Full wwPDB EM Validation Report ⓘ

Dec 7, 2022 – 04:11 PM JST

PDB ID	:	7VMP
EMDB ID	:	EMD-33939
Title	:	Structure of recombinant RyR2 (Ca2+ dataset, class 2, open state)
Authors	:	Kobayashi, T.; Tsutsumi, A.; Kurebayashi, N.; Kodama, M.; Kikkawa, M.; Murayama, T.; Ogawa, H.
Deposited on	:	2021-10-09
Resolution	:	3.50 Å(reported)

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:

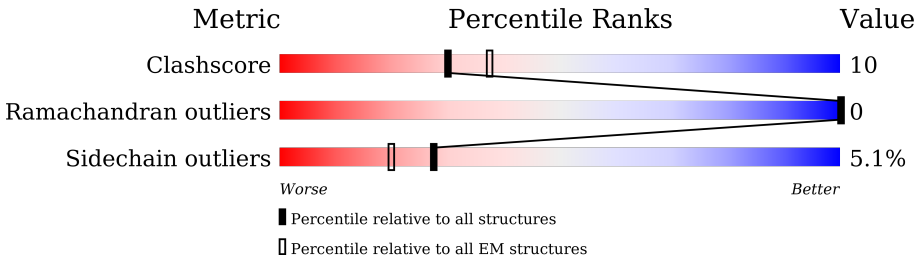
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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	4966	28% 62% 17% • 20%
1	B	4966	28% 62% 18% • 20%
1	C	4966	28% 62% 18% • 20%
1	D	4966	29% 61% 18% • 20%
2	G	176	11% 40% 19% • 39%
2	H	176	10% 41% 19% • 39%
2	I	176	11% 40% 20% • 39%
2	J	176	10% 41% 19% • 39%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 122036 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 Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3991	Total	C	N	O	S	0	0
			29688	18782	5180	5553	173		
1	B	3991	Total	C	N	O	S	0	0
			29688	18782	5180	5553	173		
1	C	3991	Total	C	N	O	S	0	0
			29688	18782	5180	5553	173		
1	D	3991	Total	C	N	O	S	0	0
			29688	18782	5180	5553	173		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	H	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	I	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	J	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-67	MET	-	initiating methionine	UNP P68106
G	-66	GLY	-	expression tag	UNP P68106
G	-65	SER	-	expression tag	UNP P68106
G	-64	SER	-	expression tag	UNP P68106
G	-63	HIS	-	expression tag	UNP P68106
G	-62	HIS	-	expression tag	UNP P68106
G	-61	HIS	-	expression tag	UNP P68106
G	-60	HIS	-	expression tag	UNP P68106
G	-59	HIS	-	expression tag	UNP P68106

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	-58	HIS	-	expression tag	UNP P68106
G	-57	SER	-	expression tag	UNP P68106
G	-56	SER	-	expression tag	UNP P68106
G	-55	GLY	-	expression tag	UNP P68106
G	-54	LEU	-	expression tag	UNP P68106
G	-53	VAL	-	expression tag	UNP P68106
G	-52	PRO	-	expression tag	UNP P68106
G	-51	ARG	-	expression tag	UNP P68106
G	-50	GLY	-	expression tag	UNP P68106
G	-49	SER	-	expression tag	UNP P68106
G	-48	HIS	-	expression tag	UNP P68106
G	-47	MET	-	expression tag	UNP P68106
G	-46	ALA	-	expression tag	UNP P68106
G	-45	SER	-	expression tag	UNP P68106
G	-44	MET	-	expression tag	UNP P68106
G	-43	ASP	-	expression tag	UNP P68106
G	-42	GLU	-	expression tag	UNP P68106
G	-41	LYS	-	expression tag	UNP P68106
G	-40	THR	-	expression tag	UNP P68106
G	-39	THR	-	expression tag	UNP P68106
G	-38	GLY	-	expression tag	UNP P68106
G	-37	TRP	-	expression tag	UNP P68106
G	-36	ARG	-	expression tag	UNP P68106
G	-35	GLY	-	expression tag	UNP P68106
G	-34	GLY	-	expression tag	UNP P68106
G	-33	HIS	-	expression tag	UNP P68106
G	-32	VAL	-	expression tag	UNP P68106
G	-31	VAL	-	expression tag	UNP P68106
G	-30	GLU	-	expression tag	UNP P68106
G	-29	GLY	-	expression tag	UNP P68106
G	-28	LEU	-	expression tag	UNP P68106
G	-27	ALA	-	expression tag	UNP P68106
G	-26	GLY	-	expression tag	UNP P68106
G	-25	GLU	-	expression tag	UNP P68106
G	-24	LEU	-	expression tag	UNP P68106
G	-23	GLU	-	expression tag	UNP P68106
G	-22	GLN	-	expression tag	UNP P68106
G	-21	LEU	-	expression tag	UNP P68106
G	-20	ARG	-	expression tag	UNP P68106
G	-19	ALA	-	expression tag	UNP P68106
G	-18	ARG	-	expression tag	UNP P68106
G	-17	LEU	-	expression tag	UNP P68106

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	-16	GLU	-	expression tag	UNP P68106
G	-15	HIS	-	expression tag	UNP P68106
G	-14	HIS	-	expression tag	UNP P68106
G	-13	PRO	-	expression tag	UNP P68106
G	-12	GLN	-	expression tag	UNP P68106
G	-11	GLY	-	expression tag	UNP P68106
G	-10	GLN	-	expression tag	UNP P68106
G	-9	ARG	-	expression tag	UNP P68106
G	-8	GLU	-	expression tag	UNP P68106
G	-7	PRO	-	expression tag	UNP P68106
G	-6	GLY	-	expression tag	UNP P68106
G	-5	SER	-	expression tag	UNP P68106
G	-4	GLY	-	expression tag	UNP P68106
G	-3	GLY	-	expression tag	UNP P68106
G	-2	SER	-	expression tag	UNP P68106
G	-1	GLY	-	expression tag	UNP P68106
G	0	GLY	-	expression tag	UNP P68106
G	1	THR	-	expression tag	UNP P68106
H	-67	MET	-	initiating methionine	UNP P68106
H	-66	GLY	-	expression tag	UNP P68106
H	-65	SER	-	expression tag	UNP P68106
H	-64	SER	-	expression tag	UNP P68106
H	-63	HIS	-	expression tag	UNP P68106
H	-62	HIS	-	expression tag	UNP P68106
H	-61	HIS	-	expression tag	UNP P68106
H	-60	HIS	-	expression tag	UNP P68106
H	-59	HIS	-	expression tag	UNP P68106
H	-58	HIS	-	expression tag	UNP P68106
H	-57	SER	-	expression tag	UNP P68106
H	-56	SER	-	expression tag	UNP P68106
H	-55	GLY	-	expression tag	UNP P68106
H	-54	LEU	-	expression tag	UNP P68106
H	-53	VAL	-	expression tag	UNP P68106
H	-52	PRO	-	expression tag	UNP P68106
H	-51	ARG	-	expression tag	UNP P68106
H	-50	GLY	-	expression tag	UNP P68106
H	-49	SER	-	expression tag	UNP P68106
H	-48	HIS	-	expression tag	UNP P68106
H	-47	MET	-	expression tag	UNP P68106
H	-46	ALA	-	expression tag	UNP P68106
H	-45	SER	-	expression tag	UNP P68106
H	-44	MET	-	expression tag	UNP P68106

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	-43	ASP	-	expression tag	UNP P68106
H	-42	GLU	-	expression tag	UNP P68106
H	-41	LYS	-	expression tag	UNP P68106
H	-40	THR	-	expression tag	UNP P68106
H	-39	THR	-	expression tag	UNP P68106
H	-38	GLY	-	expression tag	UNP P68106
H	-37	TRP	-	expression tag	UNP P68106
H	-36	ARG	-	expression tag	UNP P68106
H	-35	GLY	-	expression tag	UNP P68106
H	-34	GLY	-	expression tag	UNP P68106
H	-33	HIS	-	expression tag	UNP P68106
H	-32	VAL	-	expression tag	UNP P68106
H	-31	VAL	-	expression tag	UNP P68106
H	-30	GLU	-	expression tag	UNP P68106
H	-29	GLY	-	expression tag	UNP P68106
H	-28	LEU	-	expression tag	UNP P68106
H	-27	ALA	-	expression tag	UNP P68106
H	-26	GLY	-	expression tag	UNP P68106
H	-25	GLU	-	expression tag	UNP P68106
H	-24	LEU	-	expression tag	UNP P68106
H	-23	GLU	-	expression tag	UNP P68106
H	-22	GLN	-	expression tag	UNP P68106
H	-21	LEU	-	expression tag	UNP P68106
H	-20	ARG	-	expression tag	UNP P68106
H	-19	ALA	-	expression tag	UNP P68106
H	-18	ARG	-	expression tag	UNP P68106
H	-17	LEU	-	expression tag	UNP P68106
H	-16	GLU	-	expression tag	UNP P68106
H	-15	HIS	-	expression tag	UNP P68106
H	-14	HIS	-	expression tag	UNP P68106
H	-13	PRO	-	expression tag	UNP P68106
H	-12	GLN	-	expression tag	UNP P68106
H	-11	GLY	-	expression tag	UNP P68106
H	-10	GLN	-	expression tag	UNP P68106
H	-9	ARG	-	expression tag	UNP P68106
H	-8	GLU	-	expression tag	UNP P68106
H	-7	PRO	-	expression tag	UNP P68106
H	-6	GLY	-	expression tag	UNP P68106
H	-5	SER	-	expression tag	UNP P68106
H	-4	GLY	-	expression tag	UNP P68106
H	-3	GLY	-	expression tag	UNP P68106
H	-2	SER	-	expression tag	UNP P68106

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	GLY	-	expression tag	UNP P68106
H	0	GLY	-	expression tag	UNP P68106
H	1	THR	-	expression tag	UNP P68106
I	-67	MET	-	initiating methionine	UNP P68106
I	-66	GLY	-	expression tag	UNP P68106
I	-65	SER	-	expression tag	UNP P68106
I	-64	SER	-	expression tag	UNP P68106
I	-63	HIS	-	expression tag	UNP P68106
I	-62	HIS	-	expression tag	UNP P68106
I	-61	HIS	-	expression tag	UNP P68106
I	-60	HIS	-	expression tag	UNP P68106
I	-59	HIS	-	expression tag	UNP P68106
I	-58	HIS	-	expression tag	UNP P68106
I	-57	SER	-	expression tag	UNP P68106
I	-56	SER	-	expression tag	UNP P68106
I	-55	GLY	-	expression tag	UNP P68106
I	-54	LEU	-	expression tag	UNP P68106
I	-53	VAL	-	expression tag	UNP P68106
I	-52	PRO	-	expression tag	UNP P68106
I	-51	ARG	-	expression tag	UNP P68106
I	-50	GLY	-	expression tag	UNP P68106
I	-49	SER	-	expression tag	UNP P68106
I	-48	HIS	-	expression tag	UNP P68106
I	-47	MET	-	expression tag	UNP P68106
I	-46	ALA	-	expression tag	UNP P68106
I	-45	SER	-	expression tag	UNP P68106
I	-44	MET	-	expression tag	UNP P68106
I	-43	ASP	-	expression tag	UNP P68106
I	-42	GLU	-	expression tag	UNP P68106
I	-41	LYS	-	expression tag	UNP P68106
I	-40	THR	-	expression tag	UNP P68106
I	-39	THR	-	expression tag	UNP P68106
I	-38	GLY	-	expression tag	UNP P68106
I	-37	TRP	-	expression tag	UNP P68106
I	-36	ARG	-	expression tag	UNP P68106
I	-35	GLY	-	expression tag	UNP P68106
I	-34	GLY	-	expression tag	UNP P68106
I	-33	HIS	-	expression tag	UNP P68106
I	-32	VAL	-	expression tag	UNP P68106
I	-31	VAL	-	expression tag	UNP P68106
I	-30	GLU	-	expression tag	UNP P68106
I	-29	GLY	-	expression tag	UNP P68106

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	-28	LEU	-	expression tag	UNP P68106
I	-27	ALA	-	expression tag	UNP P68106
I	-26	GLY	-	expression tag	UNP P68106
I	-25	GLU	-	expression tag	UNP P68106
I	-24	LEU	-	expression tag	UNP P68106
I	-23	GLU	-	expression tag	UNP P68106
I	-22	GLN	-	expression tag	UNP P68106
I	-21	LEU	-	expression tag	UNP P68106
I	-20	ARG	-	expression tag	UNP P68106
I	-19	ALA	-	expression tag	UNP P68106
I	-18	ARG	-	expression tag	UNP P68106
I	-17	LEU	-	expression tag	UNP P68106
I	-16	GLU	-	expression tag	UNP P68106
I	-15	HIS	-	expression tag	UNP P68106
I	-14	HIS	-	expression tag	UNP P68106
I	-13	PRO	-	expression tag	UNP P68106
I	-12	GLN	-	expression tag	UNP P68106
I	-11	GLY	-	expression tag	UNP P68106
I	-10	GLN	-	expression tag	UNP P68106
I	-9	ARG	-	expression tag	UNP P68106
I	-8	GLU	-	expression tag	UNP P68106
I	-7	PRO	-	expression tag	UNP P68106
I	-6	GLY	-	expression tag	UNP P68106
I	-5	SER	-	expression tag	UNP P68106
I	-4	GLY	-	expression tag	UNP P68106
I	-3	GLY	-	expression tag	UNP P68106
I	-2	SER	-	expression tag	UNP P68106
I	-1	GLY	-	expression tag	UNP P68106
I	0	GLY	-	expression tag	UNP P68106
I	1	THR	-	expression tag	UNP P68106
J	-67	MET	-	initiating methionine	UNP P68106
J	-66	GLY	-	expression tag	UNP P68106
J	-65	SER	-	expression tag	UNP P68106
J	-64	SER	-	expression tag	UNP P68106
J	-63	HIS	-	expression tag	UNP P68106
J	-62	HIS	-	expression tag	UNP P68106
J	-61	HIS	-	expression tag	UNP P68106
J	-60	HIS	-	expression tag	UNP P68106
J	-59	HIS	-	expression tag	UNP P68106
J	-58	HIS	-	expression tag	UNP P68106
J	-57	SER	-	expression tag	UNP P68106
J	-56	SER	-	expression tag	UNP P68106

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	-55	GLY	-	expression tag	UNP P68106
J	-54	LEU	-	expression tag	UNP P68106
J	-53	VAL	-	expression tag	UNP P68106
J	-52	PRO	-	expression tag	UNP P68106
J	-51	ARG	-	expression tag	UNP P68106
J	-50	GLY	-	expression tag	UNP P68106
J	-49	SER	-	expression tag	UNP P68106
J	-48	HIS	-	expression tag	UNP P68106
J	-47	MET	-	expression tag	UNP P68106
J	-46	ALA	-	expression tag	UNP P68106
J	-45	SER	-	expression tag	UNP P68106
J	-44	MET	-	expression tag	UNP P68106
J	-43	ASP	-	expression tag	UNP P68106
J	-42	GLU	-	expression tag	UNP P68106
J	-41	LYS	-	expression tag	UNP P68106
J	-40	THR	-	expression tag	UNP P68106
J	-39	THR	-	expression tag	UNP P68106
J	-38	GLY	-	expression tag	UNP P68106
J	-37	TRP	-	expression tag	UNP P68106
J	-36	ARG	-	expression tag	UNP P68106
J	-35	GLY	-	expression tag	UNP P68106
J	-34	GLY	-	expression tag	UNP P68106
J	-33	HIS	-	expression tag	UNP P68106
J	-32	VAL	-	expression tag	UNP P68106
J	-31	VAL	-	expression tag	UNP P68106
J	-30	GLU	-	expression tag	UNP P68106
J	-29	GLY	-	expression tag	UNP P68106
J	-28	LEU	-	expression tag	UNP P68106
J	-27	ALA	-	expression tag	UNP P68106
J	-26	GLY	-	expression tag	UNP P68106
J	-25	GLU	-	expression tag	UNP P68106
J	-24	LEU	-	expression tag	UNP P68106
J	-23	GLU	-	expression tag	UNP P68106
J	-22	GLN	-	expression tag	UNP P68106
J	-21	LEU	-	expression tag	UNP P68106
J	-20	ARG	-	expression tag	UNP P68106
J	-19	ALA	-	expression tag	UNP P68106
J	-18	ARG	-	expression tag	UNP P68106
J	-17	LEU	-	expression tag	UNP P68106
J	-16	GLU	-	expression tag	UNP P68106
J	-15	HIS	-	expression tag	UNP P68106
J	-14	HIS	-	expression tag	UNP P68106

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	-13	PRO	-	expression tag	UNP P68106
J	-12	GLN	-	expression tag	UNP P68106
J	-11	GLY	-	expression tag	UNP P68106
J	-10	GLN	-	expression tag	UNP P68106
J	-9	ARG	-	expression tag	UNP P68106
J	-8	GLU	-	expression tag	UNP P68106
J	-7	PRO	-	expression tag	UNP P68106
J	-6	GLY	-	expression tag	UNP P68106
J	-5	SER	-	expression tag	UNP P68106
J	-4	GLY	-	expression tag	UNP P68106
J	-3	GLY	-	expression tag	UNP P68106
J	-2	SER	-	expression tag	UNP P68106
J	-1	GLY	-	expression tag	UNP P68106
J	0	GLY	-	expression tag	UNP P68106
J	1	THR	-	expression tag	UNP P68106

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Zn 1 1	0
3	B	1	Total Zn 1 1	0
3	C	1	Total Zn 1 1	0
3	D	1	Total Zn 1 1	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

