	1:B:1723:GLU:HG2	2.55	0.41
1:B:2104:UNK:CA	1:B:2107:UNK:HG3	2.50	0.41
1:B:2212:TRP:O	1:B:2229:LYS:HB3	2.21	0.41
1:B:2405:MET:O	1:B:2409:ALA:HB3	2.21	0.41
1:B:2989:LEU:HD12	1:B:2989:LEU:HA	1.77	0.41
1:B:3057:ASP:N	1:B:3057:ASP:OD1	2.54	0.41
1:B:3062:HIS:H	1:B:3066:GLU:HG3	1.86	0.41
1:C:233:LEU:HB3	1:C:251:THR:OG1	2.21	0.41
1:C:436:THR:HG22	1:C:460:GLY:HA3	2.03	0.41
1:C:936:UNK:HA	1:C:939:UNK:CG	2.51	0.41
1:C:1002:UNK:CG	1:C:1005:UNK:HB2	2.51	0.41
1:C:1099:PRO:HB2	1:C:1295:TRP:HE1	1.86	0.41
1:C:1491:ASP:HB2	1:C:1495:ARG:HB2	2.02	0.41
1:C:1986:LEU:HA	1:C:1989:PHE:CD2	2.56	0.41
1:C:2010:GLN:OE1	1:C:2013:LEU:HD11	2.21	0.41
1:C:2492:VAL:HG12	1:C:2526:ILE:HG22	2.02	0.41
1:C:2889:ILE:HD12	1:C:2993:LEU:HD23	2.03	0.41
1:C:2978:ARG:HG3	1:C:2979:GLU:HG3	2.03	0.41
1:C:3057:ASP:OD1	1:C:3057:ASP:N	2.54	0.41
1:A:793:ARG:HH12	1:A:2523:GLU:CD	2.24	0.41
1:A:2098:UNK:HG2	1:A:2099:UNK:N	2.36	0.41
1:A:2212:TRP:O	1:A:2229:LYS:HB3	2.21	0.41
1:A:2334:HIS:CD2	1:A:2391:LYS:HG3	2.50	0.41
1:B:594:LEU:O	1:B:598:TYR:HB2	2.21	0.41
1:B:1462:ALA:HB2	1:B:1468:TYR:CE1	2.56	0.41
1:B:2919:GLY:O	1:B:2921:PRO:HD3	2.21	0.41
1:B:2927:GLN:HE21	1:B:2927:GLN:HB3	1.70	0.41
1:C:278:ARG:HD2	1:C:674:TRP:CE3	2.56	0.41
1:C:594:LEU:O	1:C:598:TYR:HB2	2.21	0.41
1:C:709:LEU:HD11	1:C:872:ARG:CZ	2.51	0.41
1:C:2483:VAL:HG13	1:C:2954:VAL:HG11	2.03	0.41
1:C:2989:LEU:HD12	1:C:2989:LEU:HA	1.77	0.41
1:A:1087:PHE:CD1	1:B:198:ILE:HG23	2.56	0.40
1:A:1095:LEU:HD13	1:A:1289:PRO:CB	2.52	0.40
1:A:1120:GLU:HA	1:A:1125:VAL:CG2	2.50	0.40
1:A:2086:UNK:HA	1:A:2089:UNK:CG	2.51	0.40
1:A:2093:UNK:HB2	1:A:2129:UNK:HB2	2.03	0.40
1:B:358:ASP:OD2	1:B:361:THR:HB	2.21	0.40
1:C:180:ALA:O	1:C:184:LEU:HG	2.21	0.40
1:C:273:ARG:HD2	1:C:282:VAL:CG1	2.51	0.40
1:C:602:ARG:NH2	1:C:641:ASP:OD1	2.27	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:984:UNK:HG2	1:C:984:UNK:O	2.20	0.40
1:C:1133:VAL:N	1:C:1193:ALA:O	2.48	0.40
1:C:1224:UNK:O	1:C:1224:UNK:HG2	2.20	0.40
1:C:2300:PHE:HZ	1:C:2398:LEU:HB3	1.85	0.40
1:A:278:ARG:HD2	1:A:674:TRP:HE3	1.87	0.40
1:A:709:LEU:HD11	1:A:872:ARG:CZ	2.51	0.40
1:A:1462:ALA:HB2	1:A:1468:TYR:CE1	2.56	0.40
1:A:1604:ASP:N	1:A:1604:ASP:OD1	2.55	0.40
1:A:1695:LEU:HD12	1:A:1695:LEU:HA	1.71	0.40
1:A:1702:GLU:OE1	1:A:1711:VAL:HG22	2.22	0.40
1:A:2010:GLN:OE1	1:A:2013:LEU:HD11	2.21	0.40
1:A:2120:UNK:C	1:A:2123:UNK:HG3	2.50	0.40
1:A:2405:MET:HE2	1:A:2405:MET:HA	2.03	0.40
1:A:2710:LEU:HD12	1:A:2713:VAL:HG21	2.03	0.40
1:B:133:GLN:O	1:B:137:VAL:HG23	2.21	0.40
1:B:417:LEU:HD21	1:B:625:LEU:HD21	2.02	0.40
1:B:756:LEU:HD13	1:B:859:PHE:CD2	2.55	0.40
1:B:999:UNK:HG2	1:B:1007:UNK:HG3	1.96	0.40
1:B:1087:PHE:CD1	1:C:198:ILE:HG23	2.56	0.40
1:B:1237:ARG:HH11	1:B:1237:ARG:HG2	1.86	0.40
1:B:1381:ASP:OD1	1:B:1391:SER:OG	2.22	0.40
1:B:1533:VAL:N	1:B:1543:ALA:O	2.52	0.40
1:B:1604:ASP:OD1	1:B:1604:ASP:N	2.55	0.40
1:B:2400:ASP:OD1	1:B:2400:ASP:N	2.45	0.40
1:B:2978:ARG:HG3	1:B:2979:GLU:HG3	2.03	0.40
1:C:133:GLN:O	1:C:137:VAL:HG23	2.21	0.40
1:C:393:VAL:O	1:C:395:GLU:N	2.52	0.40
1:C:544:ILE:C	1:C:546:HIS:H	2.22	0.40
1:C:1215:UNK:CG	1:C:1216:UNK:N	2.84	0.40
1:C:1400:PRO:O	1:C:1415:GLY:HA2	2.21	0.40
1:C:2114:UNK:O	1:C:2117:UNK:HG3	2.21	0.40
1:C:2449:UNK:O	1:C:2449:UNK:CG	2.68	0.40
1:C:2892:HIS:HA	1:C:2942:GLN:HE22	1.85	0.40
1:A:198:ILE:HG23	1:C:1087:PHE:CD1	2.56	0.40
1:A:487:PHE:O	1:A:521:VAL:N	2.51	0.40
1:A:618:PRO:HB3	1:A:915:PHE:HA	2.02	0.40
1:A:2286:ARG:HD3	1:A:2331:SER:OG	2.20	0.40
1:A:2346:MET:O	1:A:2349:ASN:N	2.55	0.40
1:B:984:UNK:HG2	1:B:984:UNK:O	2.20	0.40
1:B:1095:LEU:HD13	1:B:1289:PRO:CB	2.52	0.40
1:B:1616:PRO:HG2	1:B:1619:VAL:HB	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2014:SER:H	1:C:2591:ARG:NH1	2.19	0.40
1:B:2093:UNK:HB2	1:B:2129:UNK:HB2	2.03	0.40
1:B:2114:UNK:O	1:B:2117:UNK:HG3	2.21	0.40
1:B:2672:TRP:CZ3	1:B:2830:LYS:HG2	2.56	0.40
1:C:745:THR:HG22	1:C:747:LEU:N	2.37	0.40
1:C:793:ARG:HH12	1:C:2523:GLU:CD	2.24	0.40
1:C:794:LEU:HD12	1:C:830:TYR:HB3	2.04	0.40
1:C:799:PHE:CZ	1:C:2433:UNK:CG	2.99	0.40
1:C:976:UNK:O	1:C:976:UNK:CG	2.68	0.40
1:C:995:UNK:HB1	1:C:1011:UNK:HG2	1.99	0.40
1:C:1237:ARG:HG2	1:C:1237:ARG:HH11	1.86	0.40
1:C:2141:VAL:HG22	1:C:2238:PHE:CD2	2.56	0.40
1:C:2405:MET:O	1:C:2409:ALA:HB3	2.21	0.40
1:C:2574:GLU:HG3	1:C:2599:TRP:CE2	2.57	0.40
1:C:2672:TRP:CZ3	1:C:2830:LYS:HG2	2.56	0.40
1:C:2770:LEU:CB	1:C:2815:GLN:HB3	2.51	0.40
1:A:180:ALA:O	1:A:184:LEU:HG	2.21	0.40
1:A:417:LEU:HD21	1:A:625:LEU:HD21	2.02	0.40
1:A:745:THR:HG22	1:A:747:LEU:N	2.37	0.40
1:A:1706:LYS:HA	1:A:1735:GLU:HG3	2.03	0.40
1:A:2611:VAL:HA	1:A:2612:PRO:HD3	1.86	0.40
1:A:2618:SER:HB3	1:A:2786:ASP:OD1	2.21	0.40
1:A:2672:TRP:CZ3	1:A:2830:LYS:HG2	2.56	0.40
1:B:142:ARG:HD3	1:B:142:ARG:HA	1.91	0.40
1:B:336:TRP:HE1	1:B:364:THR:HG22	1.86	0.40
1:B:544:ILE:C	1:B:546:HIS:H	2.22	0.40
1:B:587:TRP:CZ2	1:B:694:ASP:OD2	2.74	0.40
1:B:1002:UNK:CG	1:B:1005:UNK:HB2	2.51	0.40
1:B:1087:PHE:HZ	1:C:203:ASP:OD2	2.05	0.40
1:B:1353:PRO:HB2	1:B:1707:SER:HB2	2.04	0.40
1:B:1380:ALA:HB1	1:B:1474:LEU:CD1	2.50	0.40
1:B:2907:HIS:HA	1:B:2910:ILE:HG12	2.04	0.40
1:C:1095:LEU:HD12	1:C:1096:THR:N	2.35	0.40
1:C:1535:PHE:O	1:C:1679:TRP:N	2.48	0.40
1:C:1616:PRO:HG2	1:C:1619:VAL:HB	2.04	0.40
1:C:1619:VAL:HA	1:C:1620:PRO:HD2	1.80	0.40
1:C:2093:UNK:HB2	1:C:2129:UNK:HB2	2.03	0.40
1:A:358:ASP:OD2	1:A:361:THR:HB	2.21	0.40
1:A:374:GLY:C	1:A:375:ILE:HG13	2.41	0.40
1:A:544:ILE:C	1:A:546:HIS:H	2.22	0.40
1:A:1013:UNK:CG	1:A:1014:UNK:N	2.58	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1629:PHE:O	1:A:1633:ILE:HG13	2.22	0.40
1:A:2114:UNK:O	1:A:2117:UNK:HG3	2.22	0.40
1:A:2205:ASP:O	1:A:2209:LEU:HB2	2.21	0.40
1:A:2405:MET:O	1:A:2409:ALA:HB3	2.21	0.40
1:A:2503:LYS:HG3	1:A:2513:TYR:HB2	2.02	0.40
1:A:2836:LEU:HD23	1:A:2836:LEU:HA	1.87	0.40
1:B:273:ARG:HD2	1:B:282:VAL:CG1	2.51	0.40
1:B:541:GLU:HG3	1:B:542:VAL:N	2.37	0.40
1:B:585:HIS:HB3	1:B:694:ASP:HB2	2.03	0.40
1:B:985:UNK:O	1:B:988:UNK:HG3	2.21	0.40
1:B:1099:PRO:HB2	1:B:1295:TRP:HE1	1.86	0.40
1:B:2346:MET:O	1:B:2349:ASN:N	2.55	0.40
1:B:2492:VAL:HG12	1:B:2526:ILE:HG22	2.02	0.40
1:B:2557:LEU:HD23	1:B:2558:LEU:N	2.37	0.40
1:B:2611:VAL:HA	1:B:2612:PRO:HD3	1.86	0.40
1:C:408:VAL:HG23	1:C:418:GLU:HB2	2.04	0.40
1:C:2930:LEU:HD23	1:C:2930:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2637/3089 (85%)	2489 (94%)	140 (5%)	8 (0%)	41	77
1	B	2637/3089 (85%)	2489 (94%)	140 (5%)	8 (0%)	41	77
1	C	2637/3089 (85%)	2489 (94%)	139 (5%)	9 (0%)	41	77
1	D	2637/3089 (85%)	2488 (94%)	140 (5%)	9 (0%)	41	77
1	E	2637/3089 (85%)	2488 (94%)	141 (5%)	8 (0%)	41	77
1	F	2637/3089 (85%)	2488 (94%)	140 (5%)	9 (0%)	41	77
All	All	15822/18534 (85%)	14931 (94%)	840 (5%)	51 (0%)	44	77

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1148	GLU
1	E	1148	GLU
1	F	1148	GLU
1	A	1148	GLU
1	B	1148	GLU
1	C	1148	GLU
1	D	1724	TYR
1	E	1724	TYR
1	F	1724	TYR
1	A	1724	TYR
1	B	1724	TYR
1	C	1724	TYR
1	D	149	ALA
1	D	1652	TRP
1	D	1705	VAL
1	E	149	ALA
1	E	1652	TRP
1	E	1705	VAL
1	F	149	ALA
1	F	1652	TRP
1	F	1705	VAL
1	A	149	ALA
1	A	1652	TRP
1	A	1705	VAL
1	B	149	ALA
1	B	1652	TRP
1	B	1705	VAL
1	C	149	ALA
1	C	1652	TRP
1	C	1705	VAL
1	D	89	GLU
1	E	89	GLU
1	F	89	GLU
1	A	89	GLU
1	B	89	GLU
1	C	89	GLU
1	D	1068	VAL
1	D	1285	LYS
1	E	1068	VAL
1	E	1285	LYS
1	F	1068	VAL
1	F	1285	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1068	VAL
1	A	1285	LYS
1	B	1068	VAL
1	B	1285	LYS
1	C	1068	VAL
1	C	1285	LYS
1	D	2585	PRO
1	F	2585	PRO
1	C	2585	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2076/2264 (92%)	1987 (96%)	89 (4%)	29	53
1	B	2076/2264 (92%)	1986 (96%)	90 (4%)	29	53
1	C	2076/2264 (92%)	1987 (96%)	89 (4%)	29	53
1	D	2076/2264 (92%)	1987 (96%)	89 (4%)	29	53
1	E	2076/2264 (92%)	1987 (96%)	89 (4%)	29	53
1	F	2076/2264 (92%)	1987 (96%)	89 (4%)	29	53
All	All	12456/13584 (92%)	11921 (96%)	535 (4%)	33	53