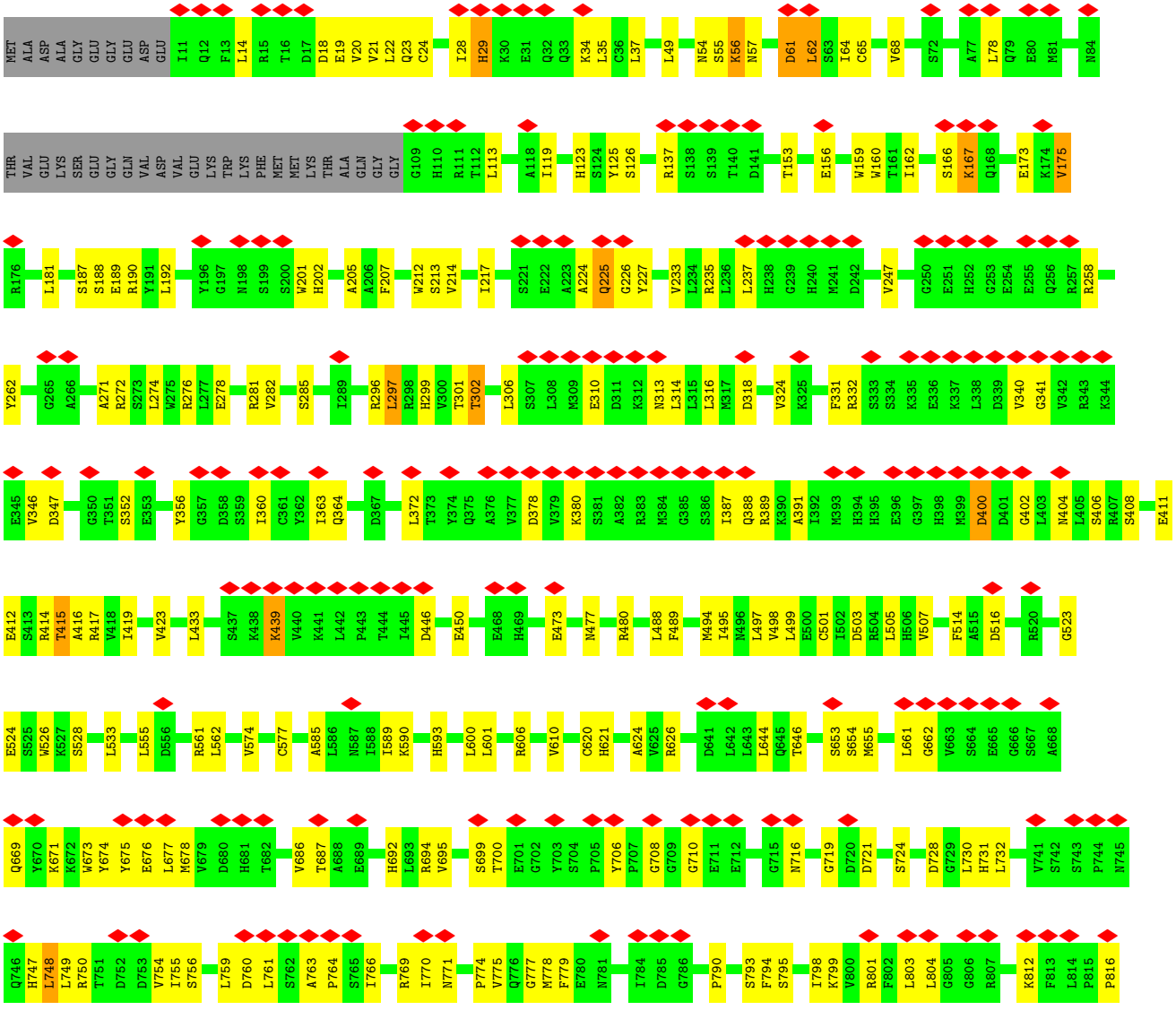
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Ca 1 1	0
4	B	1	Total Ca 1 1	0
4	C	1	Total Ca 1 1	0
4	D	1	Total Ca 1 1	0

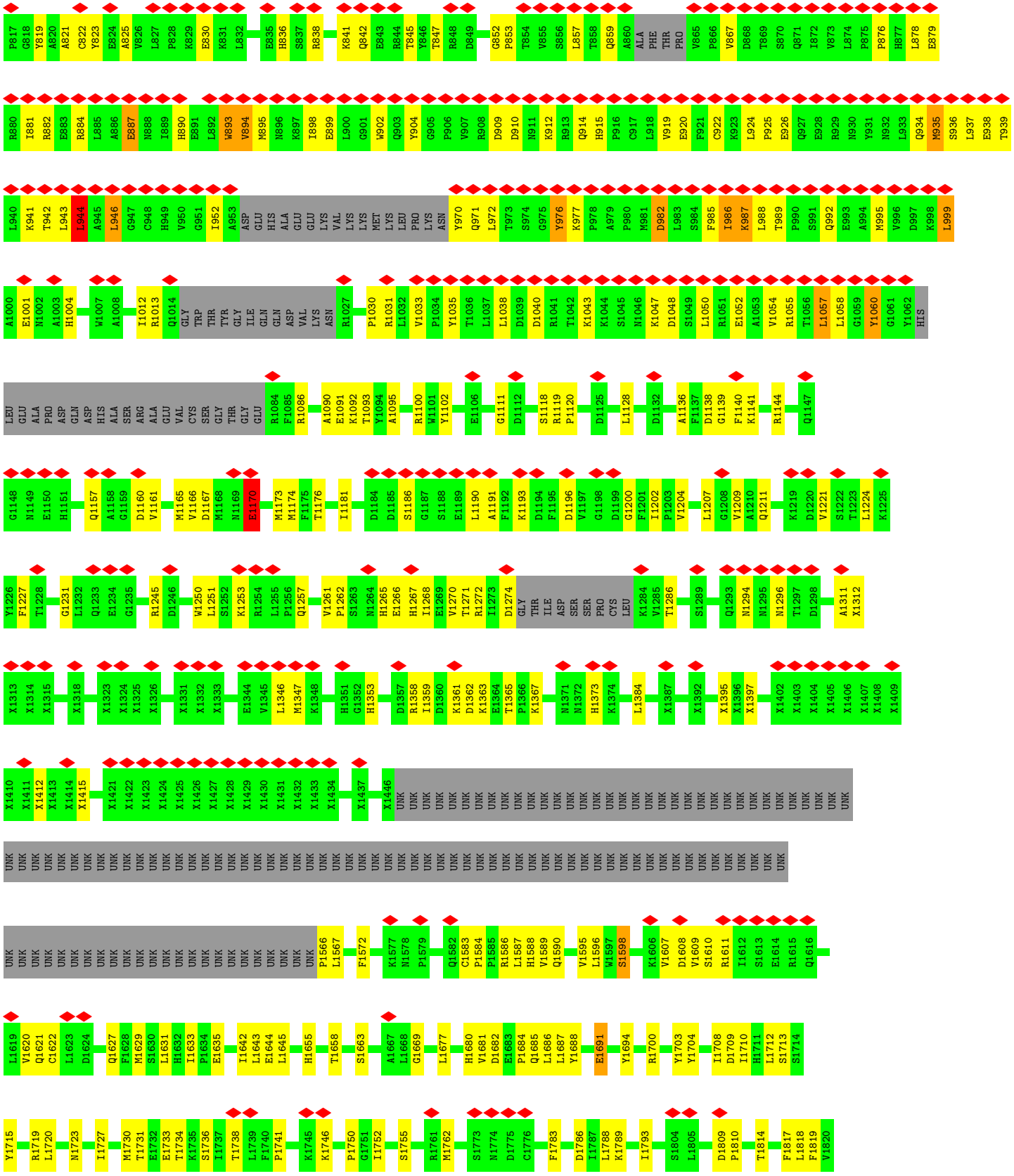
3 Residue-property plots (i)

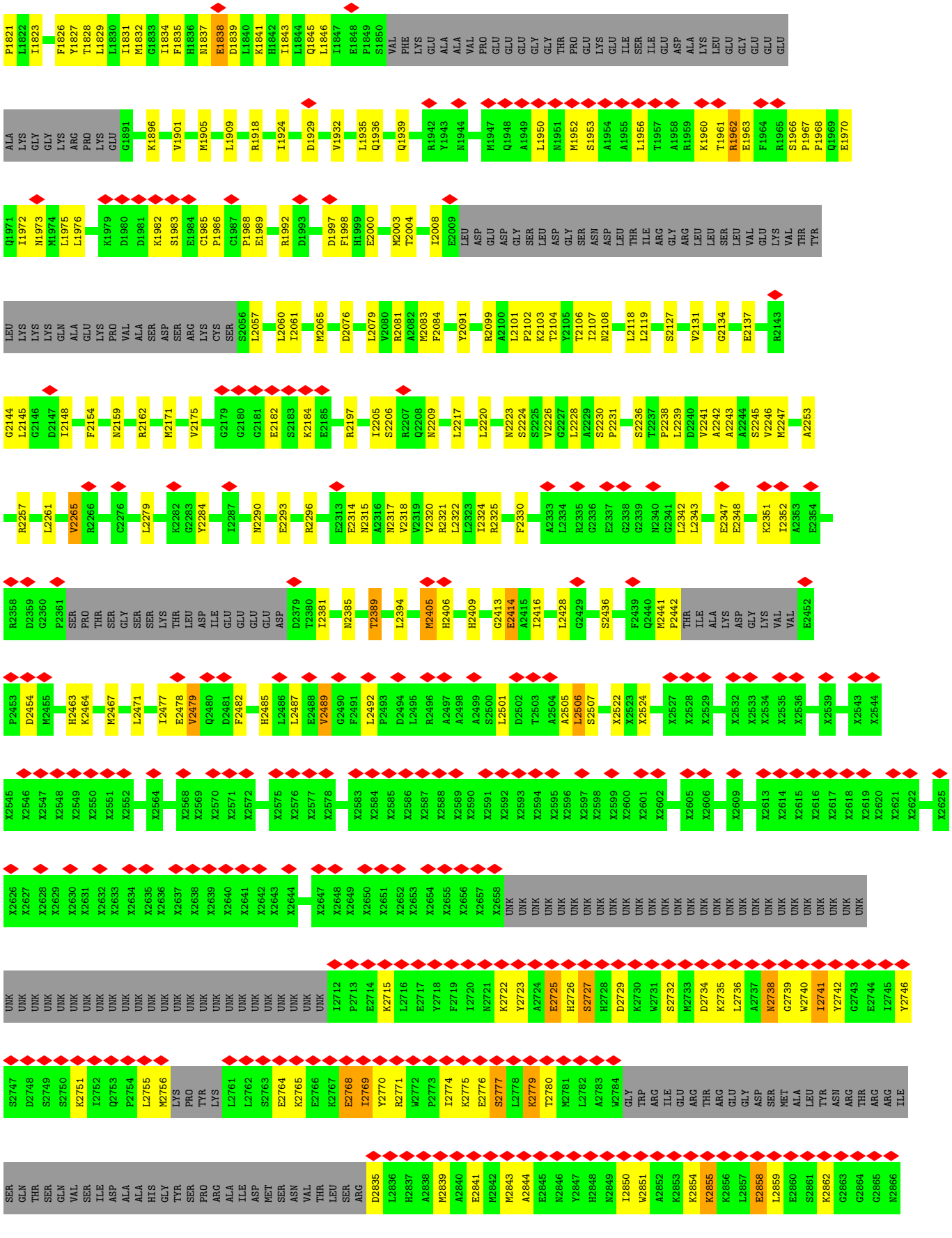
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

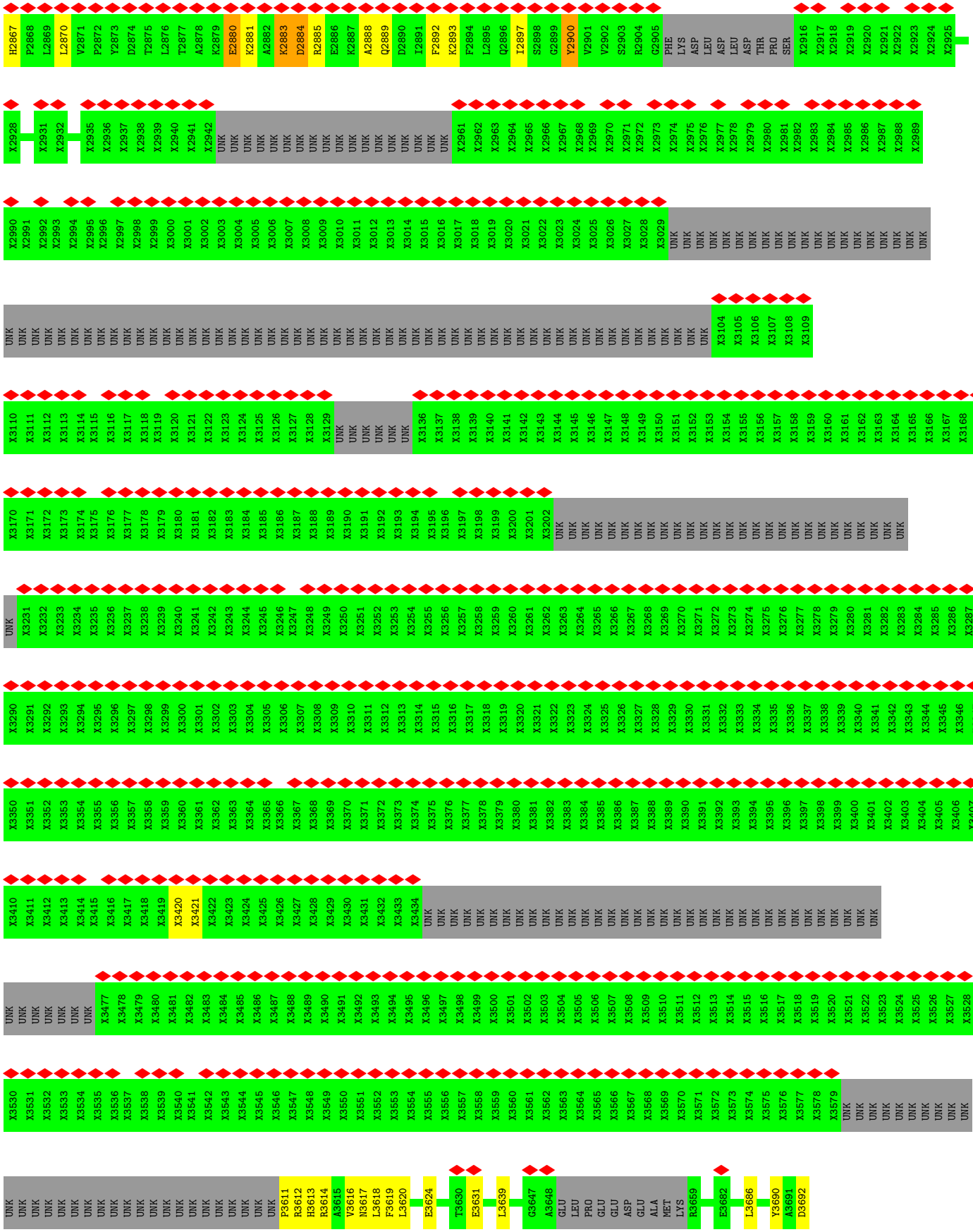
- Molecule 1: Ryanodine receptor 2

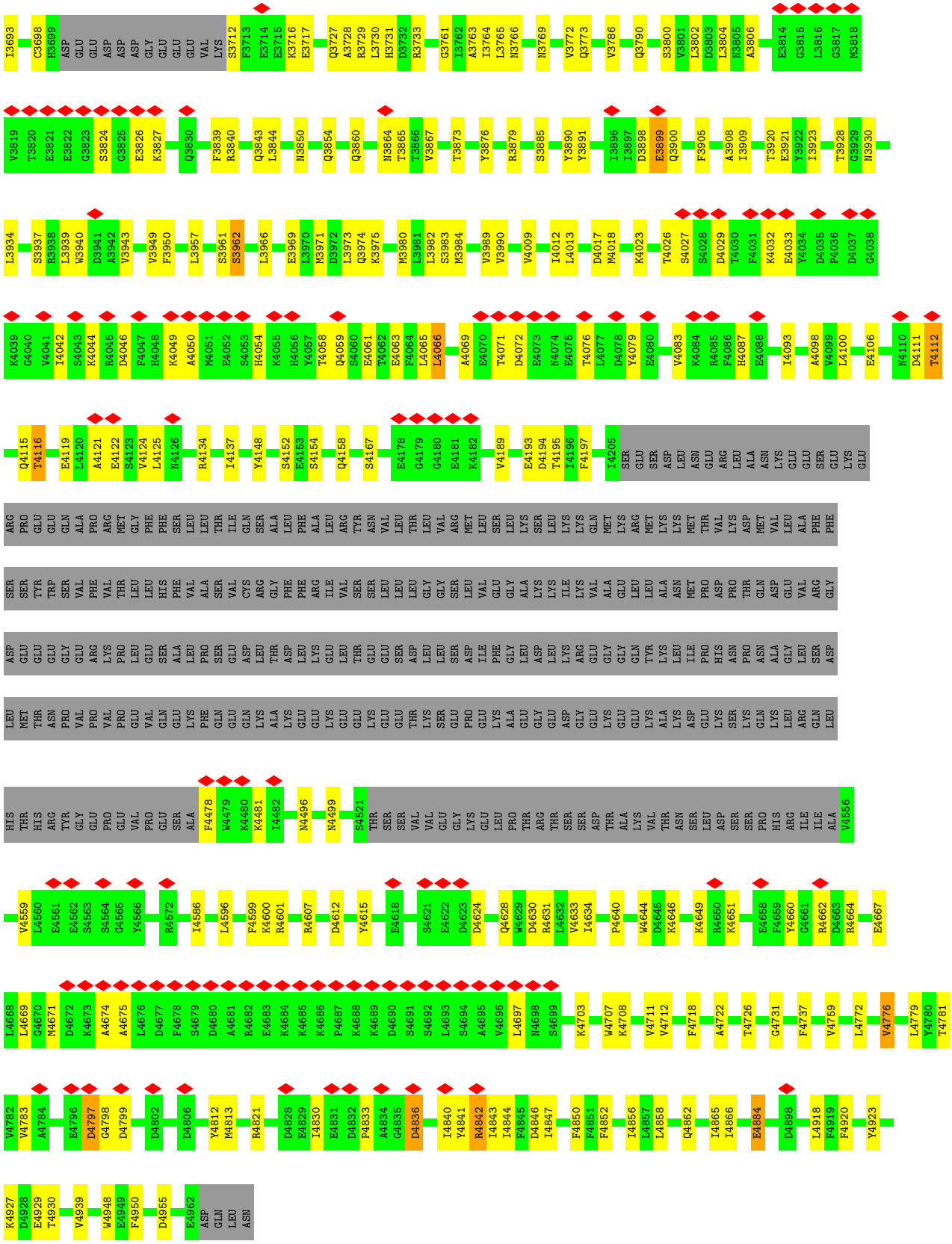
Chain A:




P817 G818 Y819 A820 A821 C822 Y823 E824 A825 V826 L827 P828 K829 E830 K831 L832 E835 H836 S837 R838 K841 Q842 E843 R844 T845 Y846 T847 R848 D849 G852 P853 T854 V855 S856 L857 T858 Q859 A860 ALA PHE THR PRO V865 P866 V867 D868 T869 S870 Q871 I872 V873 L874 P875 P876 H877 L878 E879
R880 I881 R882 E883 R884 L885 A886 E887 N888 I889 H890 E891 L892 W893 V894 M895 N896 K897 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918 V919 E920 F921 C922 K923 L924 P925 E926 Q927 E928 R929 N930 Y931 N932 L933 Q934 M935 S936 L937 E938 T939
L940 K941 T942 L943 L944 A945 L946 G947 C948 H949 V950 G951 I952 A953 ASP GLU HIS ALA GLU GLU LYS VAL LYS LYS MET LYS LEU PRO LYS ASN Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 T989 P990 S991 Q992 E993 A994 M995 V996 D997 K998 L999
A1000 E1001 N1002 A1003 H1004 W1007 A1008 I1012 R1013 Q1014 GLY TRP THR TYR GLY ILE GLN GLN ASP VAL LYS ASN R1027 P1030 R1031 L1032 V1033 P1034 Y1035 T1036 L1037 L1038 D1039 D1040 R1041 T1042 K1043 K1044 S1045 N1046 K1047 D1048 S1049 L1050 R1051 E1052 A1053 V1054 R1055 T1056 L1057 L1058 G1059 Y1060 G1061 Y1062 HIS
LEU GLU ALA PRO ASP GLN ASP HIS ALA SER ARG ALA GLU VAL CYS SER GLY THR GLY GLU R1084 F1085 R1086 A1090 E1091 K1092 T1093 Y1094 A1095 R1100 W1101 Y1102 E1106 G1111 D1112 S1118 R1119 P1120 D1125 L1128 D1132 A1136 F1137 D1138 G1139 F1140 K1141 R1144 Q1147
G1148 N1149 E1150 H1151 Q1157 A1158 G1159 D1160 V1161 M1165 V1166 D1167 M1168 N1169 E1170 M1173 M1174 F1175 T1176 I1181 D1184 D1185 S1186 G1187 S1188 E1189 L1190 A1191 F1192 K1193 D1194 F1195 D1196 V1197 G1198 D1199 G1200 F1201 I1202 P1203 V1204 L1207 G1208 V1209 A1210 Q1211 K1219 D1220 V1221 S1222 T1223 L1224 K1225
Y1226 F1227 T1228 G1231 L1232 Q1233 E1234 G1235 R1245 D1246 W1250 L1251 S1252 K1253 R1254 L1255 P1256 Q1257 V1261 P1262 S1263 N1264 H1265 E1266 H1267 I1268 E1269 V1270 T1271 R1272 I1273 D1274 GLY THR ILE ASP SER SER PRO CYS LEU K1284 V1285 T1286 S1289 Q1293 N1294 N1295 N1296 T1297 D1298 A1311 X1312
X1313 X1314 X1315 X1318 X1323 X1324 X1325 X1326 X1331 X1332 X1333 E1344 V1345 L1346 M1347 K1348 H1351 G1352 H1353 D1357 R1358 I1359 D1360 K1361 D1362 K1363 E1364 T1365 P1366 K1367 N1371 N1372 H1373 K1374 L1384 X1387 X1392 X1395 X1396 X1397 X1402 X1403 X1404 X1405 X1406 X1407 X1408 X1409
X1410 X1411 X1412 X1413 X1414 X1415 X1421 X1422 X1423 X1424 X1425 X1426 X1427 X1428 X1429 X1430 X1431 X1432 X1433 X1434 X1437 X1446 UNK
UNK
UNK
UNK P1566 L1567 F1572 K1577 N1578 P1579 Q1582 C1583 P1584 P1585 R1586 L1587 H1588 V1589 Q1590 V1595 L1596 W1597 S1598 K1606 V1607 D1608 V1609 S1610 R1611 I1612 S1613 E1614 R1615 Q1616
L1619 V1620 Q1621 C1622 L1623 D1624 Q1627 F1628 M1629 S1630 L1631 H1632 I1633 P1634 E1635 I1642 L1643 E1644 L1645 H1655 T1658 S1663 A1667 L1668 G1669 L1677 H1680 V1681 D1682 E1683 P1684 Q1685 L1686 L1687 Y1688 E1691 Y1694 R1700 Y1703 Y1704 I1708 D1709 I1710 H1711 L1712 S1713 S1714
Y1715 R1719 L1720 N1723 I1727 M1730 T1731 E1732 E1733 T1734 K1735 S1736 I1737 T1738 L1739 F1740 P1741 K1745 K1746 P1750 G1751 I1752 S1755 R1761 M1762 S1773 N1774 D1775 C1776 F1783 D1786 I1787 L1788 K1789 I1793 S1804 L1805 D1809 P1810 T1814 F1817 L1818 F1819 V1820

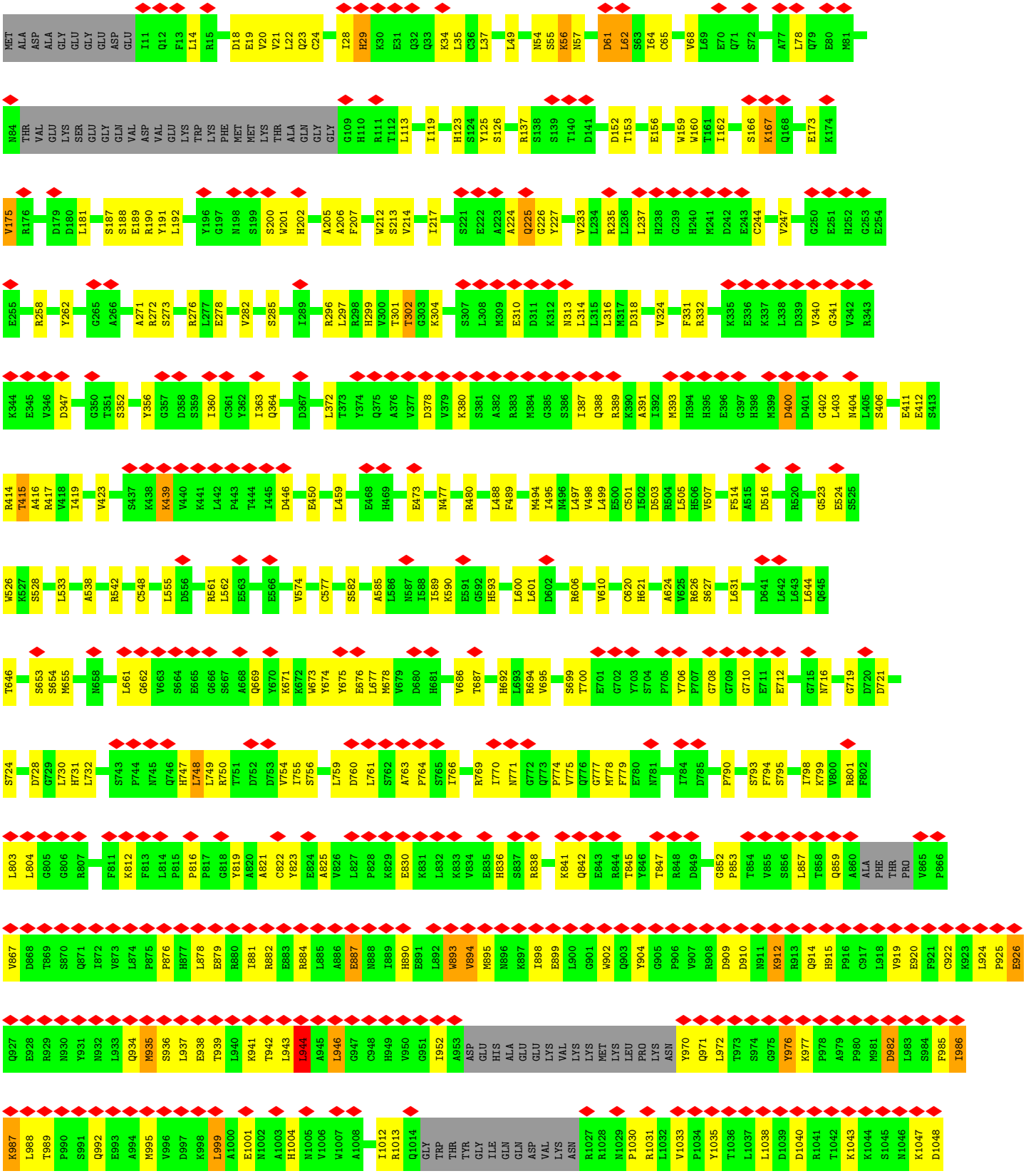


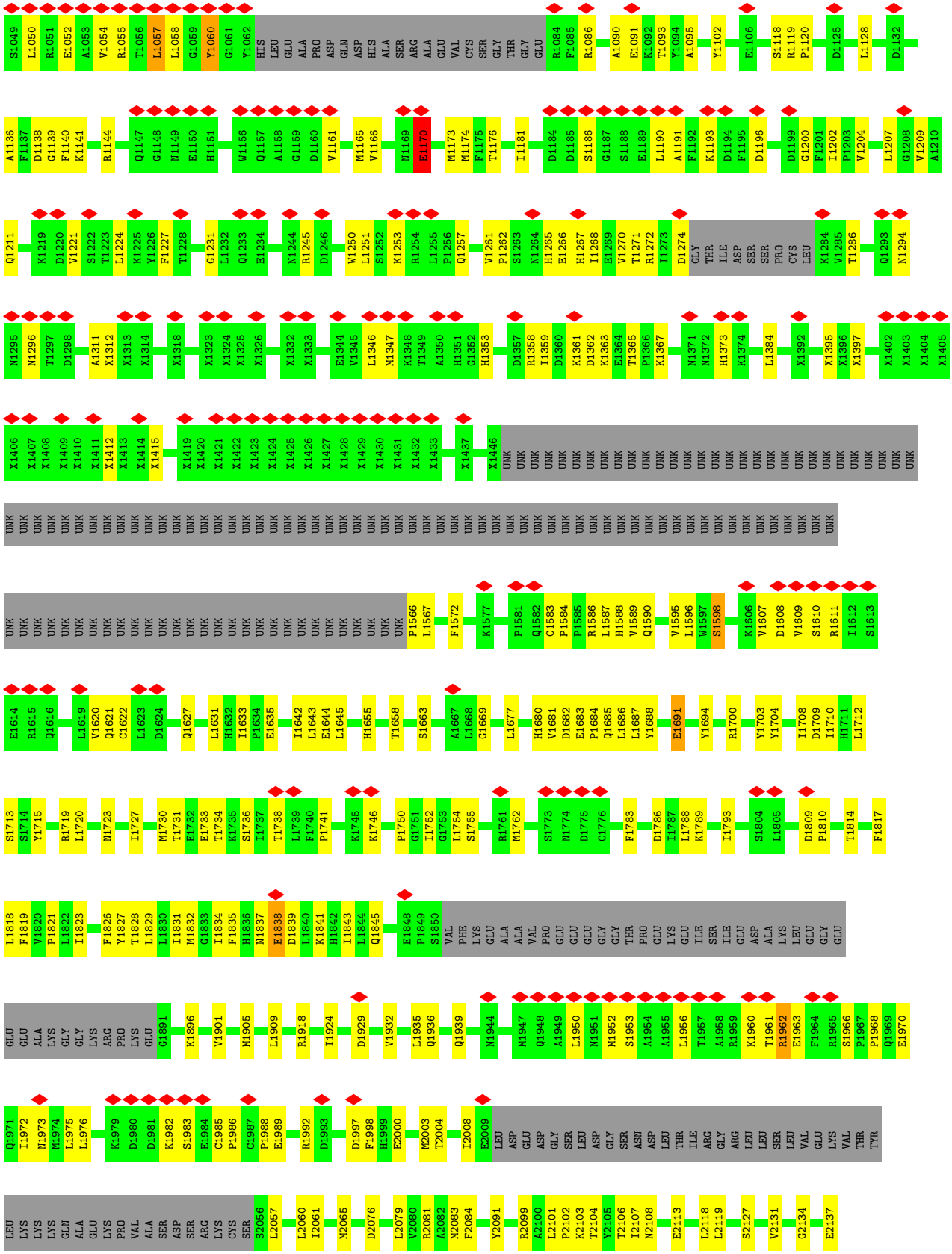

H2867 P2868 L2869 L2870 V2871 P2872 Y2873 D2874 T2875 L2876 T2877 A2878 K2879 E2880 K2881 A2882 K2883 D2884 R2885 E2886 K2887 A2888 Q2889 D2890 I2891 F2892 K2893 F2894 L2895 Q2896 I2897 S2898 G2899 Y2900 V2901 V2902 S2903 R2904 G2905 PHE LYS ASP LEU ASP LEU ASP THR PRO SER X2916 X2917 X2918 X2919 X2920 X2921 X2922 X2923 X2924 X2925
X2928 X2931 X2932 X2935 X2936 X2937 X2938 X2939 X2940 X2941 X2942 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK X2961 X2962 X2963 X2964 X2965 X2966 X2967 X2968 X2969 X2970 X2971 X2972 X2973 X2974 X2975 X2976 X2977 X2978 X2979 X2980 X2981 X2982 X2983 X2984 X2985 X2986 X2987 X2988 X2989
X2990 X2991 X2992 X2993 X2994 X2995 X2996 X2997 X2998 X2999 X3000 X3001 X3002 X3003 X3004 X3005 X3006 X3007 X3008 X3009 X3010 X3011 X3012 X3013 X3014 X3015 X3016 X3017 X3018 X3019 X3020 X3021 X3022 X3023 X3024 X3025 X3026 X3027 X3028 X3029 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