All (535) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	90	LEU
1	D	208	VAL
1	D	209	SER
1	D	232	VAL
1	D	233	LEU
1	D	248	ILE
1	D	251	THR
1	D	342	GLU
1	D	344	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	358	ASP
1	D	361	THR
1	D	389	THR
1	D	390	VAL
1	D	400	TRP
1	D	409	LYS
1	D	424	LEU
1	D	427	ARG
1	D	439	THR
1	D	456	GLU
1	D	517	ILE
1	D	544	ILE
1	D	580	ARG
1	D	584	HIS
1	D	595	LEU
1	D	606	ASN
1	D	621	SER
1	D	638	MET
1	D	644	LEU
1	D	654	GLU
1	D	694	ASP
1	D	696	HIS
1	D	699	ASP
1	D	791	GLU
1	D	857	VAL
1	D	1021	LEU
1	D	1096	THR
1	D	1105	ARG
1	D	1127	GLU
1	D	1162	THR
1	D	1253	ARG
1	D	1358	GLN
1	D	1421	GLN
1	D	1468	TYR
1	D	1471	GLU
1	D	1488	VAL
1	D	1508	ILE
1	D	1544	ILE
1	D	1551	LEU
1	D	1564	ILE
1	D	1618	LEU
1	D	1651	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1662	ARG
1	D	1672	GLN
1	D	1673	PHE
1	D	1745	ASP
1	D	2059	ARG
1	D	2067	LEU
1	D	2070	LEU
1	D	2192	THR
1	D	2196	VAL
1	D	2209	LEU
1	D	2294	SER
1	D	2297	ARG
1	D	2299	MET
1	D	2303	ASP
1	D	2306	TYR
1	D	2395	THR
1	D	2401	ILE
1	D	2620	THR
1	D	2692	MET
1	D	2742	THR
1	D	2784	THR
1	D	2800	PHE
1	D	2802	ARG
1	D	2809	LEU
1	D	2827	LEU
1	D	2861	LEU
1	D	2871	THR
1	D	2879	LEU
1	D	2894	THR
1	D	2916	ARG
1	D	2930	LEU
1	D	2935	LYS
1	D	2962	ASP
1	D	3001	HIS
1	D	3019	ASP
1	D	3076	SER
1	D	3077	THR
1	D	3080	ARG
1	E	90	LEU
1	E	208	VAL
1	E	209	SER
1	E	232	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	233	LEU
1	E	248	ILE
1	E	251	THR
1	E	342	GLU
1	E	344	HIS
1	E	358	ASP
1	E	361	THR
1	E	389	THR
1	E	390	VAL
1	E	400	TRP
1	E	409	LYS
1	E	424	LEU
1	E	427	ARG
1	E	439	THR
1	E	456	GLU
1	E	517	ILE
1	E	544	ILE
1	E	580	ARG
1	E	584	HIS
1	E	595	LEU
1	E	606	ASN
1	E	621	SER
1	E	638	MET
1	E	644	LEU
1	E	654	GLU
1	E	694	ASP
1	E	696	HIS
1	E	699	ASP
1	E	791	GLU
1	E	857	VAL
1	E	1021	LEU
1	E	1096	THR
1	E	1105	ARG
1	E	1127	GLU
1	E	1162	THR
1	E	1253	ARG
1	E	1358	GLN
1	E	1421	GLN
1	E	1468	TYR
1	E	1471	GLU
1	E	1488	VAL
1	E	1508	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	1544	ILE
1	E	1551	LEU
1	E	1564	ILE
1	E	1618	LEU
1	E	1651	THR
1	E	1662	ARG
1	E	1672	GLN
1	E	1673	PHE
1	E	1745	ASP
1	E	2059	ARG
1	E	2067	LEU
1	E	2070	LEU
1	E	2192	THR
1	E	2196	VAL
1	E	2209	LEU
1	E	2294	SER
1	E	2297	ARG
1	E	2299	MET
1	E	2303	ASP
1	E	2306	TYR
1	E	2395	THR
1	E	2401	ILE
1	E	2620	THR
1	E	2692	MET
1	E	2742	THR
1	E	2784	THR
1	E	2800	PHE
1	E	2802	ARG
1	E	2809	LEU
1	E	2827	LEU
1	E	2861	LEU
1	E	2871	THR
1	E	2879	LEU
1	E	2894	THR
1	E	2916	ARG
1	E	2930	LEU
1	E	2935	LYS
1	E	2962	ASP
1	E	3001	HIS
1	E	3019	ASP
1	E	3076	SER
1	E	3077	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	3080	ARG
1	F	90	LEU
1	F	208	VAL
1	F	209	SER
1	F	232	VAL
1	F	233	LEU
1	F	248	ILE
1	F	251	THR
1	F	342	GLU
1	F	344	HIS
1	F	358	ASP
1	F	361	THR
1	F	389	THR
1	F	390	VAL
1	F	400	TRP
1	F	409	LYS
1	F	424	LEU
1	F	427	ARG
1	F	439	THR
1	F	456	GLU
1	F	517	ILE
1	F	544	ILE
1	F	580	ARG
1	F	584	HIS
1	F	595	LEU
1	F	606	ASN
1	F	621	SER
1	F	638	MET
1	F	644	LEU
1	F	654	GLU
1	F	694	ASP
1	F	696	HIS
1	F	699	ASP
1	F	791	GLU
1	F	857	VAL
1	F	1021	LEU
1	F	1096	THR
1	F	1105	ARG
1	F	1127	GLU
1	F	1162	THR
1	F	1253	ARG
1	F	1358	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	1421	GLN
1	F	1468	TYR
1	F	1471	GLU
1	F	1488	VAL
1	F	1508	ILE
1	F	1544	ILE
1	F	1551	LEU
1	F	1564	ILE
1	F	1618	LEU
1	F	1651	THR
1	F	1662	ARG
1	F	1672	GLN
1	F	1673	PHE
1	F	1745	ASP
1	F	2059	ARG
1	F	2067	LEU
1	F	2070	LEU
1	F	2192	THR
1	F	2196	VAL
1	F	2209	LEU
1	F	2294	SER
1	F	2297	ARG
1	F	2299	MET
1	F	2303	ASP
1	F	2306	TYR
1	F	2395	THR
1	F	2401	ILE
1	F	2620	THR
1	F	2692	MET
1	F	2742	THR
1	F	2784	THR
1	F	2800	PHE
1	F	2802	ARG
1	F	2809	LEU
1	F	2827	LEU
1	F	2861	LEU
1	F	2871	THR
1	F	2879	LEU
1	F	2894	THR
1	F	2916	ARG
1	F	2930	LEU
1	F	2935	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	2962	ASP
1	F	3001	HIS
1	F	3019	ASP
1	F	3076	SER
1	F	3077	THR
1	F	3080	ARG
1	A	90	LEU
1	A	208	VAL
1	A	209	SER
1	A	232	VAL
1	A	233	LEU
1	A	248	ILE
1	A	251	THR
1	A	342	GLU
1	A	344	HIS
1	A	358	ASP
1	A	361	THR
1	A	389	THR
1	A	390	VAL
1	A	400	TRP
1	A	409	LYS
1	A	424	LEU
1	A	427	ARG
1	A	439	THR
1	A	456	GLU
1	A	517	ILE
1	A	544	ILE
1	A	580	ARG
1	A	584	HIS
1	A	595	LEU
1	A	606	ASN
1	A	621	SER
1	A	638	MET
1	A	644	LEU
1	A	654	GLU
1	A	694	ASP
1	A	696	HIS
1	A	699	ASP
1	A	791	GLU
1	A	857	VAL
1	A	1021	LEU
1	A	1096	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1105	ARG
1	A	1127	GLU
1	A	1162	THR
1	A	1253	ARG
1	A	1358	GLN
1	A	1421	GLN
1	A	1468	TYR
1	A	1471	GLU
1	A	1488	VAL
1	A	1508	ILE
1	A	1544	ILE
1	A	1551	LEU
1	A	1564	ILE
1	A	1618	LEU
1	A	1651	THR
1	A	1662	ARG
1	A	1672	GLN
1	A	1673	PHE
1	A	1745	ASP
1	A	2059	ARG
1	A	2067	LEU
1	A	2070	LEU
1	A	2192	THR
1	A	2196	VAL
1	A	2209	LEU
1	A	2294	SER
1	A	2297	ARG
1	A	2299	MET
1	A	2303	ASP
1	A	2306	TYR
1	A	2395	THR
1	A	2401	ILE
1	A	2620	THR
1	A	2692	MET
1	A	2742	THR
1	A	2784	THR
1	A	2800	PHE
1	A	2802	ARG
1	A	2809	LEU
1	A	2827	LEU
1	A	2861	LEU
1	A	2871	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2879	LEU
1	A	2894	THR
1	A	2916	ARG
1	A	2930	LEU
1	A	2935	LYS
1	A	2962	ASP
1	A	3001	HIS
1	A	3019	ASP
1	A	3076	SER
1	A	3077	THR
1	A	3080	ARG
1	B	90	LEU
1	B	208	VAL
1	B	209	SER
1	B	232	VAL
1	B	233	LEU
1	B	248	ILE
1	B	251	THR
1	B	342	GLU
1	B	344	HIS
1	B	358	ASP
1	B	361	THR
1	B	389	THR
1	B	390	VAL
1	B	400	TRP
1	B	409	LYS
1	B	424	LEU
1	B	427	ARG
1	B	439	THR
1	B	456	GLU
1	B	517	ILE
1	B	544	ILE
1	B	580	ARG
1	B	584	HIS
1	B	595	LEU
1	B	606	ASN
1	B	621	SER
1	B	638	MET
1	B	644	LEU
1	B	654	GLU
1	B	694	ASP
1	B	696	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	699	ASP
1	B	791	GLU
1	B	857	VAL
1	B	1021	LEU
1	B	1096	THR
1	B	1105	ARG
1	B	1127	GLU
1	B	1162	THR
1	B	1253	ARG
1	B	1358	GLN
1	B	1401	THR
1	B	1421	GLN
1	B	1468	TYR
1	B	1471	GLU
1	B	1488	VAL
1	B	1508	ILE
1	B	1544	ILE
1	B	1551	LEU
1	B	1564	ILE
1	B	1618	LEU
1	B	1651	THR
1	B	1662	ARG
1	B	1672	GLN
1	B	1673	PHE
1	B	1745	ASP
1	B	2059	ARG
1	B	2067	LEU
1	B	2070	LEU
1	B	2192	THR
1	B	2196	VAL
1	B	2209	LEU
1	B	2294	SER
1	B	2297	ARG
1	B	2299	MET
1	B	2303	ASP
1	B	2306	TYR
1	B	2395	THR
1	B	2401	ILE
1	B	2620	THR
1	B	2692	MET
1	B	2742	THR
1	B	2784	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2800	PHE
1	B	2802	ARG
1	B	2809	LEU
1	B	2827	LEU
1	B	2861	LEU
1	B	2871	THR
1	B	2879	LEU
1	B	2894	THR
1	B	2916	ARG
1	B	2930	LEU
1	B	2935	LYS
1	B	2962	ASP
1	B	3001	HIS
1	B	3019	ASP
1	B	3076	SER
1	B	3077	THR
1	B	3080	ARG
1	C	90	LEU
1	C	208	VAL
1	C	209	SER
1	C	232	VAL
1	C	233	LEU
1	C	248	ILE
1	C	251	THR
1	C	342	GLU
1	C	344	HIS
1	C	358	ASP
1	C	361	THR
1	C	389	THR
1	C	390	VAL
1	C	400	TRP
1	C	409	LYS
1	C	424	LEU
1	C	427	ARG
1	C	439	THR
1	C	456	GLU
1	C	517	ILE
1	C	544	ILE
1	C	580	ARG
1	C	584	HIS
1	C	595	LEU
1	C	606	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	621	SER
1	C	638	MET
1	C	644	LEU
1	C	654	GLU
1	C	694	ASP
1	C	696	HIS
1	C	699	ASP
1	C	791	GLU
1	C	857	VAL
1	C	1021	LEU
1	C	1096	THR
1	C	1105	ARG
1	C	1127	GLU
1	C	1162	THR
1	C	1253	ARG
1	C	1358	GLN
1	C	1421	GLN
1	C	1468	TYR
1	C	1471	GLU
1	C	1488	VAL
1	C	1508	ILE
1	C	1544	ILE
1	C	1551	LEU
1	C	1564	ILE
1	C	1618	LEU
1	C	1651	THR
1	C	1662	ARG
1	C	1672	GLN
1	C	1673	PHE
1	C	1745	ASP
1	C	2059	ARG
1	C	2067	LEU
1	C	2070	LEU
1	C	2192	THR
1	C	2196	VAL
1	C	2209	LEU
1	C	2294	SER
1	C	2297	ARG
1	C	2299	MET
1	C	2303	ASP
1	C	2306	TYR
1	C	2395	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	2401	ILE
1	C	2620	THR
1	C	2692	MET
1	C	2742	THR
1	C	2784	THR
1	C	2800	PHE
1	C	2802	ARG
1	C	2809	LEU
1	C	2827	LEU
1	C	2861	LEU
1	C	2871	THR
1	C	2879	LEU
1	C	2894	THR
1	C	2916	ARG
1	C	2930	LEU
1	C	2935	LYS
1	C	2962	ASP
1	C	3001	HIS
1	C	3019	ASP
1	C	3076	SER
1	C	3077	THR
1	C	3080	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	386	ASN
1	A	486	GLN
1	A	540	ASN
1	A	585	HIS
1	A	606	ASN
1	A	1057	ASN
1	A	1134	HIS
1	A	1276	GLN
1	A	1277	HIS
1	A	1355	GLN
1	A	1582	HIS
1	A	1617	ASN
1	A	1672	GLN
1	A	2288	HIS
1	A	2334	HIS
1	A	2349	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2651	ASN
1	A	2699	ASN
1	A	2815	GLN
1	A	2850	HIS
1	A	2927	GLN
1	A	2942	GLN
1	A	2973	HIS
1	B	386	ASN
1	B	486	GLN
1	B	540	ASN
1	B	575	HIS
1	B	585	HIS
1	B	1057	ASN
1	B	1134	HIS
1	B	1276	GLN
1	B	1277	HIS
1	B	1355	GLN
1	B	1582	HIS
1	B	1617	ASN
1	B	1672	GLN
1	B	2288	HIS
1	B	2296	ASN
1	B	2334	HIS
1	B	2349	ASN
1	B	2651	ASN
1	B	2699	ASN
1	B	2815	GLN
1	B	2850	HIS
1	B	2927	GLN
1	B	2942	GLN
1	B	2973	HIS
1	C	386	ASN
1	C	486	GLN
1	C	540	ASN
1	C	575	HIS
1	C	585	HIS
1	C	1057	ASN
1	C	1134	HIS
1	C	1276	GLN
1	C	1277	HIS
1	C	1355	GLN
1	C	1582	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1617	ASN
1	C	1672	GLN
1	C	2288	HIS
1	C	2296	ASN
1	C	2334	HIS
1	C	2349	ASN
1	C	2651	ASN
1	C	2699	ASN
1	C	2815	GLN
1	C	2850	HIS
1	C	2927	GLN
1	C	2942	GLN
1	C	2973	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FMN	E	4000	-	33,33,33	1.07	2 (6%)	48,50,50	1.26	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FMN	B	4000	-	33,33,33	1.08	2 (6%)	48,50,50	1.26	8 (16%)
2	FMN	F	4000	-	33,33,33	1.07	2 (6%)	48,50,50	1.26	7 (14%)
2	FMN	D	4000	-	33,33,33	1.07	2 (6%)	48,50,50	1.26	8 (16%)
2	FMN	C	4000	-	33,33,33	1.07	2 (6%)	48,50,50	1.26	7 (14%)
2	FMN	A	4000	-	33,33,33	1.07	2 (6%)	48,50,50	1.26	8 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	E	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	B	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	F	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	D	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	C	4000	-	-	5/18/18/18	0/3/3/3
2	FMN	A	4000	-	-	5/18/18/18	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4000	FMN	C4A-N5	4.13	1.38	1.30
2	E	4000	FMN	C4A-N5	4.11	1.38	1.30
2	F	4000	FMN	C4A-N5	4.08	1.38	1.30
2	C	4000	FMN	C4A-N5	4.08	1.38	1.30
2	D	4000	FMN	C4A-N5	4.08	1.38	1.30
2	A	4000	FMN	C4A-N5	4.08	1.38	1.30
2	C	4000	FMN	C10-N1	2.28	1.37	1.33
2	E	4000	FMN	C10-N1	2.25	1.37	1.33
2	D	4000	FMN	C10-N1	2.24	1.37	1.33
2	B	4000	FMN	C10-N1	2.24	1.37	1.33
2	F	4000	FMN	C10-N1	2.23	1.37	1.33
2	A	4000	FMN	C10-N1	2.22	1.37	1.33

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	4000	FMN	C4-N3-C2	-3.01	120.08	125.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	4000	FMN	C4-N3-C2	-3.00	120.09	125.64
2	E	4000	FMN	C4-N3-C2	-2.99	120.11	125.64
2	B	4000	FMN	C4-N3-C2	-2.98	120.13	125.64
2	D	4000	FMN	C4-N3-C2	-2.97	120.15	125.64
2	A	4000	FMN	C4-N3-C2	-2.97	120.15	125.64
2	E	4000	FMN	C4A-C10-N10	2.95	120.79	116.48
2	C	4000	FMN	C4A-C10-N10	2.94	120.78	116.48
2	B	4000	FMN	C4A-C10-N10	2.92	120.76	116.48
2	D	4000	FMN	C4A-C10-N10	2.92	120.74	116.48
2	A	4000	FMN	C4A-C10-N10	2.92	120.74	116.48
2	F	4000	FMN	C4A-C10-N10	2.92	120.74	116.48
2	B	4000	FMN	C4A-C4-N3	2.62	119.84	113.19
2	E	4000	FMN	C4A-C4-N3	2.61	119.82	113.19
2	C	4000	FMN	C4A-C4-N3	2.61	119.81	113.19
2	F	4000	FMN	C4A-C4-N3	2.61	119.81	113.19
2	D	4000	FMN	C4A-C4-N3	2.60	119.80	113.19
2	A	4000	FMN	C4A-C4-N3	2.60	119.80	113.19
2	E	4000	FMN	C10-C4A-N5	-2.59	119.36	124.86
2	B	4000	FMN	C10-C4A-N5	-2.56	119.42	124.86
2	D	4000	FMN	C10-C4A-N5	-2.56	119.43	124.86
2	A	4000	FMN	C10-C4A-N5	-2.56	119.43	124.86
2	C	4000	FMN	C10-C4A-N5	-2.54	119.46	124.86
2	F	4000	FMN	C10-C4A-N5	-2.53	119.48	124.86
2	D	4000	FMN	O4-C4-C4A	-2.43	120.14	126.60
2	F	4000	FMN	O4-C4-C4A	-2.42	120.17	126.60
2	E	4000	FMN	O4-C4-C4A	-2.42	120.18	126.60
2	B	4000	FMN	O4-C4-C4A	-2.42	120.18	126.60
2	A	4000	FMN	O4-C4-C4A	-2.41	120.21	126.60
2	C	4000	FMN	O4-C4-C4A	-2.40	120.22	126.60
2	E	4000	FMN	C4-C4A-N5	2.28	121.47	118.23
2	B	4000	FMN	C4-C4A-N5	2.26	121.45	118.23
2	D	4000	FMN	C4-C4A-N5	2.26	121.45	118.23
2	A	4000	FMN	C4-C4A-N5	2.26	121.45	118.23
2	F	4000	FMN	C4-C4A-N5	2.22	121.39	118.23
2	C	4000	FMN	C4-C4A-N5	2.22	121.39	118.23
2	D	4000	FMN	C9A-C5A-N5	-2.20	120.04	122.43
2	C	4000	FMN	C9A-C5A-N5	-2.20	120.04	122.43
2	F	4000	FMN	C9A-C5A-N5	-2.20	120.05	122.43
2	A	4000	FMN	C9A-C5A-N5	-2.18	120.06	122.43
2	B	4000	FMN	C9A-C5A-N5	-2.16	120.08	122.43
2	E	4000	FMN	C9A-C5A-N5	-2.15	120.10	122.43
2	B	4000	FMN	O2-C2-N1	-2.03	118.46	121.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4000	FMN	O2-C2-N1	-2.02	118.48	121.83
2	A	4000	FMN	O2-C2-N1	-2.00	118.51	121.83
2	E	4000	FMN	O2-C2-N1	-2.00	118.51	121.83

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	4000	FMN	O3'-C3'-C4'-C5'
2	E	4000	FMN	O3'-C3'-C4'-C5'
2	F	4000	FMN	O3'-C3'-C4'-C5'
2	A	4000	FMN	O3'-C3'-C4'-C5'
2	B	4000	FMN	O3'-C3'-C4'-C5'
2	C	4000	FMN	O3'-C3'-C4'-C5'
2	D	4000	FMN	C2'-C3'-C4'-C5'
2	E	4000	FMN	C2'-C3'-C4'-C5'
2	F	4000	FMN	C2'-C3'-C4'-C5'
2	A	4000	FMN	C2'-C3'-C4'-C5'
2	B	4000	FMN	C2'-C3'-C4'-C5'
2	C	4000	FMN	C2'-C3'-C4'-C5'
2	D	4000	FMN	C2'-C3'-C4'-O4'
2	E	4000	FMN	C2'-C3'-C4'-O4'
2	F	4000	FMN	C2'-C3'-C4'-O4'
2	A	4000	FMN	C2'-C3'-C4'-O4'
2	B	4000	FMN	C2'-C3'-C4'-O4'
2	C	4000	FMN	C2'-C3'-C4'-O4'
2	D	4000	FMN	C4'-C5'-O5'-P
2	E	4000	FMN	C4'-C5'-O5'-P
2	F	4000	FMN	C4'-C5'-O5'-P
2	A	4000	FMN	C4'-C5'-O5'-P
2	B	4000	FMN	C4'-C5'-O5'-P
2	C	4000	FMN	C4'-C5'-O5'-P
2	D	4000	FMN	O3'-C3'-C4'-O4'
2	E	4000	FMN	O3'-C3'-C4'-O4'
2	F	4000	FMN	O3'-C3'-C4'-O4'
2	A	4000	FMN	O3'-C3'-C4'-O4'
2	B	4000	FMN	O3'-C3'-C4'-O4'
2	C	4000	FMN	O3'-C3'-C4'-O4'

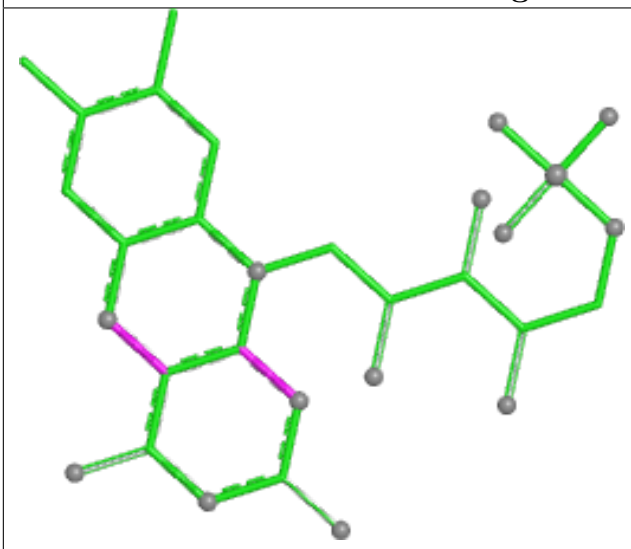
There are no ring outliers.

3 monomers are involved in 14 short contacts:

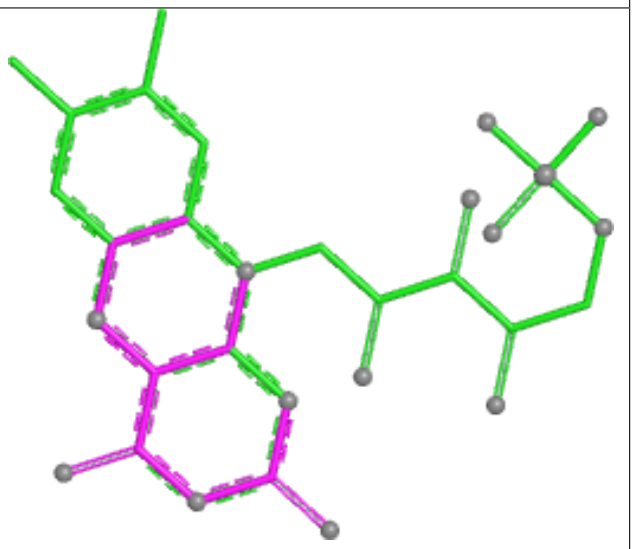
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4000	FMN	5	0
2	C	4000	FMN	4	0
2	A	4000	FMN	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