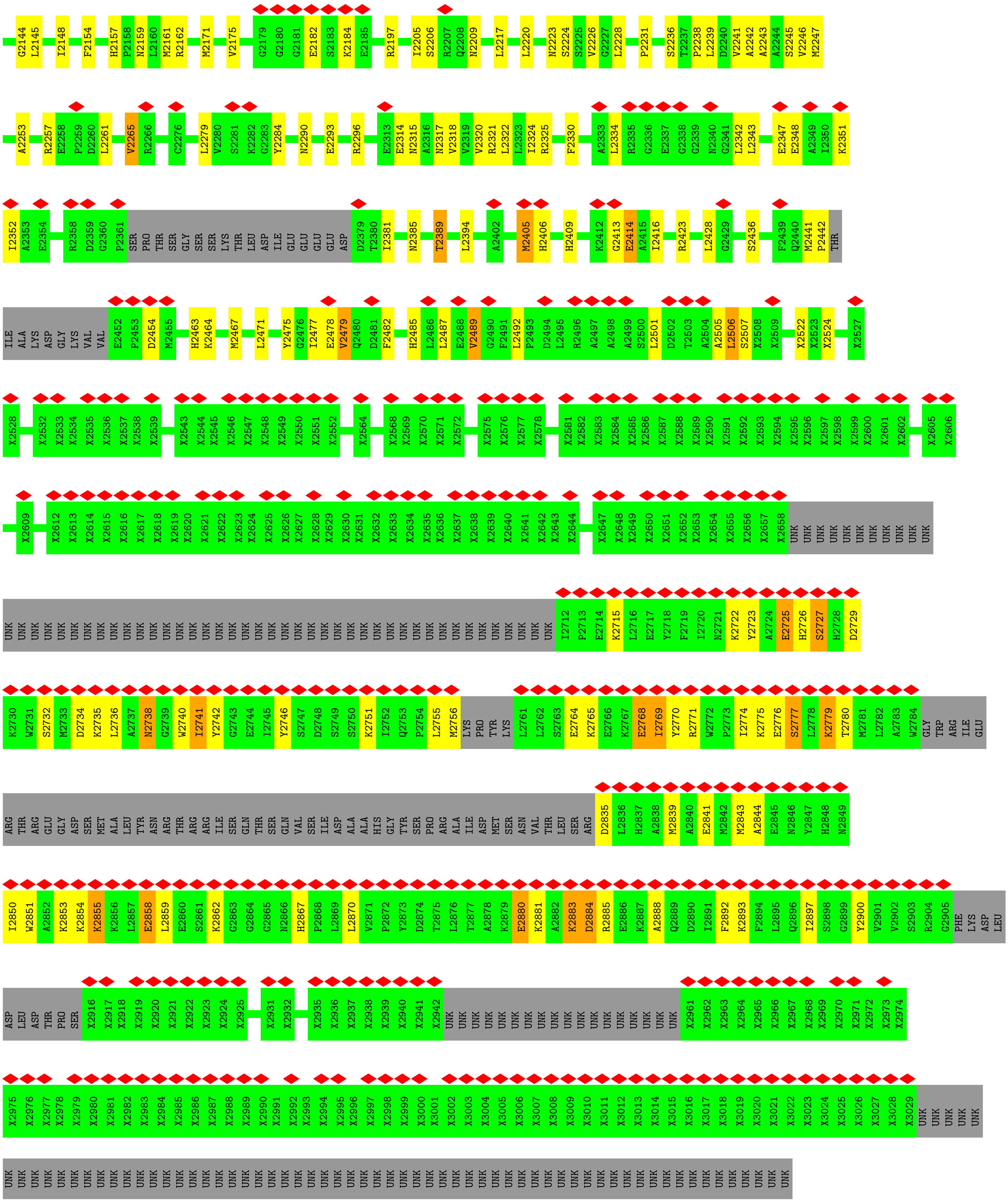


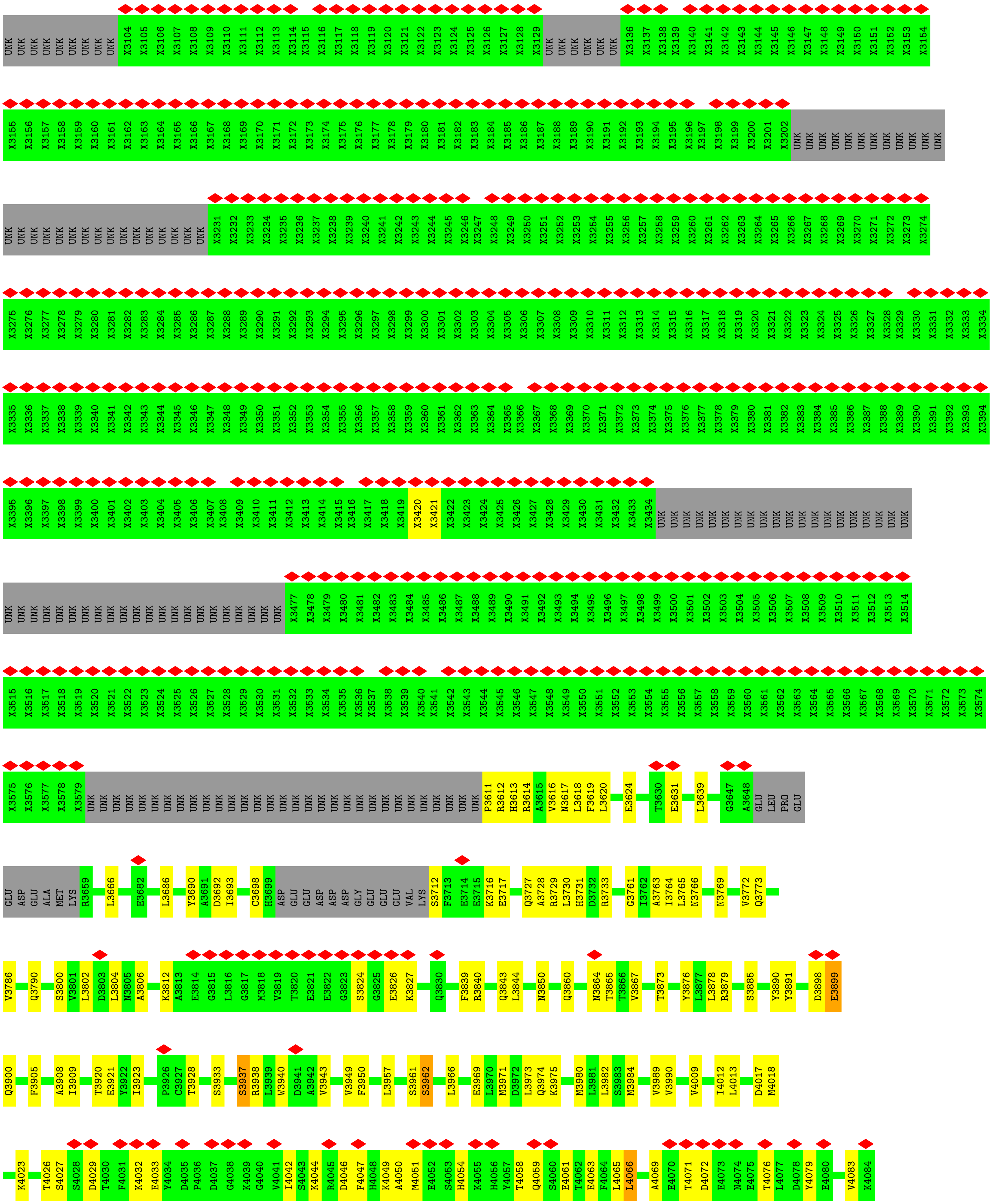
• Molecule 1: Ryanodine receptor 2

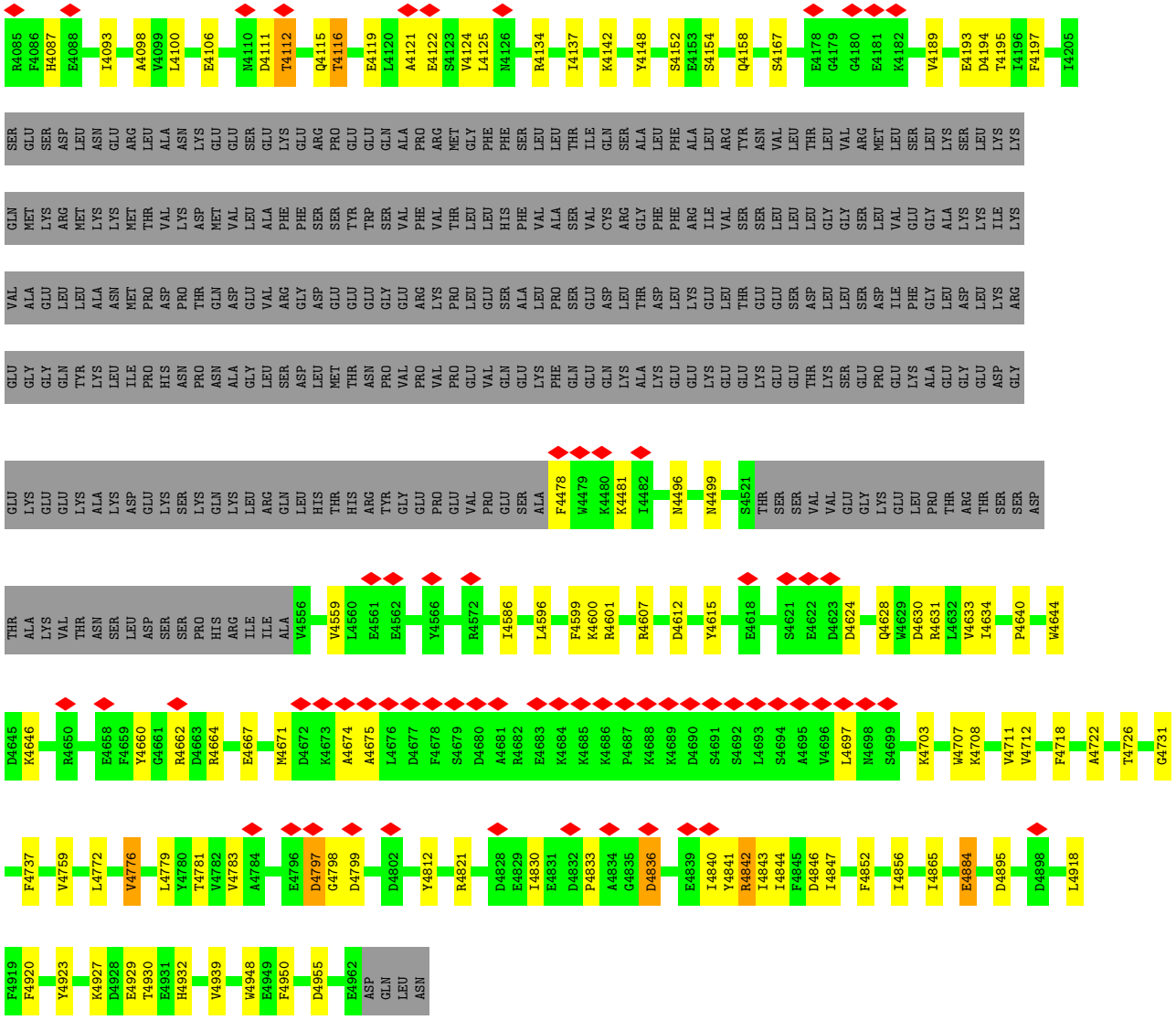
Chain B:




S1049 L1050 R1051 E1052 A1053 V1054 R1055 T1056 L1057 L1058 G1059 Y1060 G1061 Y1062 HIS LEU GLU ALA PRO ASP GLN ASP HIS ALA SER ARG ALA GLU VAL CYS SER GLY THR GLY GLU R1084 F1085 R1086 A1090 E1091 K1092 T1093 Y1094 A1095 Y1102 E1106 S1118 R1119 P1120 D1125 L1128 D1132
A1136 F1137 D1138 G1139 F1140 K1141 R1144 Q1147 G1148 N1149 E1150 H1151 W1156 Q1157 A1158 G1159 D1160 V1161 M1165 V1166 N1169 E1170 M1173 M1174 F1175 T1176 I1181 D1184 D1185 S1186 G1187 S1188 E1189 L1190 A1191 F1192 K1193 D1194 F1195 D1196 D1199 G1200 F1201 I1202 P1203 V1204 L1207 G1208 V1209 A1210
Q1211 K1219 D1220 V1221 S1222 T1223 L1224 K1225 Y1226 F1227 T1228 G1231 L1232 Q1233 E1234 N1244 R1245 D1246 W1250 L1251 S1252 K1253 R1254 L1255 P1256 Q1257 V1261 P1262 S1263 N1264 H1265 E1266 H1267 I1268 E1269 V1270 T1271 R1272 I1273 D1274 GLY THR ILE ASP SER SER PRO CYS LEU K1284 V1285 T1286 Q1293 N1294
N1295 N1296 T1297 D1298 A1311 X1312 X1313 X1314 X1318 X1323 X1324 X1325 X1326 X1332 X1333 E1344 V1345 L1346 M1347 K1348 T1349 A1350 H1351 G1352 H1353 D1357 R1358 I1359 D1360 K1361 D1362 K1363 E1364 T1365 P1366 K1367 N1371 N1372 H1373 K1374 L1384 X1392 X1395 X1396 X1397 X1402 X1403 X1404 X1405
X1406 X1407 X1408 X1409 X1410 X1411 X1412 X1413 X1414 X1415 X1419 X1420 X1421 X1422 X1423 X1424 X1425 X1426 X1427 X1428 X1429 X1430 X1431 X1432 X1433 X1437 X1446 UNK
UNK
UNK P1566 L1567 F1572 K1577 P1581 Q1582 C1583 P1584 P1585 R1586 L1587 H1588 V1589 Q1590 V1595 L1596 W1597 S1598 K1606 V1607 D1608 V1609 S1610 R1611 I1612 S1613
E1614 R1615 Q1616 L1619 V1620 Q1621 C1622 L1623 D1624 Q1627 L1631 H1632 I1633 P1634 E1635 I1642 L1643 E1644 L1645 H1655 T1658 S1663 A1667 L1668 G1669 L1677 H1680 V1681 D1682 E1683 P1684 Q1685 L1686 L1687 Y1688 E1691 Y1694 R1700 Y1703 Y1704 I1708 D1709 I1710 H1711 L1712
S1713 S1714 Y1715 R1719 L1720 N1723 I1727 M1730 T1731 E1732 E1733 T1734 K1735 S1736 I1737 T1738 L1739 F1740 P1741 K1745 K1746 P1750 G1751 I1752 G1753 L1754 S1755 R1761 M1762 S1773 N1774 D1775 C1776 F1783 D1786 I1787 L1788 K1789 I1793 S1804 L1805 D1809 P1810 T1814 F1817
L1818 F1819 Y1820 P1821 L1822 I1823 F1826 Y1827 T1828 L1829 K1830 I1831 M1832 G1833 I1834 F1835 H1836 N1837 E1838 D1839 L1840 K1841 H1842 I1843 L1844 Q1845 E1848 P1849 S1850 VAL PHE LYS GLU ALA ALA VAL PRO GLU GLU GLU GLY GLY GLY THR PRO GLU LYS GLU ILE SER ILE GLU ASP ALA LYS LEU GLU GLY GLU
GLU GLU ALA LYS GLY GLY LYS ARG PRO LYS GLU G1891 K1896 V1901 M1905 L1909 R1918 I1924 D1929 V1932 L1935 Q1936 Q1939 N1944 M1947 Q1948 A1949 L1950 N1951 M1952 S1953 A1954 A1955 L1956 T1957 A1958 R1959 K1960 T1961 R1962 E1963 F1964 R1965 S1966 P1967 P1968 Q1969 E1970
Q1971 I1972 N1973 M1974 L1975 L1976 K1979 D1980 D1981 K1982 S1983 E1984 C1985 P1986 C1987 P1988 E1989 R1992 D1993 D1997 F1998 H1999 E2000 M2003 T2004 I2008 E2009 LEU ASP GLU ASP GLY SER LEU ASP GLY SER ASN ASP LEU THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR
LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL ALA SER ASP SER ARG LYS CYS SER S2056 L2057 L2060 I2061 M2065 D2076 L2079 V2080 R2081 A2082 M2083 F2084 Y2091 R2099 A2100 L2101 P2102 K2103 T2104 Y2105 T2106 I2107 N2108 E2113 L2118 L2119 S2127 V2131 G2134 E2137

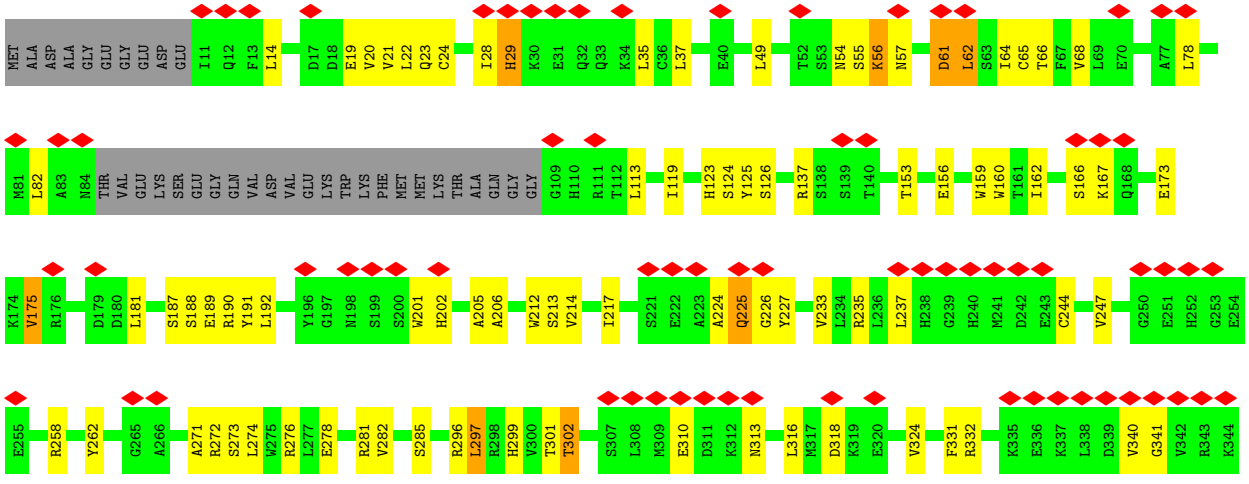

G2144 L2145 I2148 F2154 H2157 P2158 N2159 L2160 M2161 R2162 M2171 V2175 G2179 G2180 G2181 E2182 S2183 K2184 E2185 R2197 I2205 S2206 R2207 Q2208 N2209 L2217 L2220 N2223 S2224 S2225 V2226 G2227 L2228 P2231 S2236 T2237 P2238 L2239 D2240 V2241 A2242 A2243 A2244 S2245 V2246 M2247
A2253 R2257 E2258 P2259 D2260 L2261 V2265 R2266 C2276 L2279 V2280 S2281 K2282 G2283 Y2284 N2290 E2293 R2296 E2313 E2314 N2315 A2316 N2317 V2318 V2319 V2320 R2321 L2322 L2323 I2324 R2325 F2330 A2333 L2334 R2335 G2336 E2337 G2338 G2339 N2340 G2341 L2342 L2343 E2347 E2348 A2349 I2350 K2351
I2352 A2353 E2354 R2358 D2359 G2360 P2361 SER PRO THR SER GLY SER SER LYS THR LEU ASP ILE GLU GLU GLU GLU ASP D2379 T2380 I2381 N2385 T2389 L2394 A2402 M2405 H2406 H2409 K2412 G2413 E2414 A2415 I2416 R2423 L2428 G2429 S2436 F2439 Q2440 M2441 P2442 THR
ILE ALA LYS ASP GLY LYS VAL VAL E2452 P2453 D2454 M2455 H2463 K2464 M2467 L2471 Y2475 G2476 I2477 E2478 V2479 Q2480 D2481 F2482 H2485 L2486 L2487 E2488 V2489 G2490 F2491 L2492 P2493 D2494 L2495 R2496 A2497 A2498 A2499 S2500 L2501 D2502 T2503 A2504 A2505 L2506 S2507 X2508 X2509 X2522 X2523 X2524 X2527
X2528 X2532 X2533 X2534 X2535 X2536 X2537 X2538 X2539 X2543 X2544 X2545 X2546 X2547 X2548 X2549 X2550 X2551 X2552 X2564 X2568 X2569 X2570 X2571 X2572 X2575 X2576 X2577 X2578 X2581 X2582 X2583 X2584 X2585 X2586 X2587 X2588 X2589 X2590 X2591 X2592 X2593 X2594 X2595 X2596 X2597 X2598 X2599 X2600 X2601 X2602 X2605 X2606
X2609 X2612 X2613 X2614 X2615 X2616 X2617 X2618 X2619 X2620 X2621 X2622 X2623 X2624 X2625 X2626 X2627 X2628 X2629 X2630 X2631 X2632 X2633 X2634 X2635 X2636 X2637 X2638 X2639 X2640 X2641 X2642 X2643 X2644 X2647 X2648 X2649 X2650 X2651 X2652 X2653 X2654 X2655 X2656 X2657 X2658 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK
UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK I2712 P2713 E2714 K2715 L2716 E2717 Y2718 F2719 I2720 N2721 K2722 Y2723 A2724 E2725 H2726 S2727 H2728 D2729
K2730 W2731 S2732 M2733 D2734 K2735 L2736 A2737 N2738 G2739 W2740 I2741 Y2742 G2743 E2744 I2745 Y2746 S2747 D2748 S2749 S2750 K2751 I2752 Q2753 P2754 L2755 M2756 LYS PRO TYR LYS L2761 L2762 S2763 E2764 K2765 E2766 K2767 E2768 I2769 Y2770 R2771 W2772 P2773 I2774 K2775 E2776 S2777 L2778 K2779 T2780 M2781 L2782 A2783 W2784 GLY TRP ARG ILE GLU
ARG THR ARG GLU GLY ASP SER MET ALA LEU TYR ASN ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER ILE ASP ALA ALA HIS GLY TYR SER PRO ARG ALA ILE ASP MET SER ASN VAL THR LEU SER ARG D2835 L2836 H2837 A2838 M2839 A2840 E2841 M2842 M2843 A2844 E2845 N2846 Y2847 H2848 N2849
I2850 W2851 A2852 K2853 K2854 K2855 K2856 L2857 E2858 L2859 E2860 S2861 K2862 G2863 G2864 G2865 N2866 H2867 P2868 L2869 L2870 V2871 P2872 Y2873 D2874 T2875 L2876 T2877 A2878 K2879 E2880 K2881 A2882 K2883 D2884 R2885 E2886 K2887 A2888 Q2889 D2890 I2891 F2892 K2893 F2894 L2895 Q2896 I2897 S2898 G2899 Y2900 V2901 V2902 S2903 R2904 G2905 PHE LYS ASP LEU
ASP LEU ASP THR PRO SER X2916 X2917 X2918 X2919 X2920 X2921 X2922 X2923 X2924 X2925 X2931 X2932 X2935 X2936 X2937 X2938 X2939 X2940 X2941 X2942 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK X2961 X2962 X2963 X2964 X2965 X2966 X2967 X2968 X2969 X2970 X2971 X2972 X2973 X2974
X2975 X2976 X2977 X2978 X2979 X2980 X2981 X2982 X2983 X2984 X2985 X2986 X2987 X2988 X2989 X2990 X2991 X2992 X2993 X2994 X2995 X2996 X2997 X2998 X2999 X3000 X3001 X3002 X3003 X3004 X3005 X3006 X3007 X3008 X3009 X3010 X3011 X3012 X3013 X3014 X3015 X3016 X3017 X3018 X3019 X3020 X3021 X3022 X3023 X3024 X3025 X3026 X3027 X3028 X3029 UNK UNK UNK UNK UNK
UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