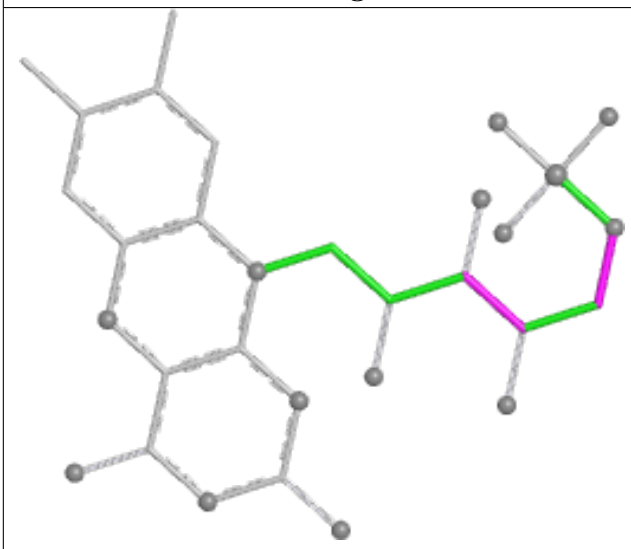
Ligand FMN E 4000



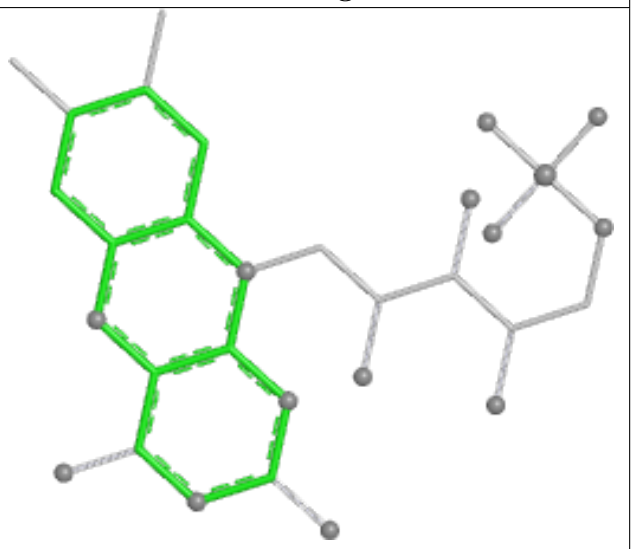
Bond lengths



Bond angles

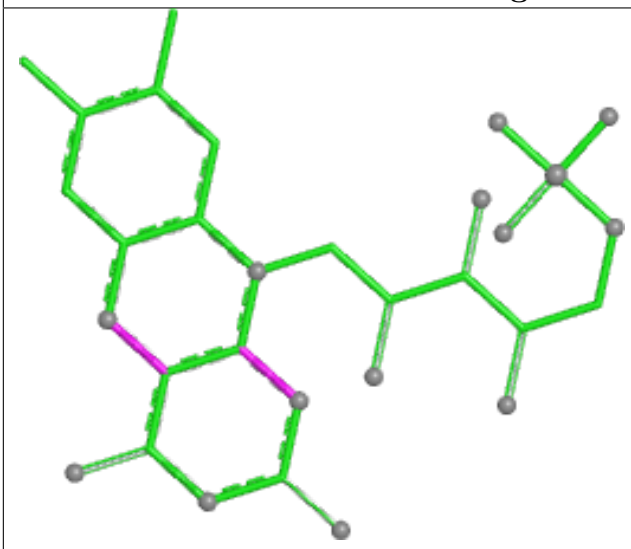


Torsions

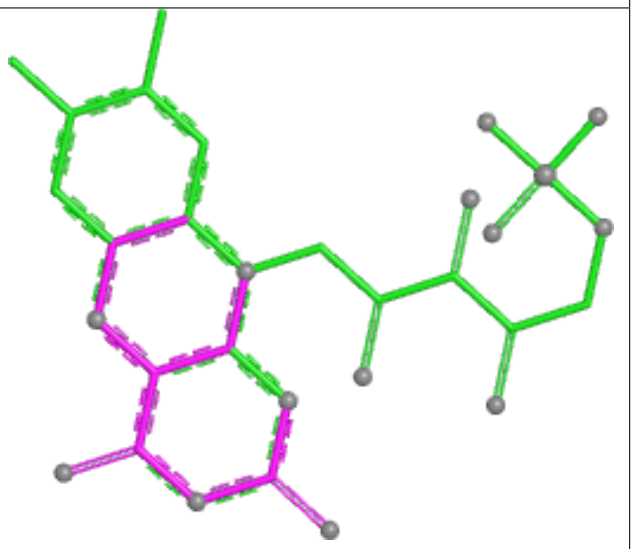


Rings

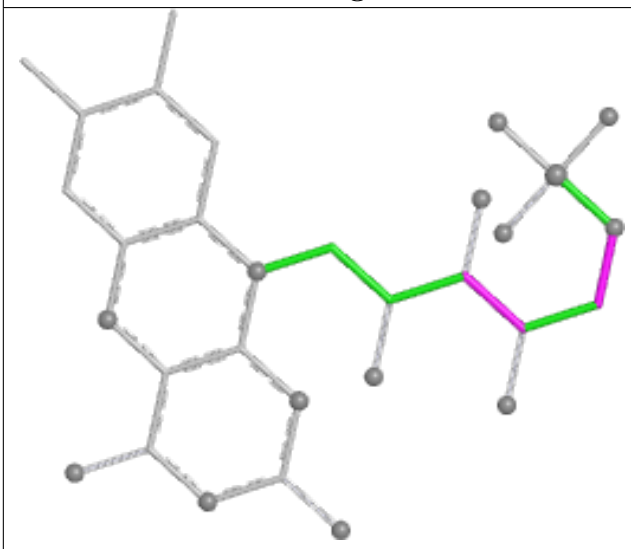
Ligand FMN B 4000



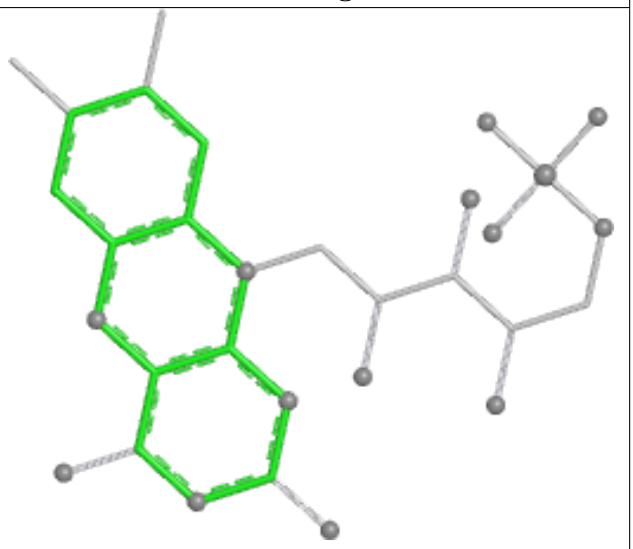
Bond lengths



Bond angles

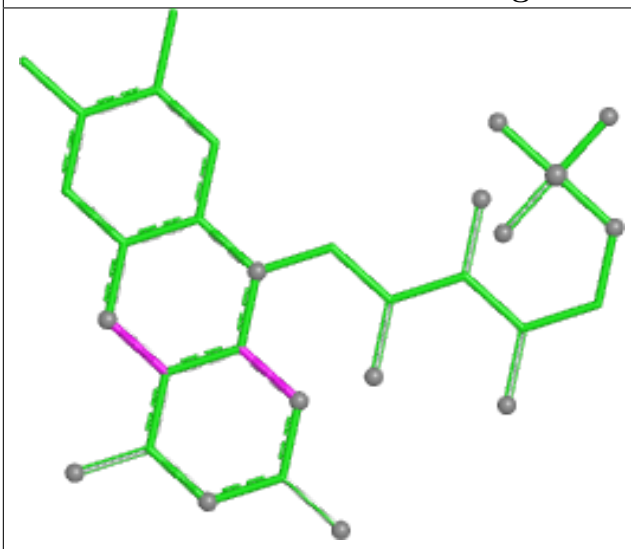


Torsions

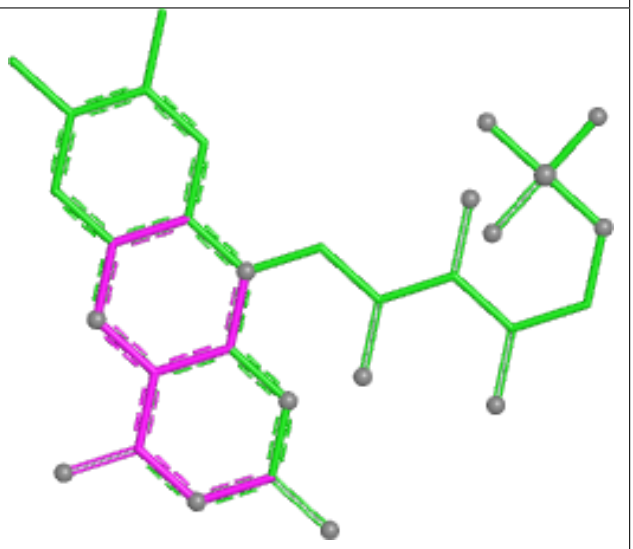


Rings

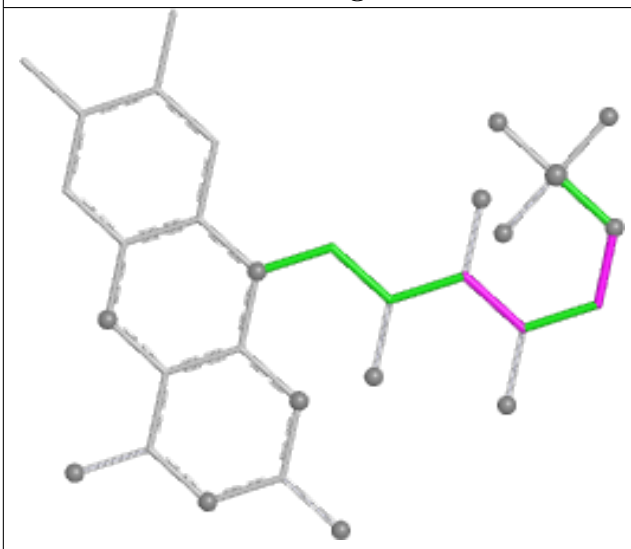
Ligand FMN F 4000



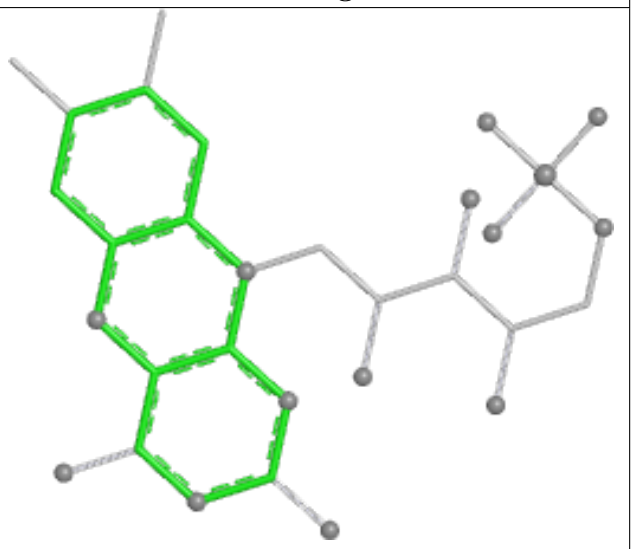
Bond lengths



Bond angles

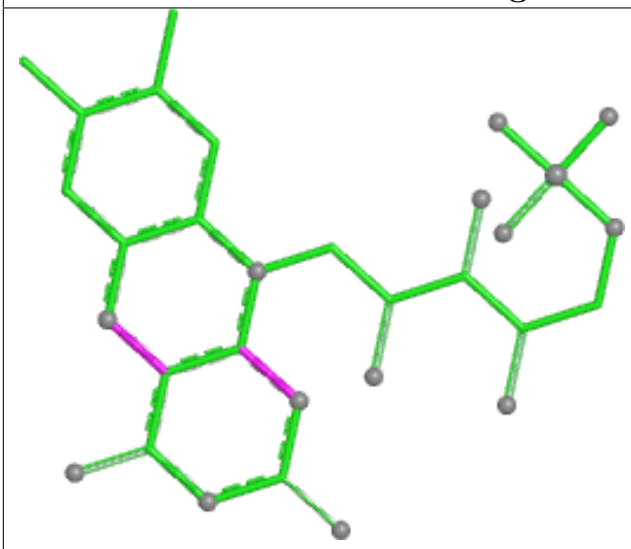


Torsions

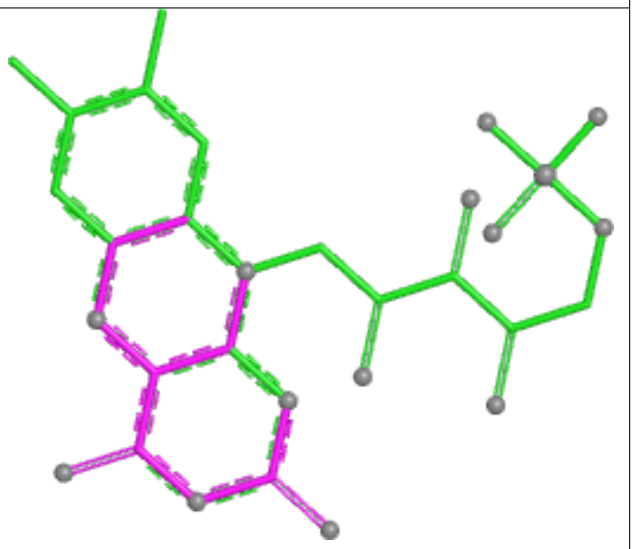


Rings

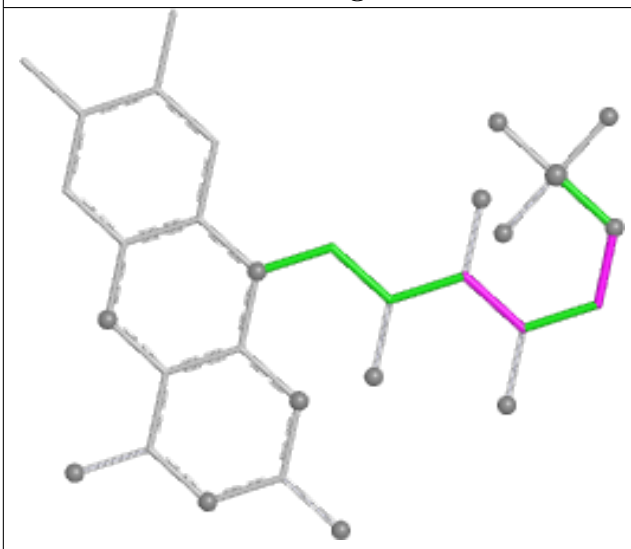
Ligand FMN D 4000



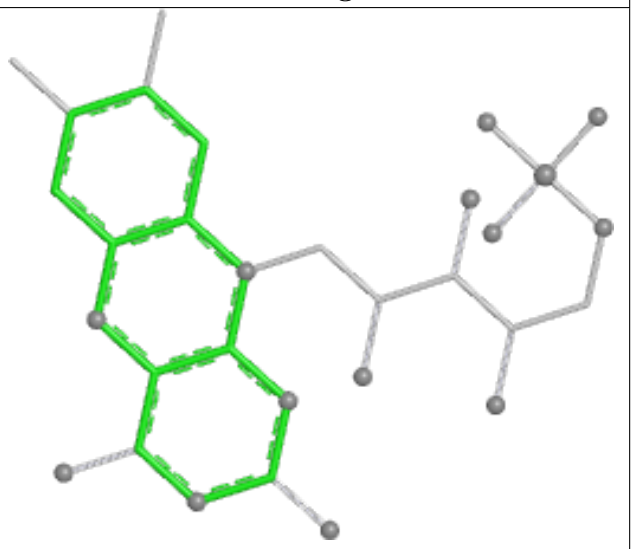
Bond lengths



Bond angles

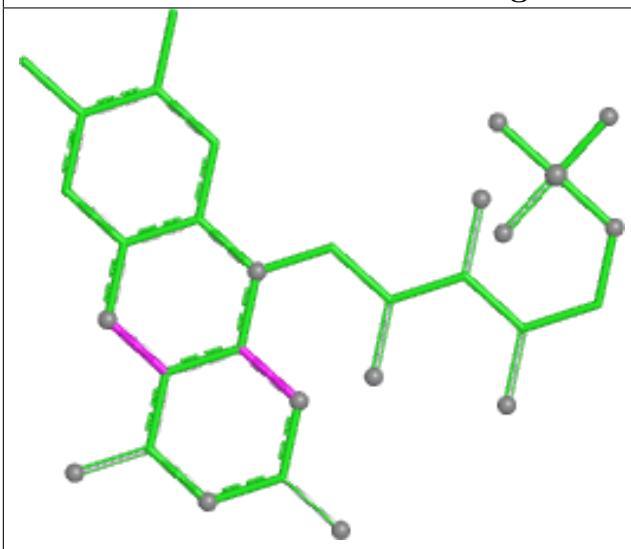


Torsions

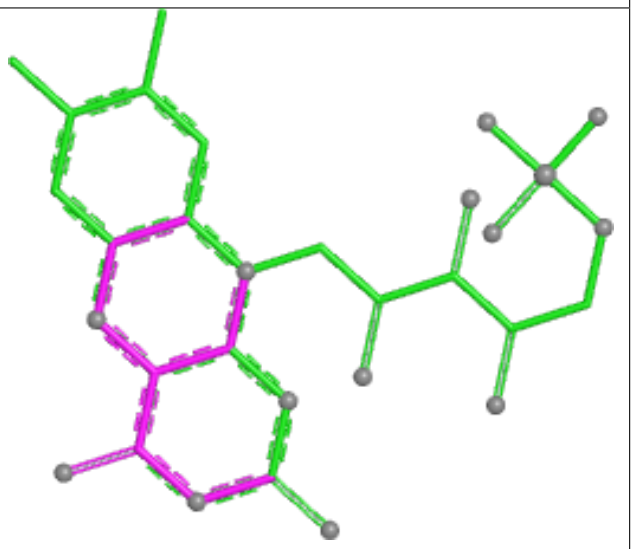