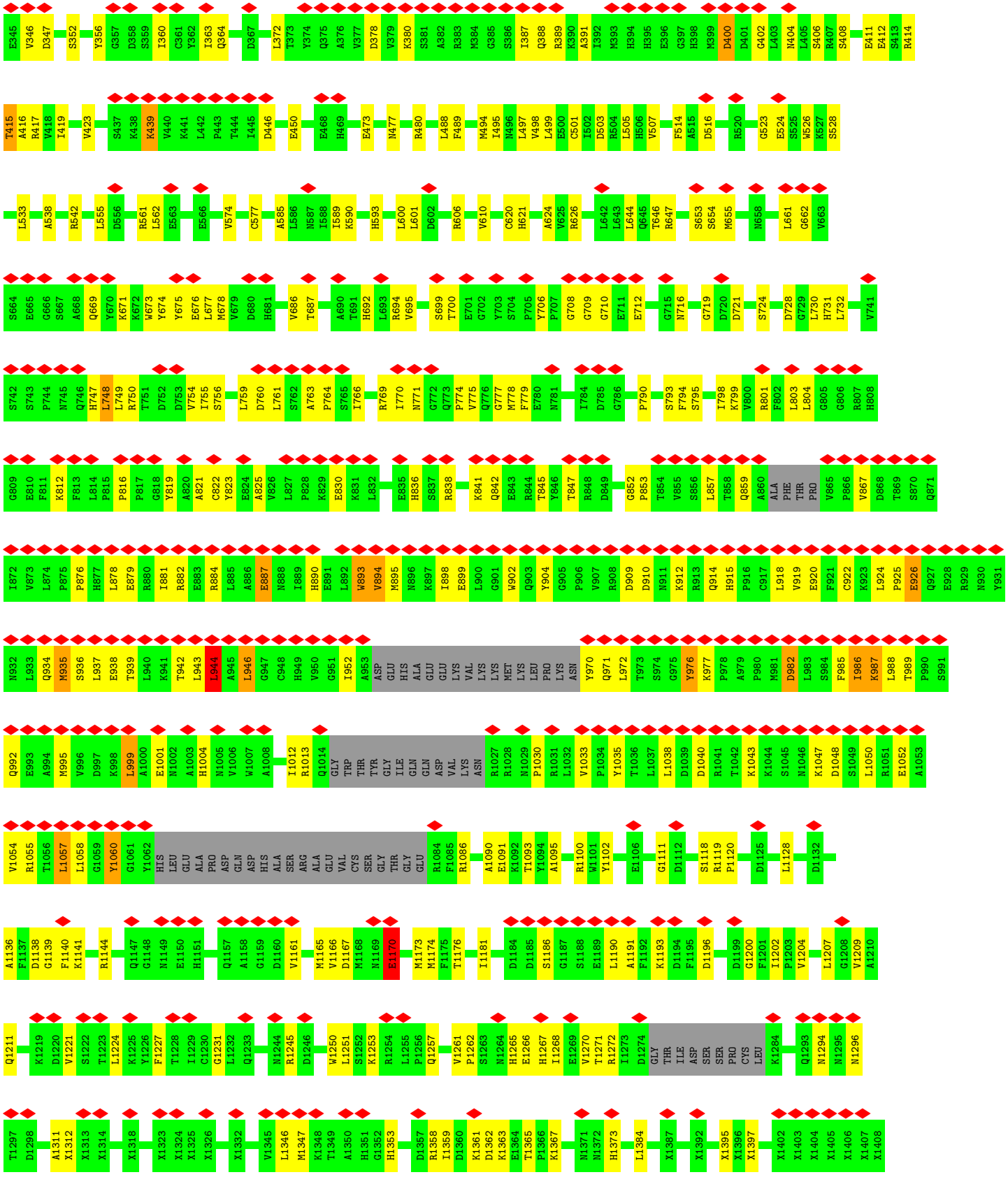

UNK UNK UNK UNK UNK UNK UNK UNK X3104 X3105 X3106 X3107 X3108 X3109 X3110 X3111 X3112 X3113 X3114 X3115 X3116 X3117 X3118 X3119 X3120 X3121 X3122 X3123 X3124 X3125 X3126 X3127 X3128 X3129 UNK UNK UNK UNK UNK X3136 X3137 X3138 X3139 X3140 X3141 X3142 X3143 X3144 X3145 X3146 X3147 X3148 X3149 X3150 X3151 X3152 X3153 X3154
X3155 X3156 X3157 X3158 X3159 X3160 X3161 X3162 X3163 X3164 X3165 X3166 X3167 X3168 X3169 X3170 X3171 X3172 X3173 X3174 X3175 X3176 X3177 X3178 X3179 X3180 X3181 X3182 X3183 X3184 X3185 X3186 X3187 X3188 X3189 X3190 X3191 X3192 X3193 X3194 X3195 X3196 X3197 X3198 X3199 X3200 X3201 X3202 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK
UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK X3231 X3232 X3233 X3234 X3235 X3236 X3237 X3238 X3239 X3240 X3241 X3242 X3243 X3244 X3245 X3246 X3247 X3248 X3249 X3250 X3251 X3252 X3253 X3254 X3255 X3256 X3257 X3258 X3259 X3260 X3261 X3262 X3263 X3264 X3265 X3266 X3267 X3268 X3269 X3270 X3271 X3272 X3273 X3274
X3275 X3276 X3277 X3278 X3279 X3280 X3281 X3282 X3283 X3284 X3285 X3286 X3287 X3288 X3289 X3290 X3291 X3292 X3293 X3294 X3295 X3296 X3297 X3298 X3299 X3300 X3301 X3302 X3303 X3304 X3305 X3306 X3307 X3308 X3309 X3310 X3311 X3312 X3313 X3314 X3315 X3316 X3317 X3318 X3319 X3320 X3321 X3322 X3323 X3324 X3325 X3326 X3327 X3328 X3329 X3330 X3331 X3332 X3333 X3334
X3335 X3336 X3337 X3338 X3339 X3340 X3341 X3342 X3343 X3344 X3345 X3346 X3347 X3348 X3349 X3350 X3351 X3352 X3353 X3354 X3355 X3356 X3357 X3358 X3359 X3360 X3361 X3362 X3363 X3364 X3365 X3366 X3367 X3368 X3369 X3370 X3371 X3372 X3373 X3374 X3375 X3376 X3377 X3378 X3379 X3380 X3381 X3382 X3383 X3384 X3385 X3386 X3387 X3388 X3389 X3390 X3391 X3392 X3393 X3394
X3395 X3396 X3397 X3398 X3399 X3400 X3401 X3402 X3403 X3404 X3405 X3406 X3407 X3408 X3409 X3410 X3411 X3412 X3413 X3414 X3415 X3416 X3417 X3418 X3419 X3420 X3421 X3422 X3423 X3424 X3425 X3426 X3427 X3428 X3429 X3430 X3431 X3432 X3433 X3434 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK
UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK X3477 X3478 X3479 X3480 X3481 X3482 X3483 X3484 X3485 X3486 X3487 X3488 X3489 X3490 X3491 X3492 X3493 X3494 X3495 X3496 X3497 X3498 X3499 X3500 X3501 X3502 X3503 X3504 X3505 X3506 X3507 X3508 X3509 X3510 X3511 X3512 X3513 X3514
X3515 X3516 X3517 X3518 X3519 X3520 X3521 X3522 X3523 X3524 X3525 X3526 X3527 X3528 X3529 X3530 X3531 X3532 X3533 X3534 X3535 X3536 X3537 X3538 X3539 X3540 X3541 X3542 X3543 X3544 X3545 X3546 X3547 X3548 X3549 X3550 X3551 X3552 X3553 X3554 X3555 X3556 X3557 X3558 X3559 X3560 X3561 X3562 X3563 X3564 X3565 X3566 X3567 X3568 X3569 X3570 X3571 X3572 X3573 X3574
X3575 X3576 X3577 X3578 X3579 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK P3611 R3612 H3613 R3614 A3615 V3616 N3617 L3618 F3619 L3620 E3624 T3630 E3631 L3639 G3647 A3648 GLU LEU PRO GLU
GLU ASP GLU ALA MET LYS R3659 L3666 E3682 L3686 Y3690 A3691 D3692 I3693 C3698 H3699 ASP GLU GLU ASP ASP GLY GLU GLU GLU VAL LYS S3712 F3713 E3714 E3715 K3716 E3717 Q3727 A3728 R3729 L3730 H3731 D3732 R3733 G3761 I3762 A3763 I3764 L3765 N3766 N3769 V3772 Q3773
V3786 Q3790 S3800 V3801 L3802 D3803 L3804 N3805 A3806 K3812 A3813 E3814 G3815 L3816 G3817 M3818 V3819 T3820 E3821 E3822 G3823 S3824 G3825 E3826 K3827 Q3830 F3839 R3840 Q3843 L3844 N3850 Q3860 N3864 T3865 T3866 V3867 T3873 Y3876 L3877 L3878 R3879 S3885 Y3890 Y3891 D3898 E3899
Q3900 F3905 A3908 I3909 T3920 E3921 Y3922 I3923 P3926 C3927 T3928 S3933 S3937 R3938 L3939 W3940 D3941 A3942 V3943 V3949 F3950 L3957 S3961 S3962 L3966 E3969 L3970 M3971 D3972 L3973 Q3974 K3975 M3980 L3981 L3982 S3983 M3984 V3989 V3990 V4009 I4012 L4013 D4017 M4018
K4023 T4026 S4027 S4028 D4029 T4030 F4031 K4032 E4033 Y4034 D4035 P4036 D4037 G4038 K4039 G4040 V4041 I4042 S4043 K4044 R4045 D4046 F4047 H4048 K4049 A4050 M4051 E4052 S4053 H4054 K4055 H4056 Y4057 T4058 Q4059 S4060 E4061 T4062 E4063 F4064 L4065 L4066 A4069 E4070 T4071 D4072 E4073 N4074 E4075 T4076 L4077 D4078 Y4079 E4080 V4083 K4084

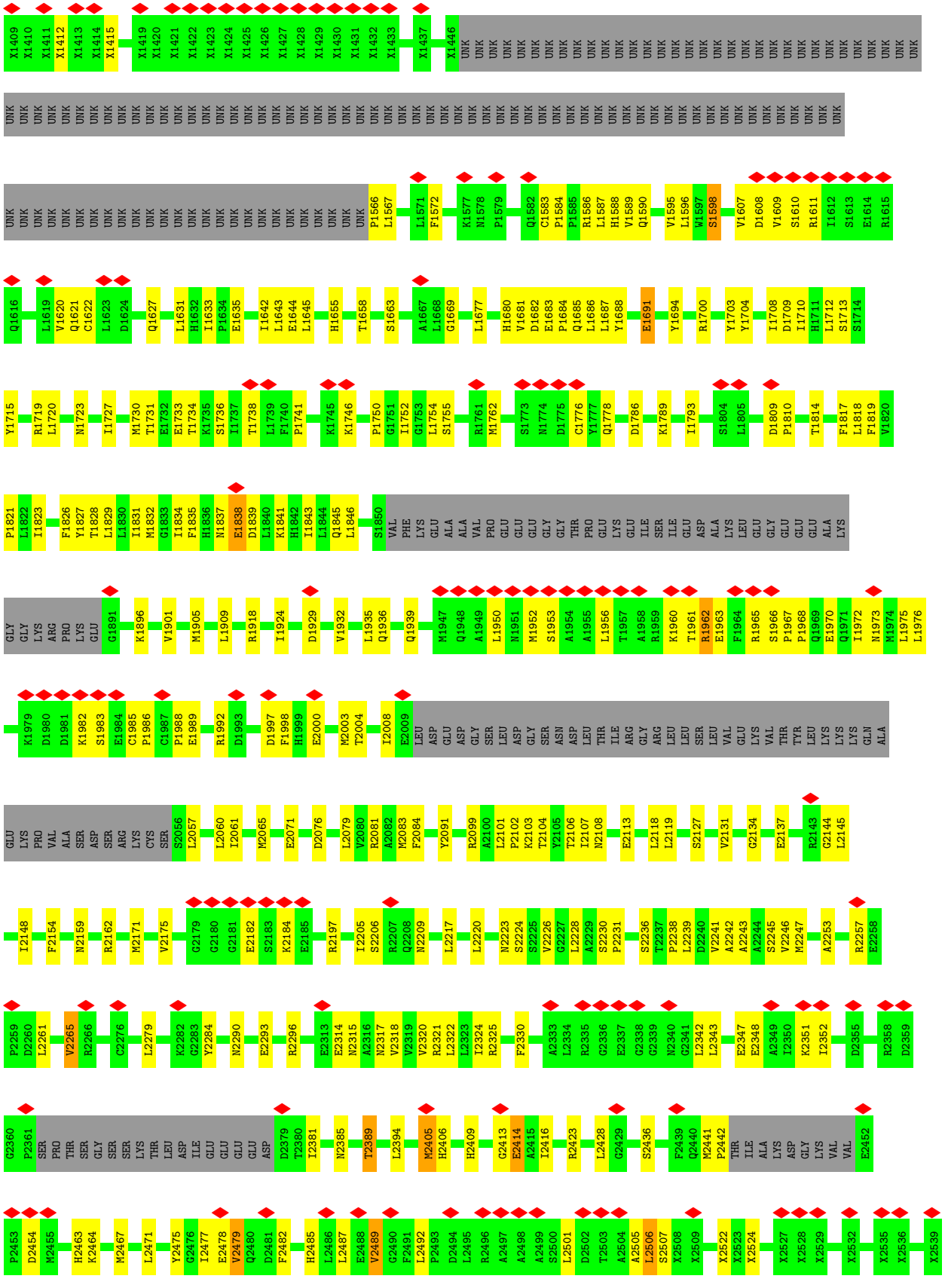


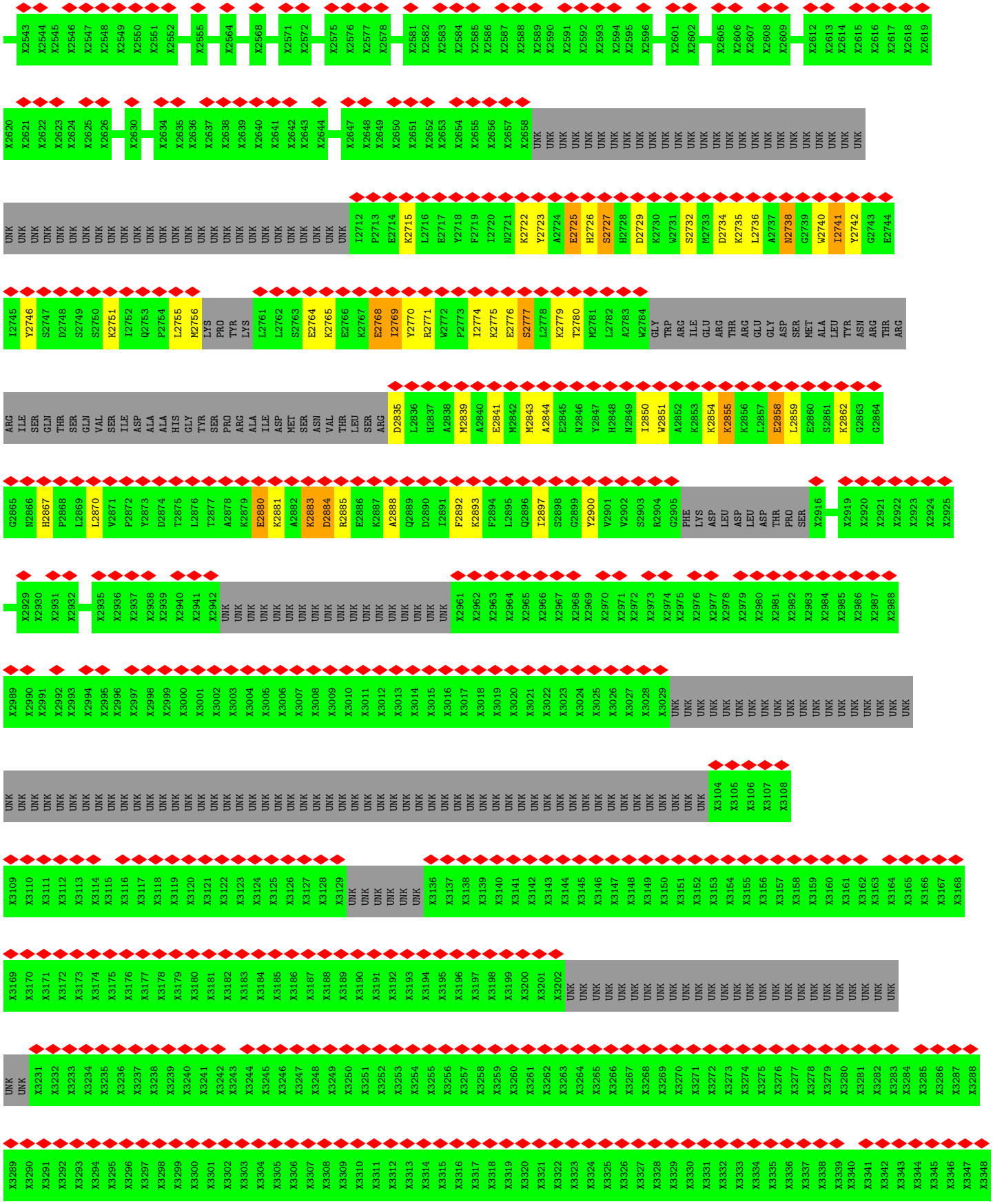
• Molecule 1: Ryanodine receptor 2

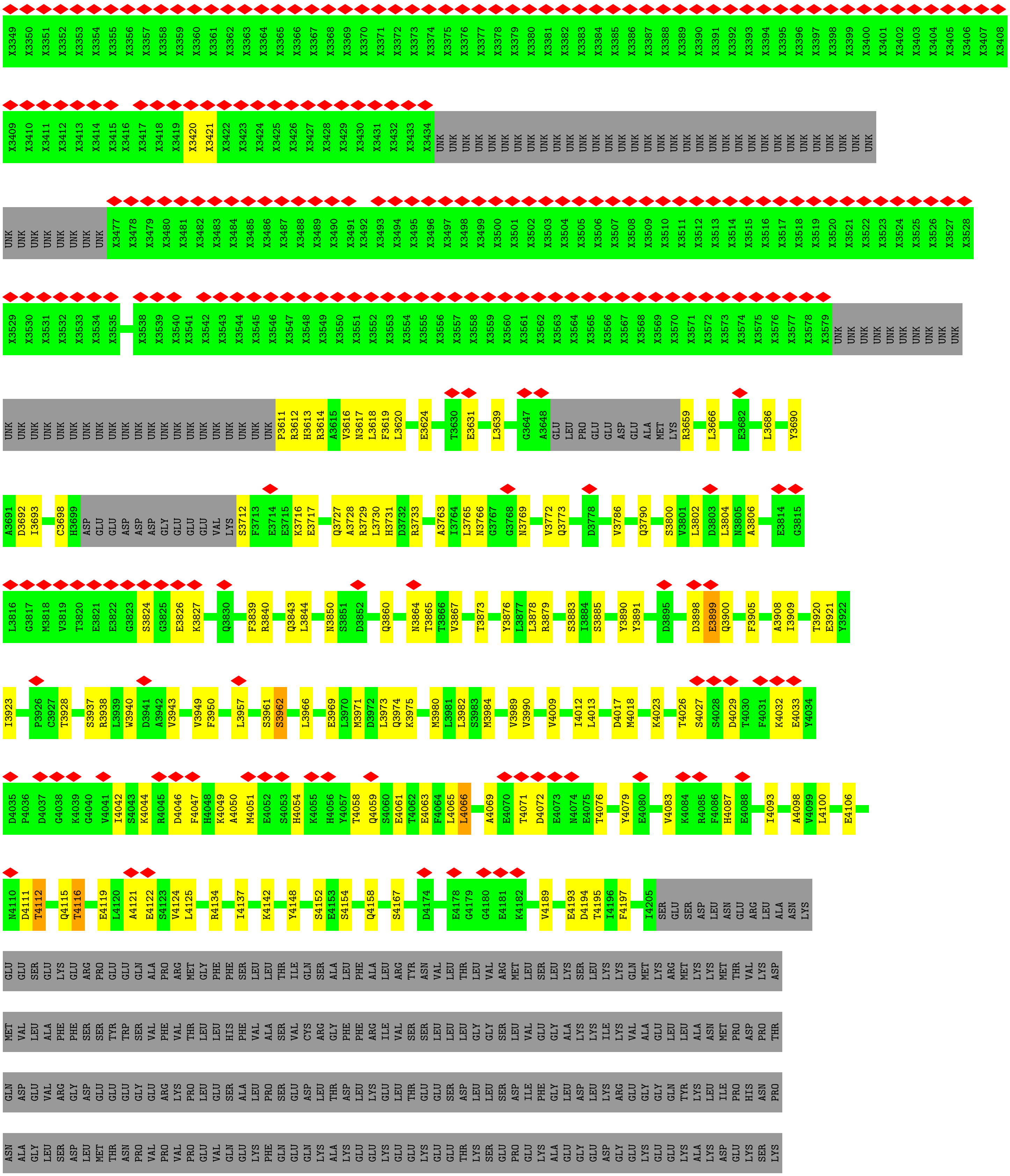
Chain C:

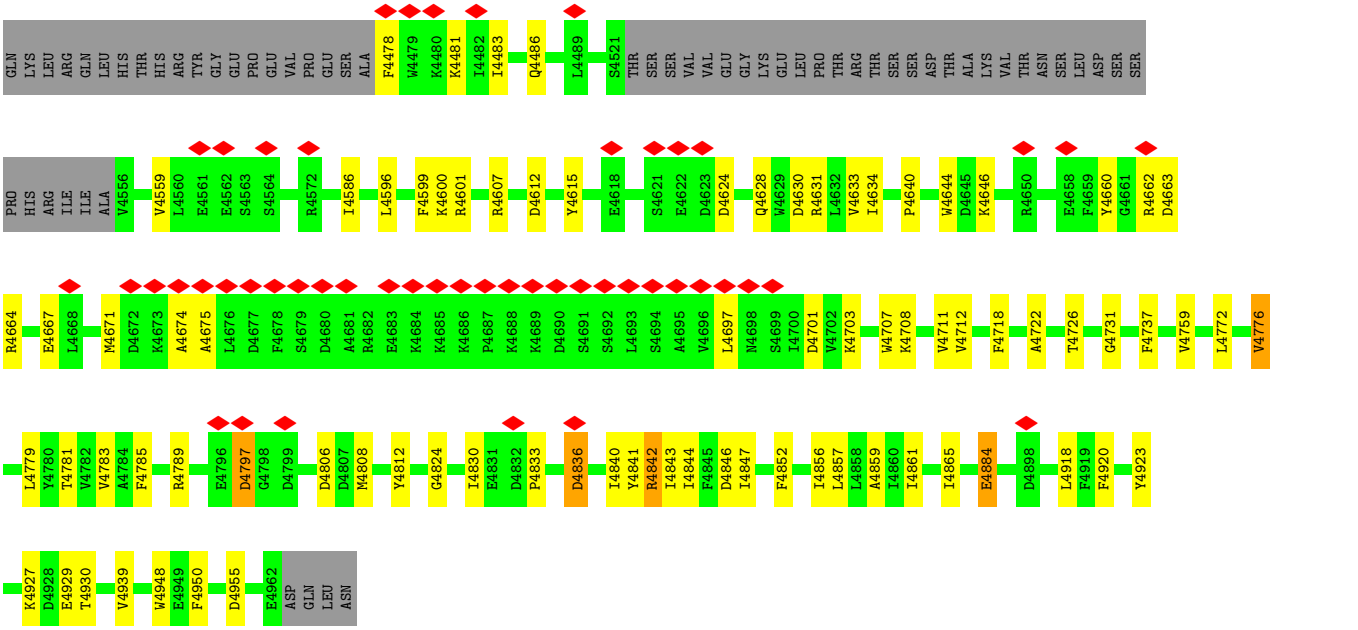



E345 V346 D347 S352 Y356 G357 D358 S359 I360 C361 Y362 I363 Q364 D367 L372 T373 Y374 Q375 A376 V377 D378 V379 K380 S381 A382 R383 M384 G385 S386 I387 Q388 R389 K390 A391 I392 M393 H394 H395 E396 G397 H398 M399 D400 D401 G402 L403 N404 L405 S406 R407 S408 E411 E412 S413 R414
T415 A416 R417 V418 I419 V423 S437 K438 K439 V440 K441 L442 P443 T444 I445 D446 E450 E468 H469 E473 N477 R480 L488 F489 M494 I495 N496 L497 V498 L499 E500 C501 I502 D503 R504 L505 H506 V507 F514 A515 D516 R520 G523 E524 S525 W526 K527 S528
L533 A538 R542 L555 D556 R561 L562 E563 E566 V574 C577 A585 L586 N587 I588 I589 K590 H593 L600 L601 D602 R606 V610 C620 H621 A624 V625 R626 L642 L643 L644 Q645 T646 R647 S653 S654 M655 N658 L661 G662 V663
S664 E665 G666 S667 A668 Q669 Y670 K671 K672 W673 Y674 Y675 E676 L677 M678 V679 D680 H681 V686 T687 A690 T691 H692 L693 R694 V695 S699 T700 E701 G702 Y703 S704 P705 Y706 P707 G708 G709 G710 E711 E712 G715 N716 G719 D720 D721 S724 D728 G729 L730 H731 L732 V741
S742 S743 P744 N745 Q746 H747 L748 L749 R750 T751 D752 D753 V754 I755 S756 L759 D760 L761 S762 A763 P764 S765 I766 R769 I770 N771 G772 Q773 P774 V775 Q776 G777 M778 F779 E780 N781 I784 D785 G786 P790 S793 F794 S795 I798 K799 V800 R801 F802 L803 L804 G805 G806 R807 H808
G809 E810 F811 K812 F813 L814 P815 P816 P817 G818 Y819 A820 A821 C822 Y823 E824 A825 V826 L827 P828 K829 E830 K831 L832 E835 H836 S837 R838 K841 Q842 E843 R844 T845 Y846 T847 R848 D849 G852 P853 T854 V855 S856 L857 T858 Q859 A860 ALA PHE THR PRO V865 P866 V867 D868 T869 S870 Q871
I872 V873 L874 P875 P876 H877 L878 E879 R880 I881 R882 E883 R884 L885 A886 E887 N888 I889 H890 E891 L892 W893 V894 M895 N896 K897 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918 V919 E920 F921 C922 K923 L924 P925 E926 Q927 E928 R929 N930 Y931
N932 L933 Q934 M935 S936 L937 E938 T939 L940 K941 T942 L943 L944 A945 L946 G947 C948 H949 V950 G951 I952 A953 ASP GLU HIS ALA GLU GLU LYS VAL LYS LYS MET LYS LEU PRO LYS ASN Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 T989 P990 S991
Q992 E993 A994 M995 V996 D997 K998 L999 A1000 E1001 N1002 A1003 H1004 N1005 V1006 W1007 A1008 I1012 R1013 Q1014 GLY TRP THR TYR GLY ILE GLN GLN ASP VAL LYS ASN R1027 R1028 N1029 P1030 R1031 L1032 V1033 P1034 Y1035 T1036 L1037 L1038 D1039 D1040 R1041 T1042 K1043 K1044 S1045 N1046 K1047 D1048 S1049 L1050 R1051 E1052 A1053
V1054 R1055 T1056 L1057 L1058 G1059 Y1060 G1061 Y1062 HIS LEU GLU ALA PRO ASP GLN ASP HIS ALA SER ARG ALA GLU VAL CYS SER GLY THR GLY GLU R1084 F1085 R1086 A1090 E1091 K1092 T1093 Y1094 A1095 R1100 W1101 Y1102 E1106 G1111 D1112 S1118 R1119 P1120 D1125 L1128 D1132
A1136 F1137 D1138 G1139 F1140 K1141 R1144 Q1147 G1148 N1149 E1150 H1151 Q1157 A1158 G1159 D1160 V1161 M1165 V1166 D1167 M1168 N1169 E1170 M1173 M1174 F1175 T1176 I1181 D1184 D1185 S1186 G1187 S1188 E1189 L1190 A1191 F1192 K1193 D1194 F1195 D1196 D1199 G1200 F1201 I1202 P1203 V1204 L1207 G1208 V1209 A1210
Q1211 K1219 D1220 V1221 S1222 T1223 L1224 K1225 Y1226 F1227 T1228 I1229 C1230 G1231 L1232 Q1233 N1244 R1245 D1246 W1250 L1251 S1252 K1253 R1254 L1255 P1256 Q1257 V1261 P1262 S1263 N1264 H1265 E1266 H1267 I1268 E1269 V1270 T1271 R1272 I1273 D1274 GLY THR ILE ASP SER SER PRO CYS LEU K1284 Q1293 N1294 N1295 N1296
T1297 D1298 A1311 X1312 X1313 X1314 X1318 X1323 X1324 X1325 X1326 X1332 V1345 L1346 M1347 K1348 T1349 A1350 H1351 G1352 H1353 D1357 R1358 I1359 D1360 K1361 D1362 K1363 E1364 T1365 P1366 K1367 N1371 N1372 H1373 L1384 X1387 X1392 X1395 X1396 X1397 X1402 X1403 X1404 X1405 X1406 X1407 X1408



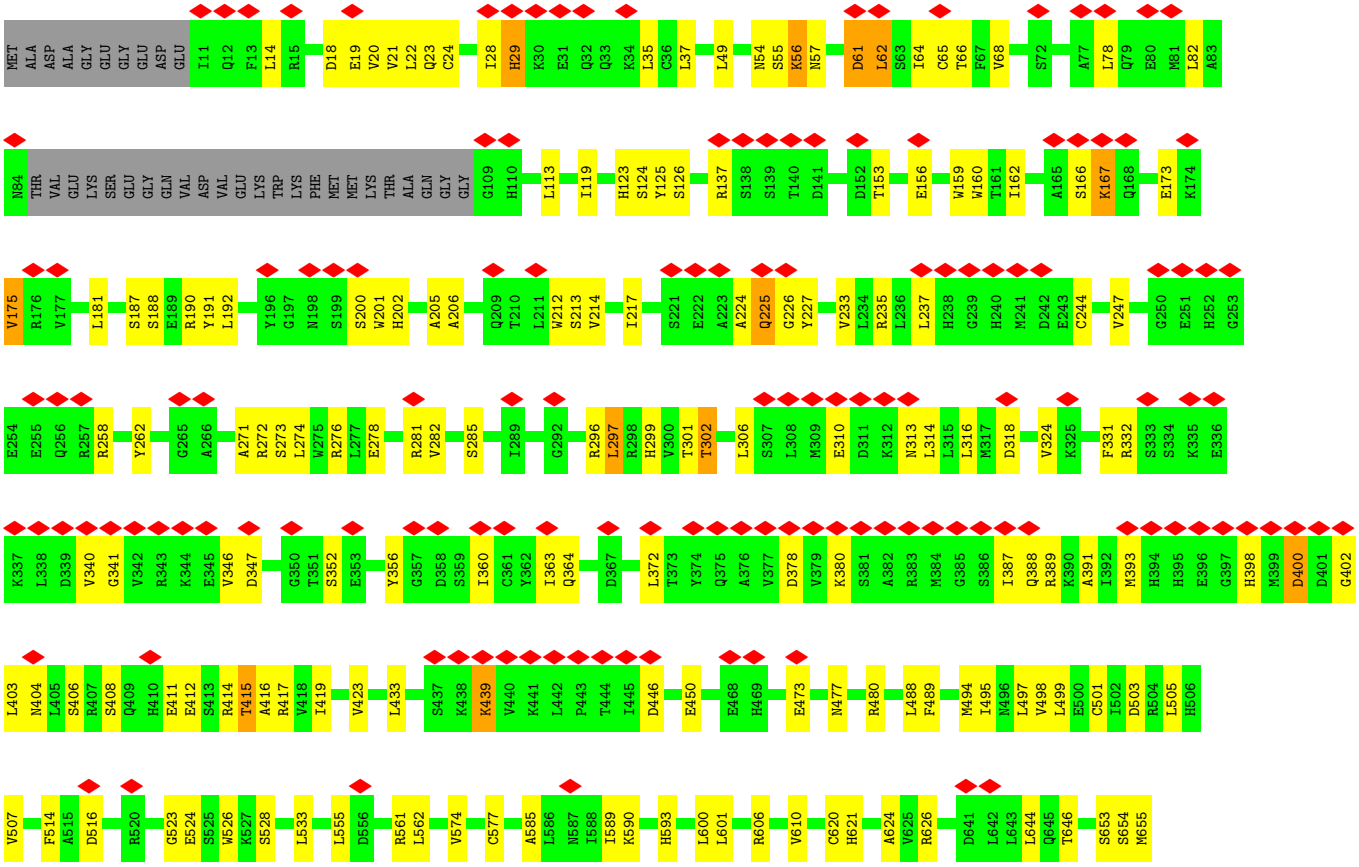

X2543 X2544 X2545 X2546 X2547 X2548 X2549 X2550 X2551 X2552 X2555 X2564 X2568 X2571 X2572 X2575 X2576 X2577 X2578 X2581 X2582 X2583 X2584 X2585 X2586 X2587 X2588 X2589 X2590 X2591 X2592 X2593 X2594 X2595 X2596 X2601 X2602 X2605 X2606 X2607 X2608 X2609 X2612 X2613 X2614 X2615 X2616 X2617 X2618 X2619
X2620 X2621 X2622 X2623 X2624 X2625 X2626 X2630 X2634 X2635 X2636 X2637 X2638 X2639 X2640 X2641 X2642 X2643 X2644 X2647 X2648 X2649 X2650 X2651 X2652 X2653 X2654 X2655 X2656 X2657 X2658 UNK
UNK I2712 P2713 E2714 K2715 L2716 E2717 Y2718 F2719 I2720 N2721 K2722 Y2723 A2724 E2725 H2726 S2727 H2728 D2729 K2730 W2731 S2732 M2733 D2734 K2735 L2736 A2737 N2738 G2739 W2740 I2741 Y2742 G2743 E2744
I2745 Y2746 S2747 D2748 S2749 S2750 K2751 I2752 Q2753 P2754 L2755 M2756 LYS PRO TYR LYS L2761 L2762 S2763 E2764 K2765 E2766 K2767 E2768 I2769 Y2770 R2771 W2772 P2773 I2774 K2775 E2776 S2777 L2778 K2779 T2780 M2781 L2782 A2783 W2784 GLY TRP ARG ILE GLU ARG THR ARG GLU GLY ASP SER MET ALA LEU TYR ASN ARG THR ARG
ARG ILE SER GLN THR SER GLN VAL SER ILE ASP ALA ALA HIS GLY TYR SER PRO ARG ALA ILE ASP MET SER ASN VAL THR LEU SER ARG D2835 L2836 H2837 A2838 M2839 A2840 E2841 M2842 M2843 A2844 E2845 N2846 Y2847 H2848 N2849 I2850 W2851 A2852 K2853 K2854 K2855 K2856 L2857 E2858 L2859 E2860 S2861 K2862 G2863 G2864
G2865 N2866 H2867 P2868 L2869 L2870 V2871 P2872 Y2873 D2874 T2875 L2876 T2877 A2878 K2879 E2880 K2881 A2882 K2883 D2884 R2885 E2886 K2887 A2888 Q2889 D2890 I2991 F2892 K2893 F2894 L2695 Q2896 I2897 S2998 G2899 Y2900 V2901 V2902 S2903 R2904 G2905 PHE LYS ASP LEU ASP LEU ASP THR PRO SER X2916 X2919 X2920 X2921 X2922 X2923 X2924 X2925
X2929 X2930 X2931 X2932 X2935 X2936 X2937 X2938 X2939 X2940 X2941 X2942 UNK X2961 X2962 X2963 X2964 X2965 X2966 X2967 X2968 X2969 X2970 X2971 X2972 X2973 X2974 X2975 X2976 X2977 X2978 X2979 X2980 X2981 X2982 X2983 X2984 X2985 X2986 X2987 X2988
X2989 X2990 X2991 X2992 X2993 X2994 X2995 X2996 X2997 X2998 X2999 X3000 X3001 X3002 X3003 X3004 X3005 X3006 X3007 X3008 X3009 X3010 X3011 X3012 X3013 X3014 X3015 X3016 X3017 X3018 X3019 X3020 X3021 X3022 X3023 X3024 X3025 X3026 X3027 X3028 X3029 UNK
UNK X3104 X3105 X3106 X3107 X3108
X3109 X3110 X3111 X3112 X3113 X3114 X3115 X3116 X3117 X3118 X3119 X3120 X3121 X3122 X3123 X3124 X3125 X3126 X3127 X3128 X3129 UNK X3136 X3137 X3138 X3139 X3140 X3141 X3142 X3143 X3144 X3145 X3146 X3147 X3148 X3149 X3150 X3151 X3152 X3153 X3154 X3155 X3156 X3157 X3158 X3159 X3160 X3161 X3162 X3163 X3164 X3165 X3166 X3167 X3168
X3169 X3170 X3171 X3172 X3173 X3174 X3175 X3176 X3177 X3178 X3179 X3180 X3181 X3182 X3183 X3184 X3185 X3186 X3187 X3188 X3189 X3190 X3191 X3192 X3193 X3194 X3195 X3196 X3197 X3198 X3199 X3200 X3201 X3202 UNK
UNK X3231 X3232 X3233 X3234 X3235 X3236 X3237 X3238 X3239 X3240 X3241 X3242 X3243 X3244 X3245 X3246 X3247 X3248 X3249 X3250 X3251 X3252 X3253 X3254 X3255 X3256 X3257 X3258 X3259 X3260 X3261 X3262 X3263 X3264 X3265 X3266 X3267 X3268 X3269 X3270 X3271 X3272 X3273 X3274 X3275 X3276 X3277 X3278 X3279 X3280 X3281 X3282 X3283 X3284 X3285 X3286 X3287 X3288
X3289 X3290 X3291 X3292 X3293 X3294 X3295 X3296 X3297 X3298 X3299 X3300 X3301 X3302 X3303 X3304 X3305 X3306 X3307 X3308 X3309 X3310 X3311 X3312 X3313 X3314 X3315 X3316 X3317 X3318 X3319 X3320 X3321 X3322 X3323 X3324 X3325 X3326 X3327 X3328 X3329 X3330 X3331 X3332 X3333 X3334 X3335 X3336 X3337 X3338 X3339 X3340 X3341 X3342 X3343 X3344 X3345 X3346 X3347 X3348