Rings

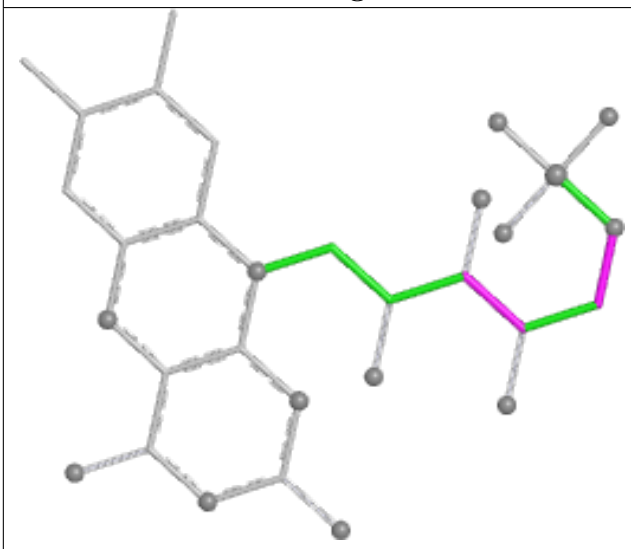
Ligand FMN C 4000



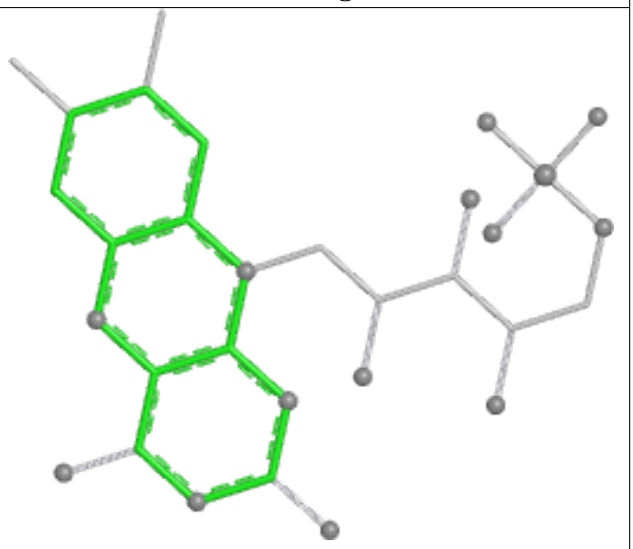
Bond lengths



Bond angles

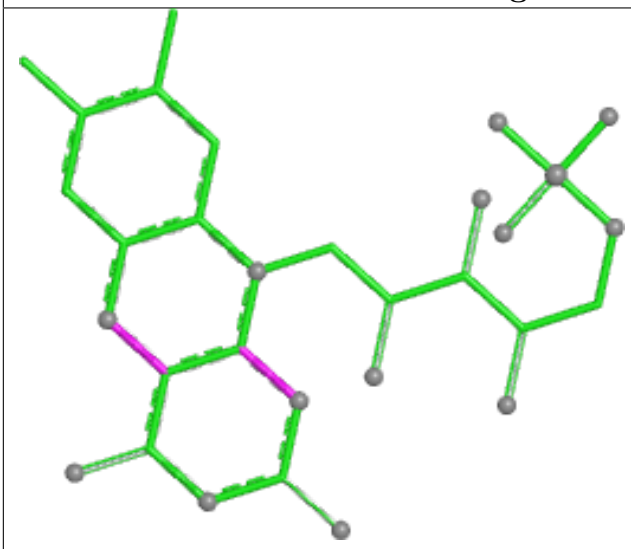


Torsions

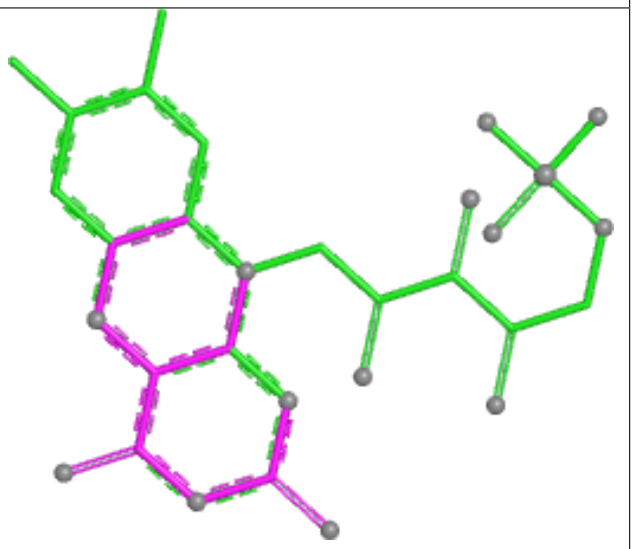


Rings

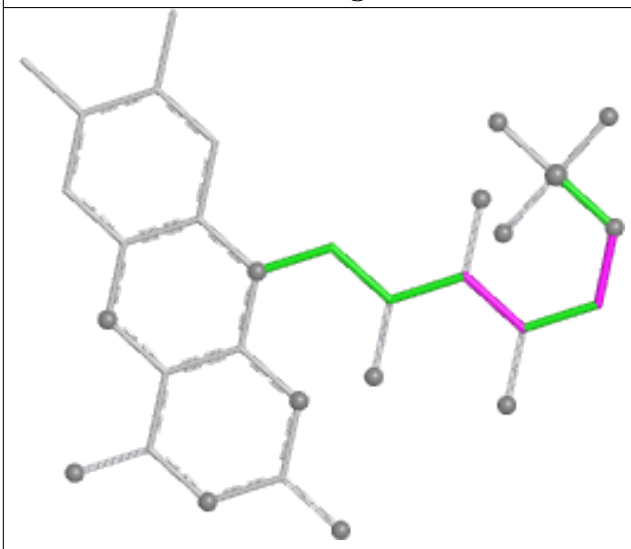
Ligand FMN A 4000



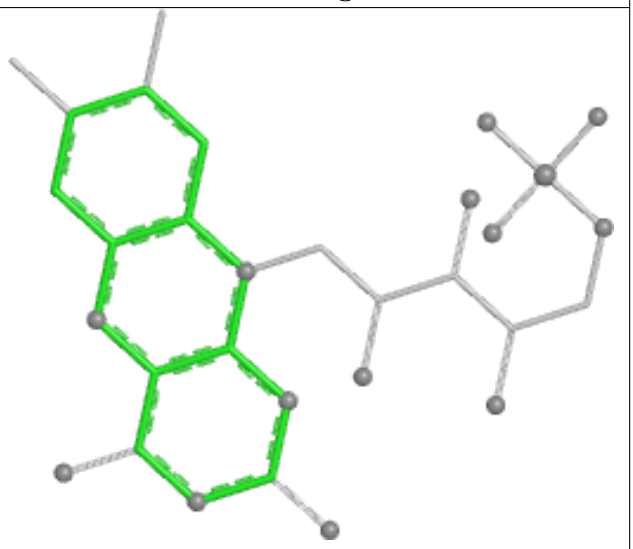
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

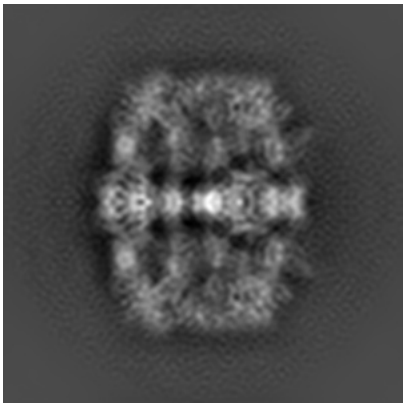
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2238. These allow visual inspection of the internal detail of the map and identification of artifacts.

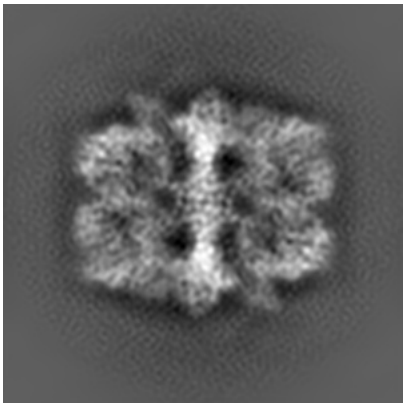
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

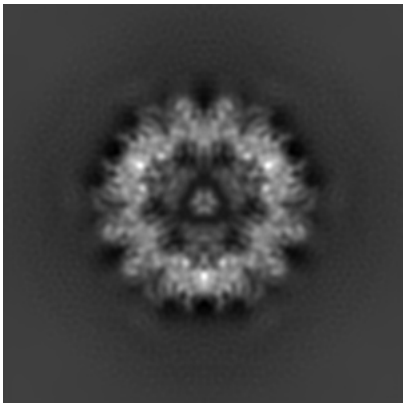
6.1.1 Primary map



X



Y

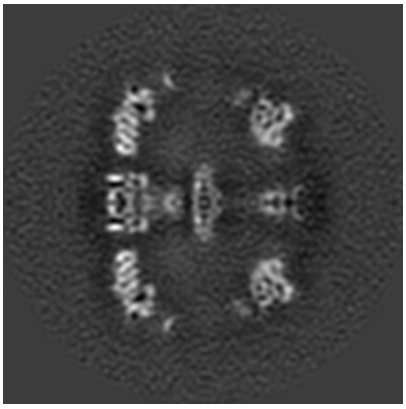


Z

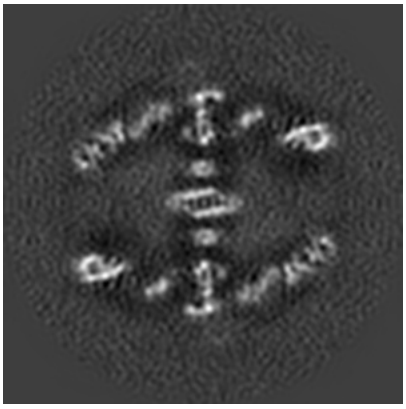
The images above show the map projected in three orthogonal directions.