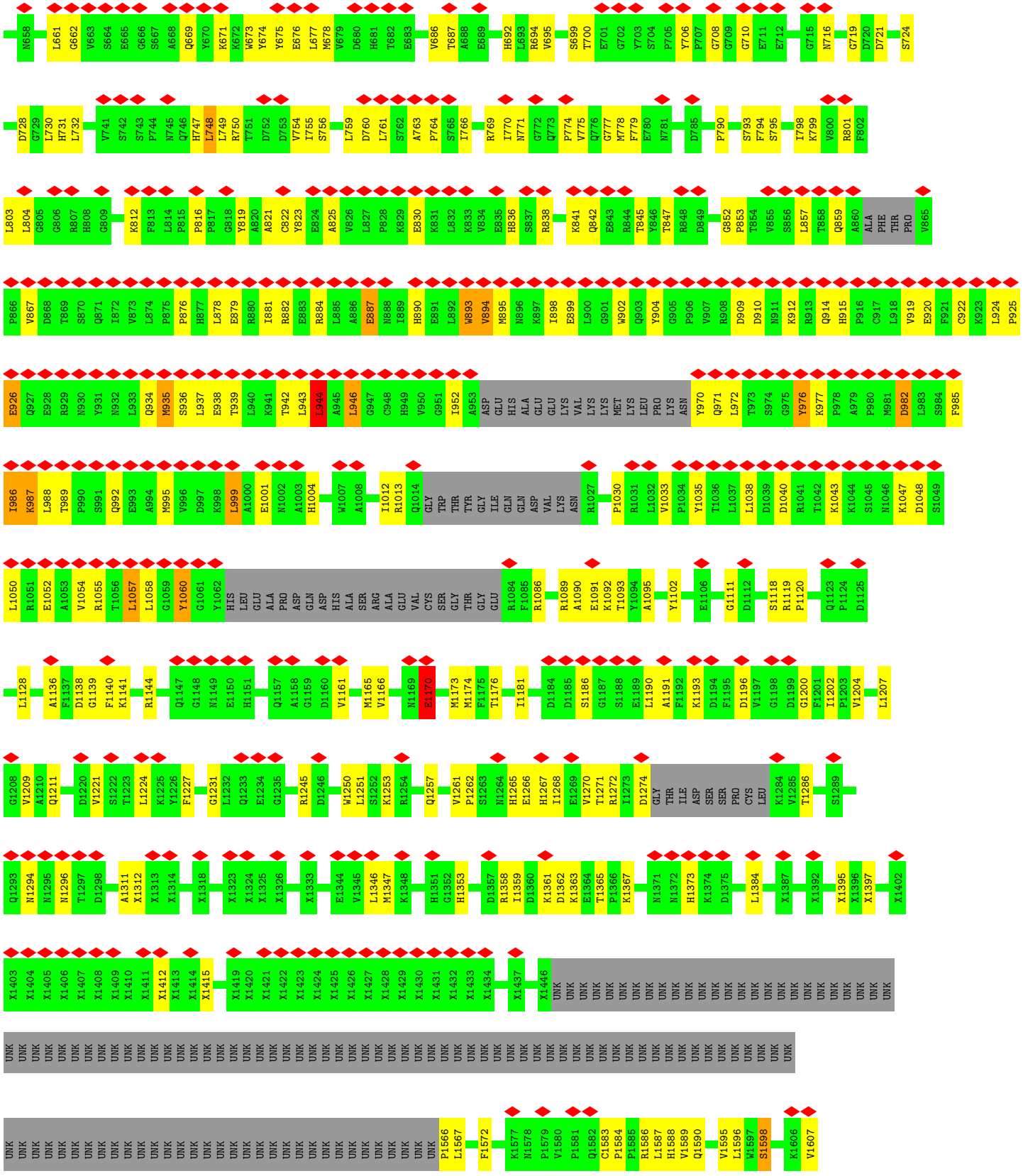

X3349 X3350 X3351 X3352 X3353 X3354 X3355 X3356 X3357 X3358 X3359 X3360 X3361 X3362 X3363 X3364 X3365 X3366 X3367 X3368 X3369 X3370 X3371 X3372 X3373 X3374 X3375 X3376 X3377 X3378 X3379 X3380 X3381 X3382 X3383 X3384 X3385 X3386 X3387 X3388 X3389 X3390 X3391 X3392 X3393 X3394 X3395 X3396 X3397 X3398 X3399 X3400 X3401 X3402 X3403 X3404 X3405 X3406 X3407 X3408
X3409 X3410 X3411 X3412 X3413 X3414 X3415 X3416 X3417 X3418 X3419 X3420 X3421 X3422 X3423 X3424 X3425 X3426 X3427 X3428 X3429 X3430 X3431 X3432 X3433 X3434 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK
UNK UNK UNK UNK UNK UNK UNK UNK X3477 X3478 X3479 X3480 X3481 X3482 X3483 X3484 X3485 X3486 X3487 X3488 X3489 X3490 X3491 X3492 X3493 X3494 X3495 X3496 X3497 X3498 X3499 X3500 X3501 X3502 X3503 X3504 X3505 X3506 X3507 X3508 X3509 X3510 X3511 X3512 X3513 X3514 X3515 X3516 X3517 X3518 X3519 X3520 X3521 X3522 X3523 X3524 X3525 X3526 X3527 X3528
X3529 X3530 X3531 X3532 X3533 X3534 X3535 X3538 X3539 X3540 X3541 X3542 X3543 X3544 X3545 X3546 X3547 X3548 X3549 X3550 X3551 X3552 X3553 X3554 X3555 X3556 X3557 X3558 X3559 X3560 X3561 X3562 X3563 X3564 X3565 X3566 X3567 X3568 X3569 X3570 X3571 X3572 X3573 X3574 X3575 X3576 X3577 X3578 X3579 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK
UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK P3611 R3612 H3613 R3614 A3615 V3616 N3617 L3618 F3619 L3620 E3624 T3630 E3631 L3639 G3647 A3648 GLU LEU PRO GLU GLU ASP GLU ALA MET LYS R3659 L3666 E3682 L3686 Y3690
A3691 D3692 I3693 C3698 H3699 ASP GLU GLU ASP ASP GLY GLU GLU GLU VAL LYS S3712 F3713 E3714 E3715 K3716 E3717 Q3727 A3728 R3729 L3730 H3731 D3732 R3733 A3763 I3764 L3765 N3766 G3767 G3768 N3769 V3772 Q3773 D3778 V3786 Q3790 S3800 V3801 L3802 D3803 L3804 N3805 A3806 E3814 G3815
L3816 G3817 M3818 V3819 T3820 E3821 E3822 G3823 S3824 G3825 E3826 K3827 Q3830 F3839 R3840 Q3843 L3844 N3850 S3851 D3852 Q3860 N3864 T3865 T3866 V3867 T3873 Y3876 L3877 L3878 R3879 S3883 I3884 S3885 Y3890 Y3891 D3895 D3898 E3899 Q3900 F3905 A3908 I3909 T3920 E3921 Y3922
I3923 P3926 C3927 T3928 S3937 R3938 L3939 W3940 D3941 A3942 V3943 V3949 F3950 L3957 S3961 S3962 L3966 E3969 L3970 M3971 D3972 L3973 Q3974 K3975 M3980 L3981 L3982 S3983 M3984 V3989 V3990 V4009 I4012 L4013 D4017 M4018 K4023 T4026 S4027 S4028 D4029 T4030 F4031 K4032 E4033 Y4034
D4035 P4036 D4037 G4038 K4039 G4040 V4041 I4042 S4043 K4044 R4045 D4046 F4047 H4048 K4049 A4050 M4051 E4052 S4053 H4054 K4055 H4056 Y4057 T4058 Q4059 S4060 E4061 T4062 E4063 F4064 L4065 L4066 A4069 E4070 T4071 D4072 E4073 N4074 E4075 T4076 Y4079 E4080 V4083 K4084 R4085 F4086 H4087 E4088 I4093 A4098 V4099 L4100 E4106
N4110 D4111 T4112 Q4115 T4116 E4119 L4120 A4121 E4122 S4123 V4124 L4125 R4134 I4137 K4142 Y4148 S4152 E4153 S4154 Q4158 S4167 D4174 E4178 G4179 G4180 E4181 K4182 V4189 E4193 D4194 T4195 I4196 F4197 I4205 SER GLU SER ASP LEU ASN GLU ARG LEU ALA ASN LYS
GLU GLU SER GLU LYS GLU ARG PRO GLU GLU GLN ALA PRO ARG MET GLY PHE PHE SER LEU LEU THR ILE GLN SER ALA LEU PHE ALA LEU ARG TYR ASN VAL LEU THR LEU VAL ARG MET LEU SER LEU LYS SER LEU LYS LYS GLN MET LYS ARG MET LYS LYS MET THR VAL LYS ASP
MET VAL LEU ALA PHE PHE SER SER TYR TRP SER VAL PHE VAL THR LEU LEU HIS PHE VAL ALA SER VAL CYS ARG GLY PHE PHE ARG ILE VAL SER SER LEU LEU LEU GLY GLY SER LEU VAL GLU GLY ALA LYS LYS ILE LYS VAL ALA GLU LEU LEU ALA ASN MET PRO ASP PRO THR
GLN ASP GLU VAL ARG GLY ASP GLU GLU GLU GLY GLU ARG LYS PRO LEU GLU SER ALA LEU PRO SER GLU ASP LEU THR ASP LEU LYS GLU LEU THR GLU GLU SER ASP LEU LEU SER ASP ILE PHE GLY LEU ASP LEU LYS ARG GLU GLY GLY GLN TYR LYS LEU ILE PRO HIS ASN PRO
ASN ALA GLY LEU SER ASP LEU MET THR ASN PRO VAL PRO VAL PRO GLU VAL GLN GLU LYS PHE GLN GLU GLN LYS ALA LYS GLU GLU LYS GLU GLU LYS GLU GLU THR LYS SER GLU PRO GLU LYS ALA GLU GLY GLU ASP GLY GLU LYS GLU GLU LYS ALA LYS ASP GLU LYS SER LYS