6.2 Central slices

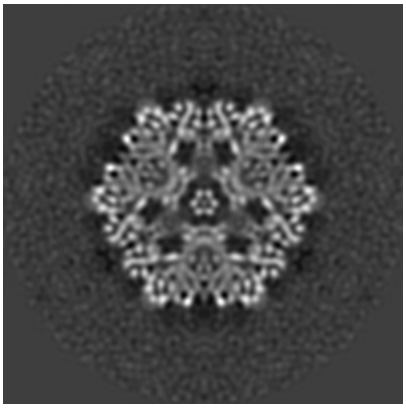
6.2.1 Primary map



X Index: 80



Y Index: 80

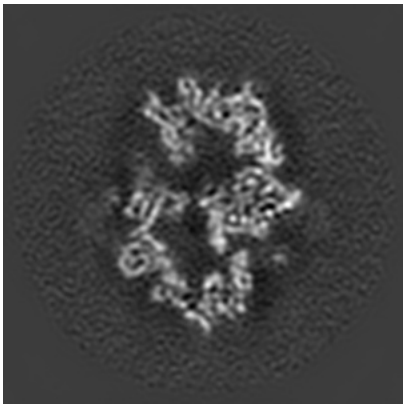


Z Index: 80

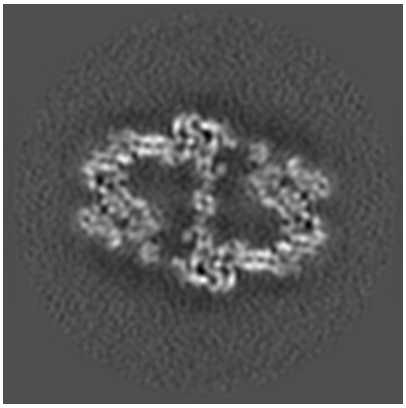
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

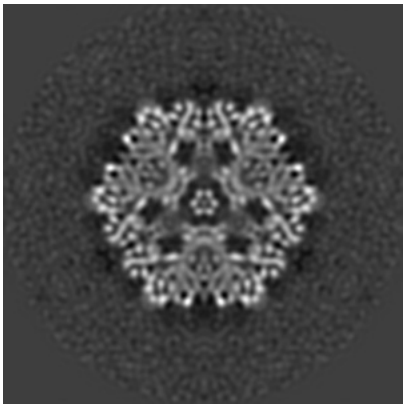
6.3.1 Primary map



X Index: 55



Y Index: 105



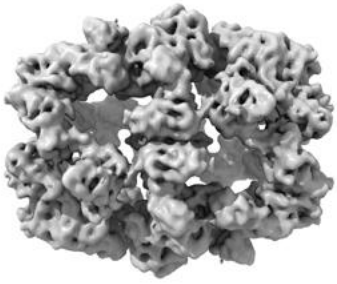
Z Index: 80

The images above show the largest variance slices of the map in three orthogonal directions.

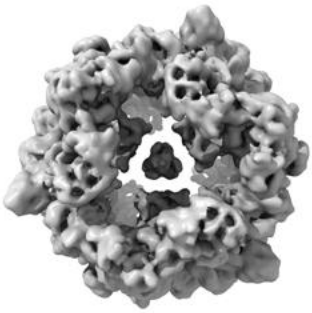
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

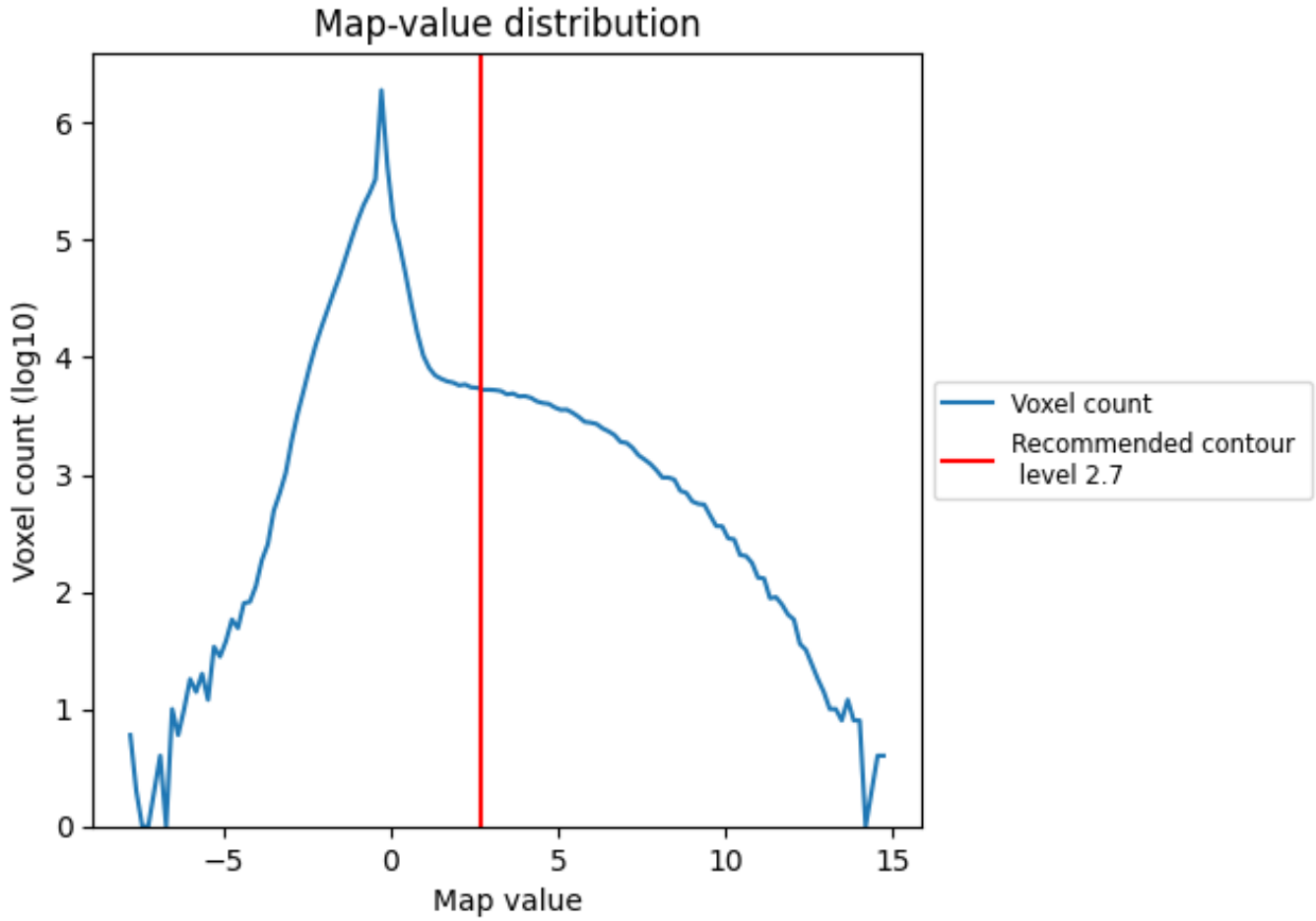
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

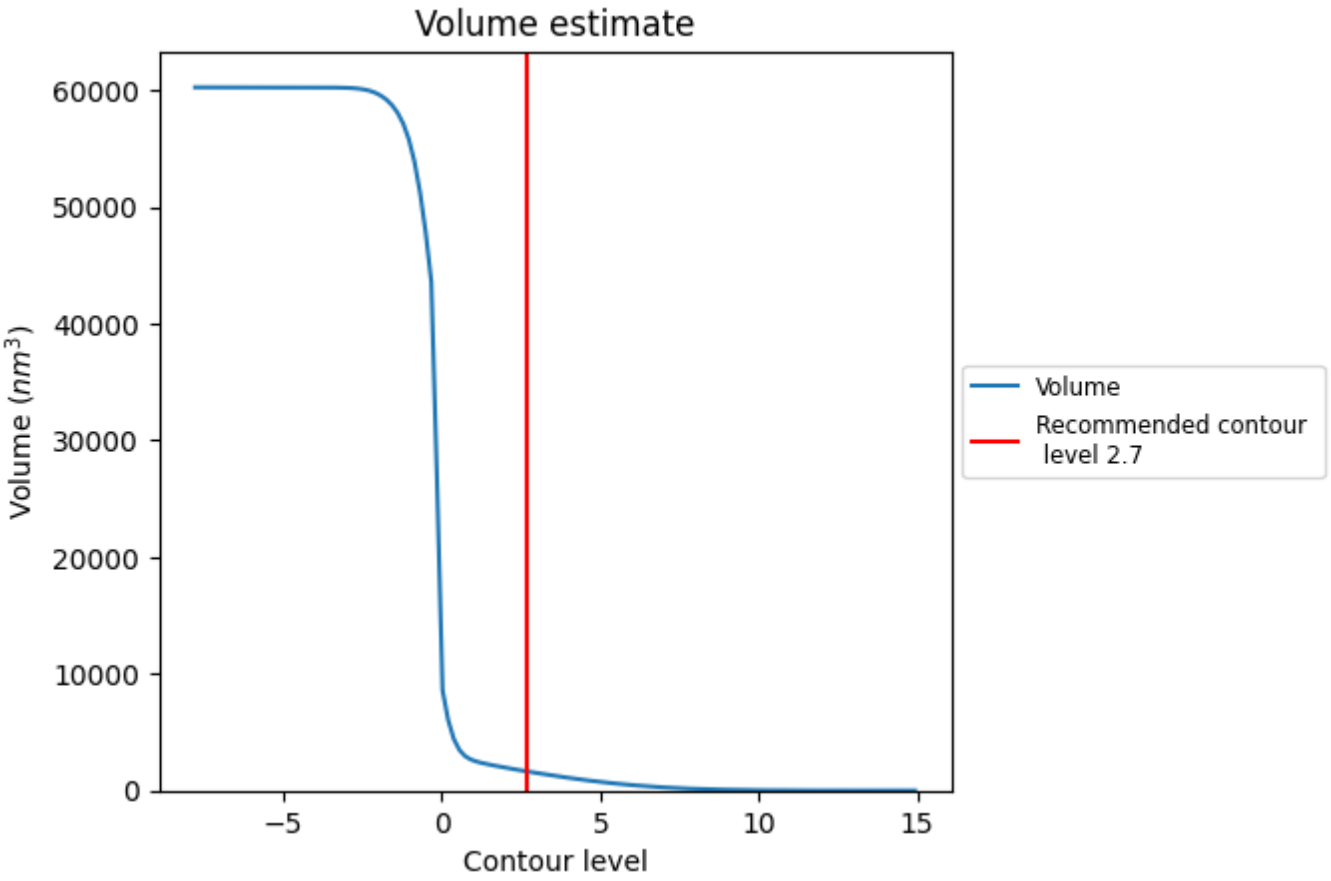
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

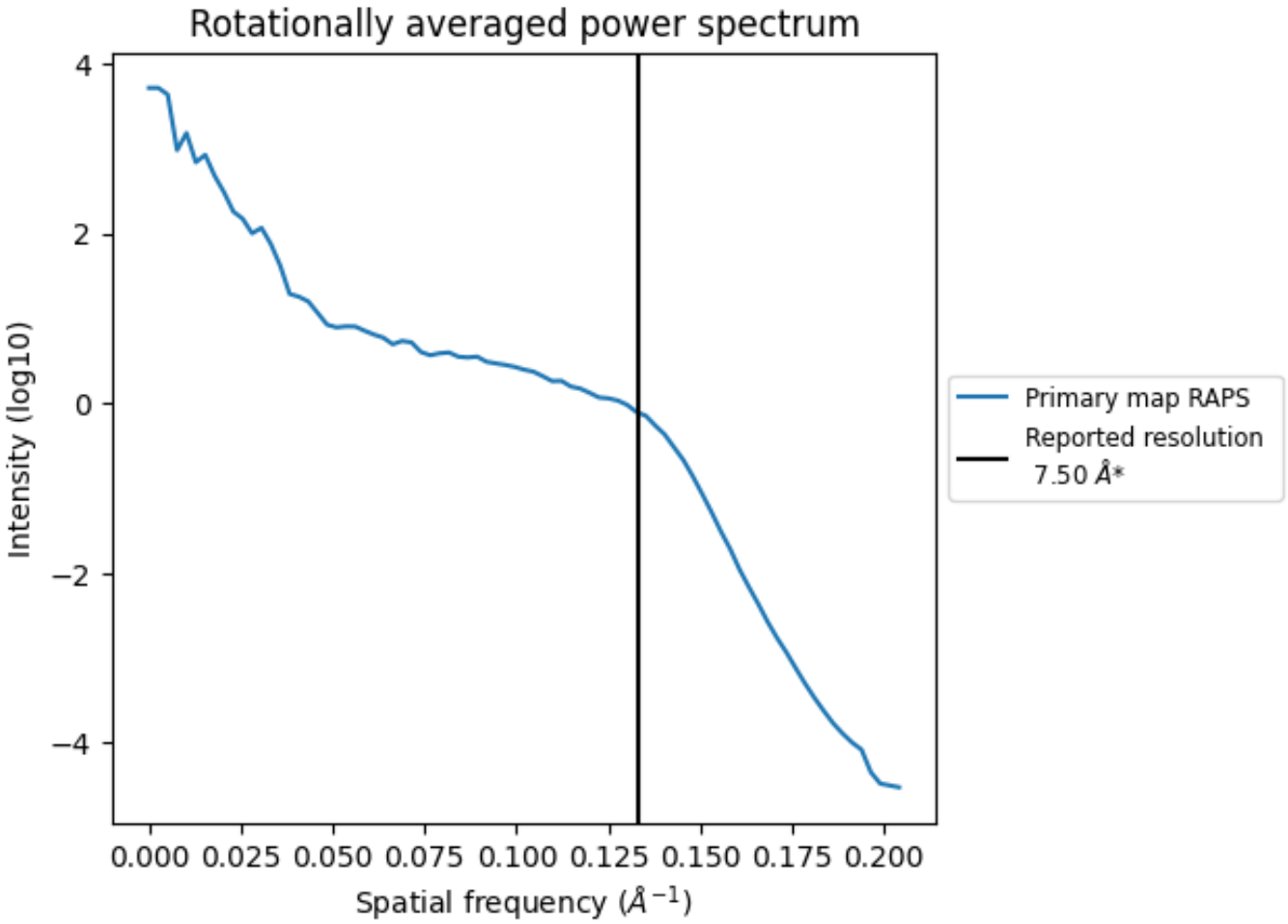
7.2 Volume estimate



The volume at the recommended contour level is 1634 nm^3; this corresponds to an approximate mass of 1476 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.133 Å^{-1}

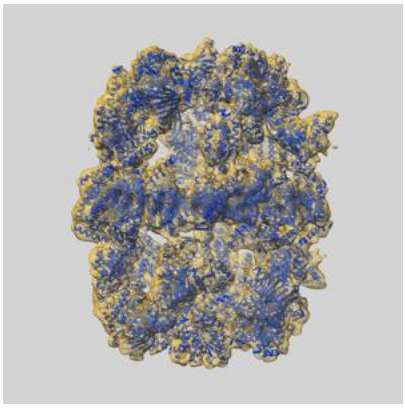
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

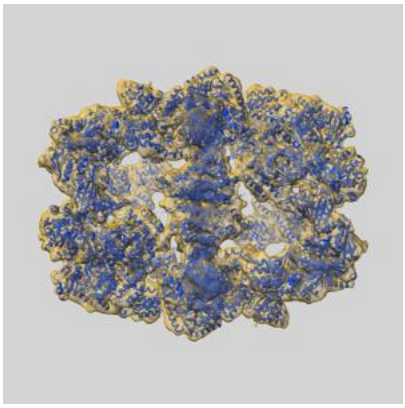
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2238 and PDB model 4V8L. Per-residue inclusion information can be found in section 3 on page 31.

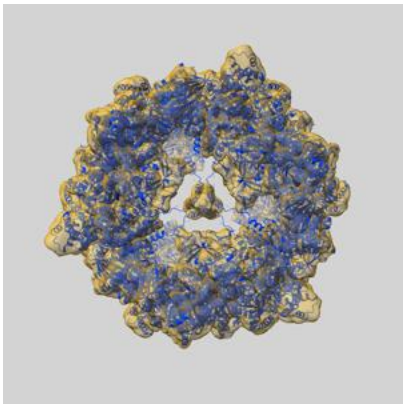
9.1 Map-model overlay



X



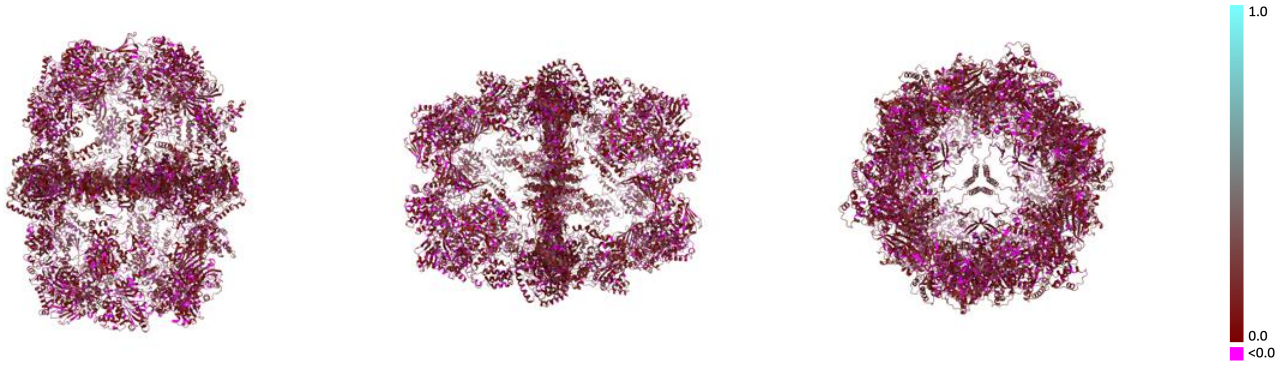
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

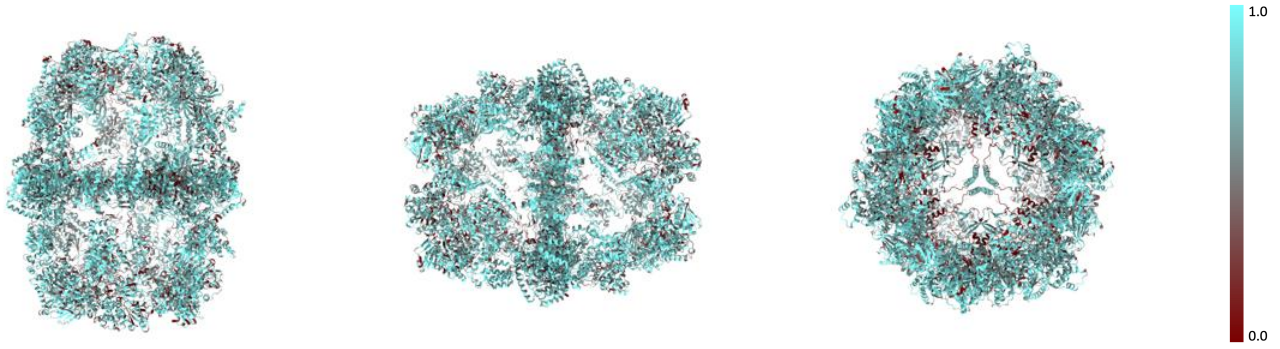
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

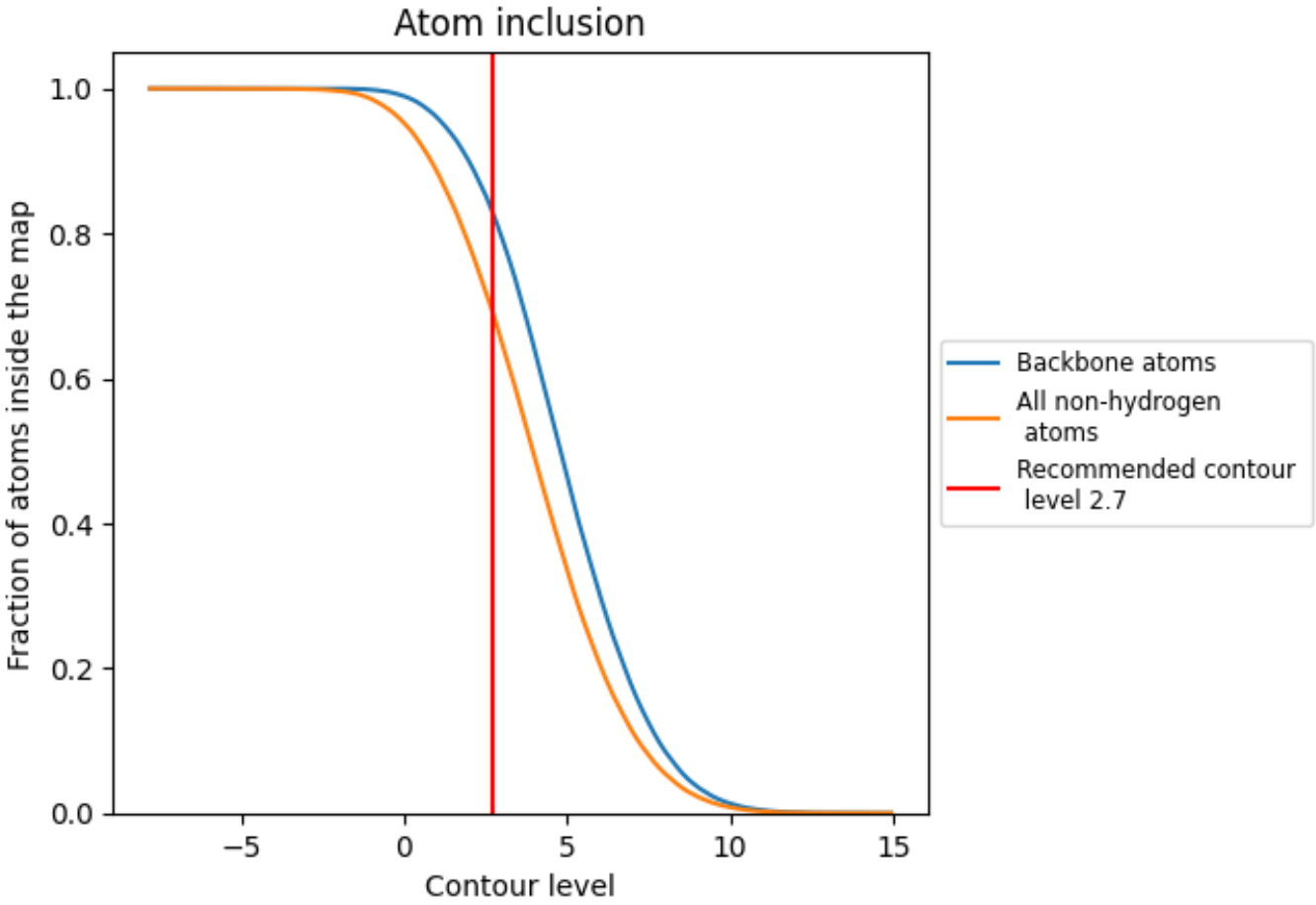
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.7).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (2.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6932	0.1100
A	0.6749	0.1000
B	0.6945	0.1130
C	0.6892	0.1090
D	0.6976	0.1120
E	0.6908	0.1080
F	0.7121	0.1200