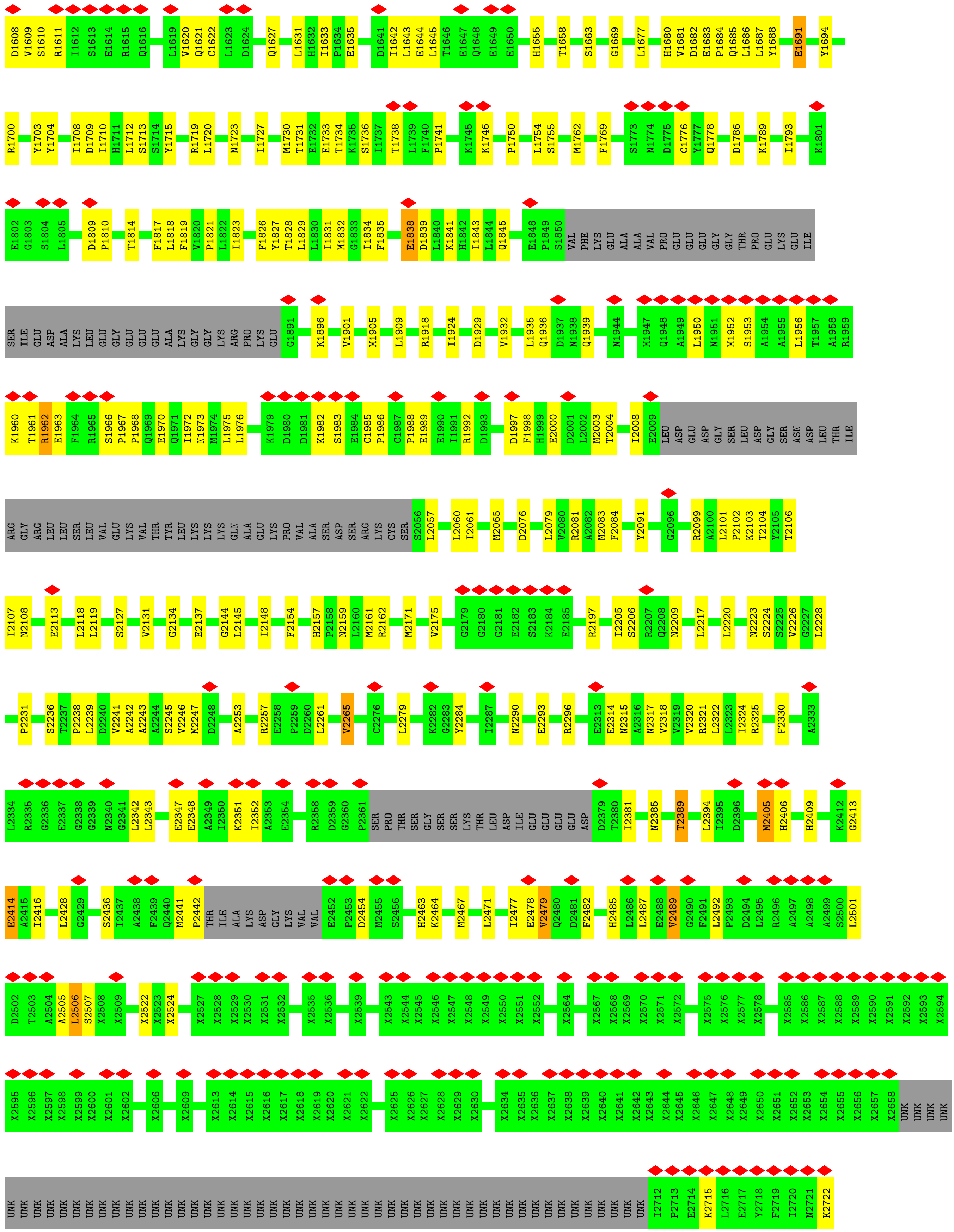


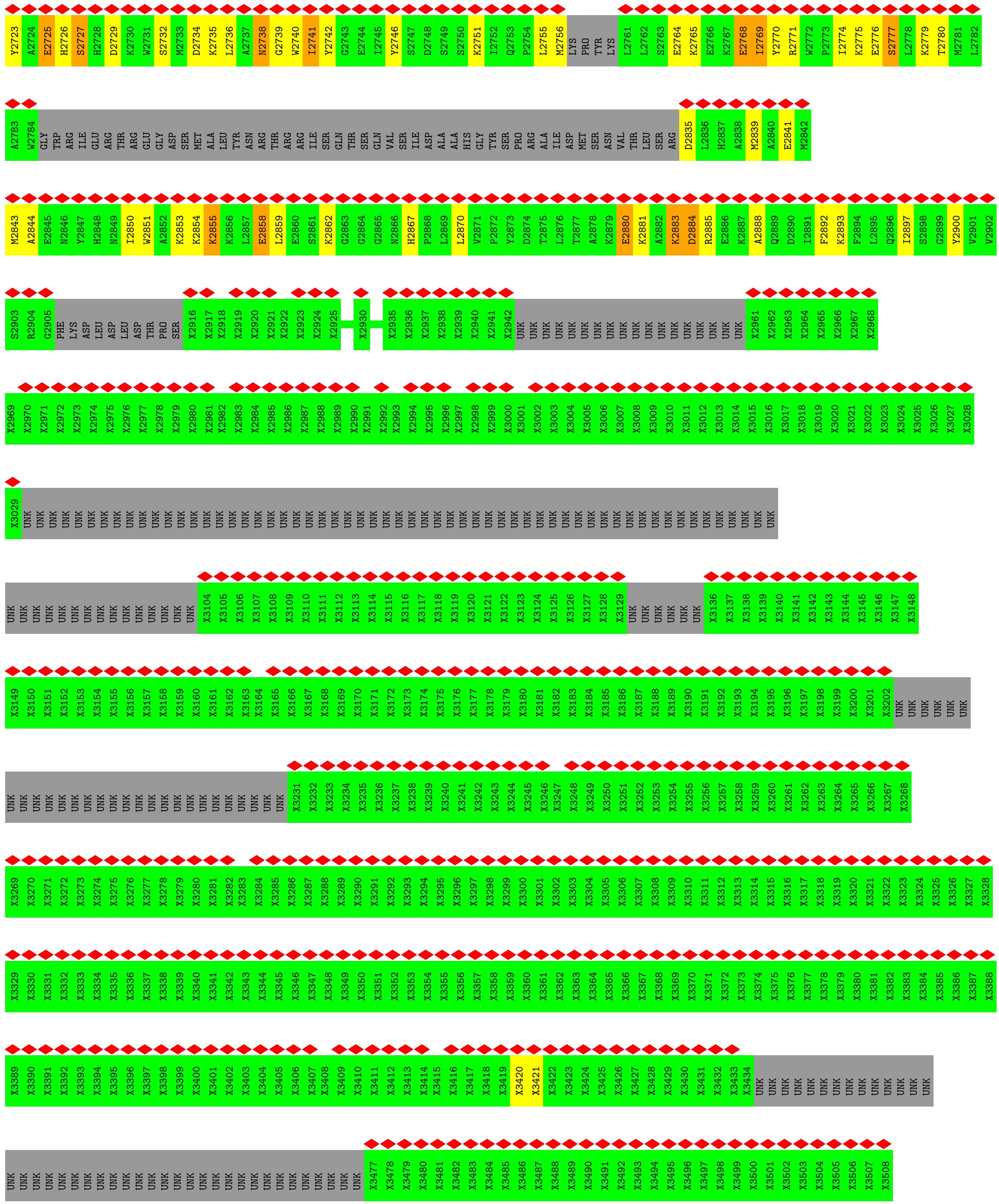
• Molecule 1: Ryanodine receptor 2

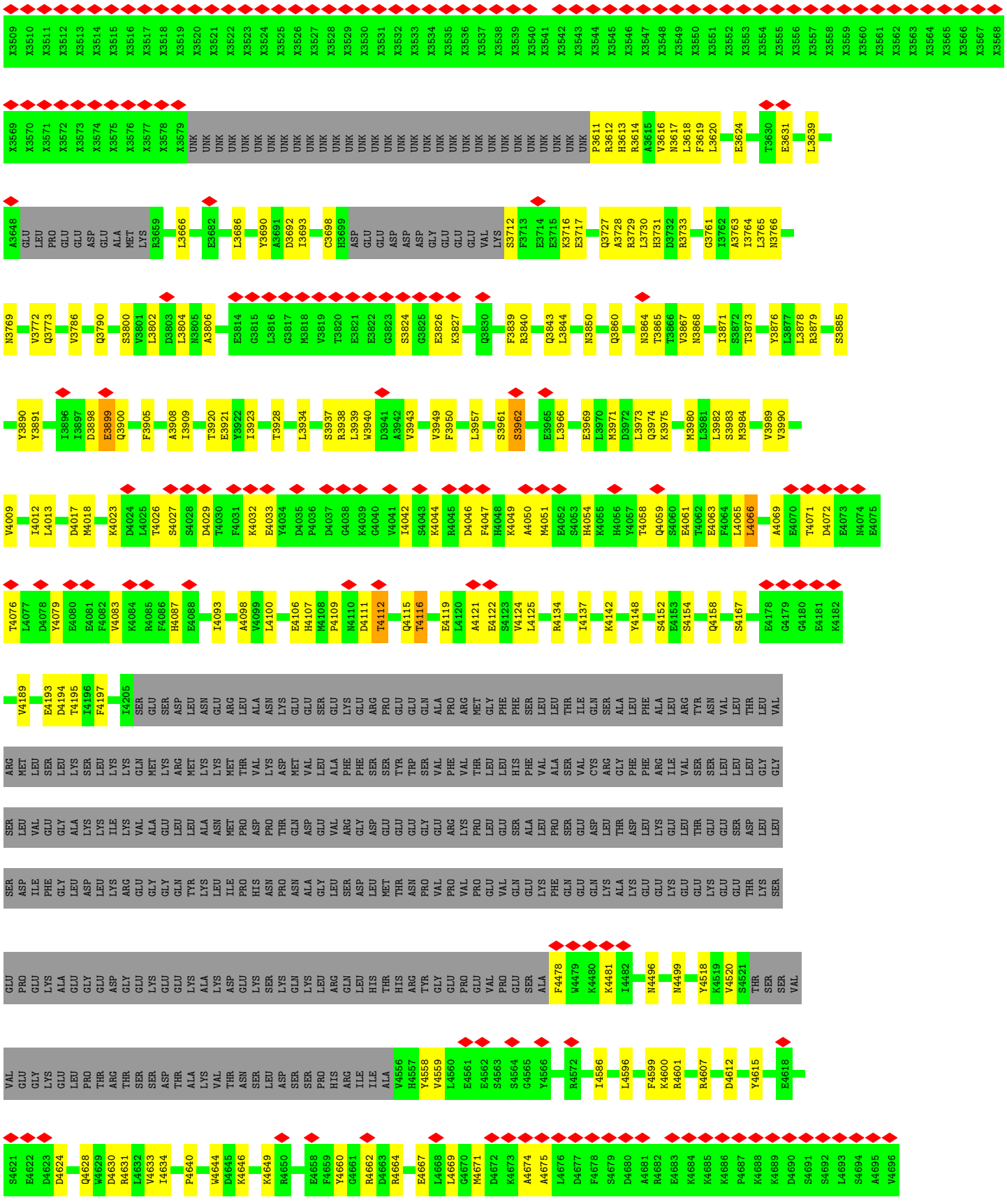
Chain D:

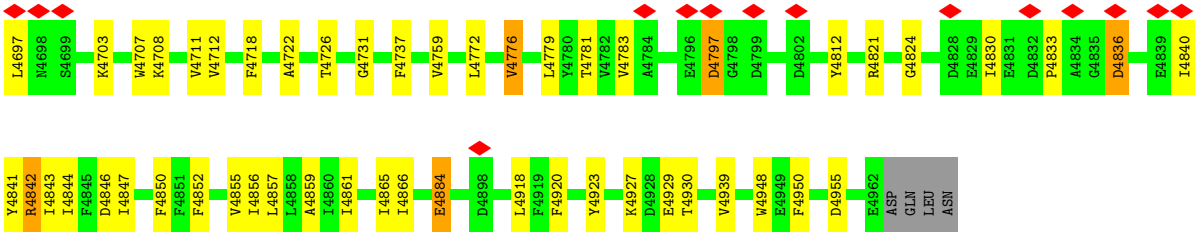



N658 L661 G662 V663 S664 E665 G666 S667 A668 Q669 Y670 K671 K672 W673 Y674 Y675 E676 L677 M678 V679 D680 H681 T682 E683 V686 T687 A688 E689 H692 L693 R694 V695 S699 T700 E701 G702 Y703 S704 P705 Y706 P707 G708 G709 G710 E711 E712 G715 N716 G719 D720 D721 S724
D728 G729 L730 H731 L732 V741 S742 S743 P744 N745 Q746 H747 L748 L749 R750 T751 D752 D753 V754 I755 S756 L759 D760 L761 S762 A763 P764 S765 I766 R769 I770 N771 G772 Q773 P774 V775 Q776 G777 M778 F779 E780 N781 D785 P790 S793 F794 S795 I798 K799 V800 R801 F802
L803 L804 G805 G806 R807 H808 G809 K812 F813 L814 P815 P816 P817 G818 Y819 A820 A821 C822 Y823 E824 A825 V826 L827 P828 K829 E830 K831 L832 K833 V834 E835 H836 S837 R838 K841 Q842 E843 R844 T845 Y846 T847 R848 D849 G852 P853 T854 V855 S856 L857 T858 Q859 A860 ALA PHE THR PRO V865
P866 V867 D868 T869 S870 Q871 I872 V873 L874 P875 P876 H877 L878 E879 R880 I881 R882 E883 R884 L885 A886 E887 N888 I889 H890 E891 L892 W893 V894 M895 N896 K897 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918 V919 E920 F921 C922 K923 L924 P925
E926 Q927 E928 R929 N930 Y931 N932 L933 Q934 M935 S936 L937 E938 T939 L940 K941 T942 L943 L944 A945 L946 G947 C948 H949 V950 G951 I952 A953 ASP GLU HIS ALA GLU GLU LYS VAL LYS LYS MET LYS LEU PRO LYS ASN Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 P980 M981 D982 L983 S984 F985
I986 K987 L988 T989 P990 S991 Q992 E993 A994 M995 V996 D997 K998 L999 A1000 E1001 N1002 A1003 H1004 W1007 A1008 I1012 R1013 Q1014 GLY TRP THR TYR GLY ILE GLN GLN ASP VAL LYS ASN R1027 P1030 R1031 L1032 V1033 P1034 Y1035 T1036 L1037 L1038 D1039 D1040 R1041 T1042 K1043 K1044 S1045 N1046 K1047 D1048 S1049
L1050 R1051 E1052 A1053 V1054 R1055 T1056 L1057 L1058 G1059 Y1060 G1061 Y1062 HIS LEU GLU ALA PRO ASP GLN ASP HIS ALA SER ARG ALA GLU VAL CYS SER GLY THR GLY GLU R1084 F1085 R1086 R1089 A1090 E1091 K1092 T1093 Y1094 A1095 Y1102 E1106 G1111 D1112 S1118 R1119 P1120 Q1123 P1124 D1125
L1128 A1136 F1137 D1138 G1139 F1140 K1141 R1144 Q1147 G1148 N1149 E1150 H1151 Q1157 A1158 G1159 D1160 V1161 M1165 V1166 N1169 E1170 M1173 M1174 F1175 T1176 I1181 D1184 D1185 S1186 G1187 S1188 E1189 L1190 A1191 F1192 K1193 D1194 F1195 D1196 V1197 G1198 D1199 G1200 F1201 I1202 P1203 V1204 L1207
G1208 V1209 A1210 Q1211 D1220 V1221 S1222 T1223 L1224 K1225 Y1226 F1227 G1231 L1232 Q1233 E1234 G1235 R1245 D1246 W1250 L1251 S1252 K1253 R1254 Q1257 V1261 P1262 S1263 N1264 H1265 E1266 H1267 I1268 E1269 V1270 T1271 R1272 I1273 D1274 GLY THR ILE ASP SER SER PRO CYS LEU K1284 V1285 T1286 S1289
Q1293 N1294 N1295 N1296 T1297 D1298 A1311 X1312 X1313 X1314 X1318 X1323 X1324 X1325 X1326 X1333 E1344 V1345 L1346 M1347 K1348 H1351 G1352 H1353 D1357 R1358 I1359 D1360 K1361 D1362 K1363 E1364 T1365 P1366 K1367 N1371 N1372 H1373 K1374 D1375 L1384 X1387 X1392 X1395 X1396 X1397 X1402
X1403 X1404 X1405 X1406 X1407 X1408 X1409 X1410 X1411 X1412 X1413 X1414 X1415 X1419 X1420 X1421 X1422 X1423 X1424 X1425 X1426 X1427 X1428 X1429 X1430 X1431 X1432 X1433 X1434 X1437 X1446 UNK
UNK
P1566 L1567 F1572 K1577 N1578 P1579 V1580 P1581 Q1582 C1583 P1584 P1585 R1586 L1587 H1588 V1589 Q1590 V1595 L1596 W1597 S1598 K1606 V1607

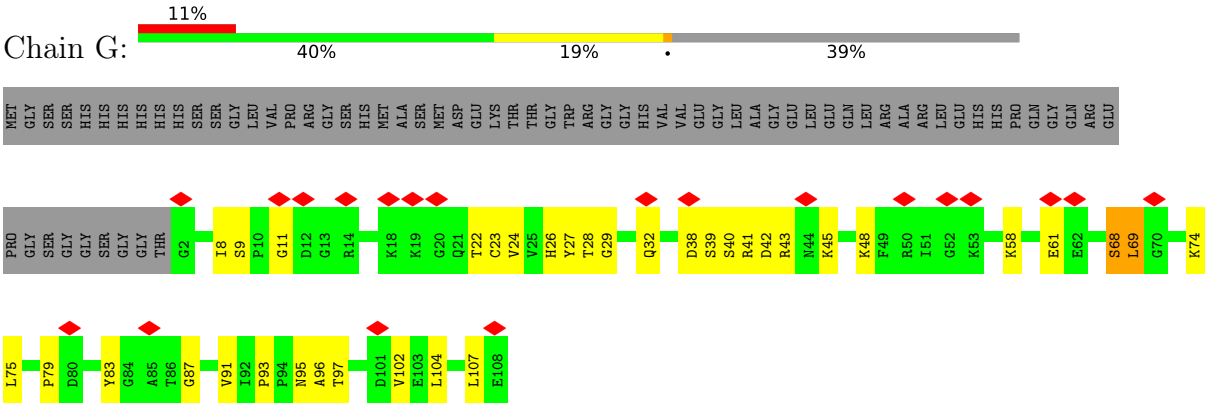

D1608 V1609 S1610 R1611 I1612 S1613 E1614 R1615 Q1616 L1619 V1620 Q1621 C1622 L1623 D1624 Q1627 L1631 H1632 I1633 P1634 E1635 D1641 I1642 L1643 E1644 L1645 T1646 E1647 Q1648 E1649 E1650 H1655 T1658 S1663 G1669 L1677 H1680 V1681 D1682 E1683 P1684 Q1685 L1686 L1687 Y1688 E1691 Y1694
R1700 Y1703 Y1704 I1708 D1709 I1710 H1711 L1712 S1713 S1714 Y1715 R1719 L1720 N1723 I1727 M1730 T1731 E1732 E1733 T1734 K1735 S1736 I1737 T1738 L1739 F1740 P1741 K1745 K1746 P1750 L1754 S1755 M1762 F1769 S1773 N1774 D1775 C1776 Y1777 Q1778 D1786 K1789 I1793 K1801
E1802 G1803 S1804 L1805 D1809 P1810 T1814 F1817 L1818 F1819 V1820 P1821 L1822 I1823 F1826 Y1827 T1828 L1829 L1830 I1831 M1832 G1833 I1834 F1835 E1838 D1839 L1840 K1841 H1842 I1843 L1844 Q1845 E1848 P1849 S1850 VAL PHE LYS GLU ALA ALA VAL PRO GLU GLU GLU GLY GLY THR PRO GLU LYS GLU ILE
SER ILE GLU ASP ALA LYS LEU GLU GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG PRO LYS GLU G1891 K1896 V1901 M1905 L1909 R1918 I1924 D1929 V1932 L1935 Q1936 D1937 N1938 Q1939 N1944 M1947 Q1948 A1949 L1950 N1951 M1952 S1953 A1954 A1955 L1956 T1957 A1958 R1959
K1960 T1961 R1962 E1963 F1964 R1965 S1966 P1967 P1968 Q1969 E1970 Q1971 I1972 N1973 M1974 L1975 L1976 K1979 D1980 D1981 K1982 S1983 E1984 C1985 P1986 C1987 P1988 E1989 E1990 I1991 R1992 D1993 D1997 F1998 H1999 E2000 D2001 L2002 M2003 T2004 I2008 E2009 LEU ASP GLU ASP GLY SER LEU ASP GLY SER ASN ASP LEU THR ILE
ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL ALA SER ASP SER ARG LYS CYS SER S2056 L2057 L2060 I2061 M2065 D2076 L2079 V2080 R2081 A2082 M2083 F2084 Y2091 G2096 R2099 A2100 L2101 P2102 K2103 T2104 Y2105 T2106
I2107 N2108 E2113 L2118 L2119 S2127 V2131 G2134 E2137 G2144 L2145 I2148 F2154 H2157 P2158 N2159 L2160 M2161 R2162 M2171 V2175 G2179 G2180 G2181 E2182 S2183 K2184 E2185 R2197 I2205 S2206 R2207 Q2208 N2209 L2217 L2220 N2223 S2224 S2225 V2226 G2227 L2228
P2231 S2236 T2237 P2238 L2239 D2240 V2241 A2242 A2243 A2244 S2245 V2246 M2247 D2248 A2253 R2257 E2258 P2259 D2260 L2261 V2265 C2276 L2279 K2282 G2283 Y2284 I2287 N2290 E2293 R2296 E2313 E2314 N2315 A2316 N2317 V2318 V2319 V2320 R2321 L2322 L2323 I2324 R2325 F2330 A2333
L2334 R2335 G2336 E2337 G2338 G2339 N2340 G2341 L2342 L2343 E2347 E2348 A2349 I2350 K2351 I2352 A2353 E2354 R2358 D2359 G2360 P2361 SER PRO THR SER GLY SER SER LYS THR LEU ASP ILE GLU GLU GLU ASP D2379 T2380 I2381 N2385 T2389 L2394 I2395 D2396 M2405 H2406 H2409 K2412 G2413
E2414 A2415 I2416 L2428 G2429 S2436 I2437 A2438 F2439 Q2440 M2441 P2442 THR ILE ALA LYS ASP GLY LYS VAL VAL E2452 P2453 D2454 M2455 S2456 H2463 K2464 M2467 L2471 I2477 E2478 V2479 Q2480 D2481 F2482 H2485 L2486 L2487 E2488 V2489 G2490 F2491 L2492 P2493 D2494 L2495 R2496 A2497 A2498 A2499 S2500 L2501
D2502 T2503 A2504 A2505 L2506 S2507 X2508 X2509 X2522 X2523 X2524 X2527 X2528 X2529 X2530 X2531 X2532 X2535 X2536 X2539 X2543 X2544 X2545 X2546 X2547 X2548 X2549 X2550 X2551 X2552 X2564 X2567 X2568 X2569 X2570 X2571 X2572 X2575 X2576 X2577 X2578 X2585 X2586 X2587 X2588 X2589 X2590 X2591 X2592 X2593 X2594
X2595 X2596 X2597 X2598 X2599 X2600 X2601 X2602 X2606 X2609 X2613 X2614 X2615 X2616 X2617 X2618 X2619 X2620 X2621 X2622 X2625 X2626 X2627 X2628 X2629 X2630 X2634 X2635 X2636 X2637 X2638 X2639 X2640 X2641 X2642 X2643 X2644 X2645 X2646 X2647 X2648 X2649 X2650 X2651 X2652 X2653 X2654 X2655 X2656 X2657 X2658 UNK UNK UNK UNK
UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK I2712 P2713 E2714 K2715 L2716 E2717 Y2718 F2719 I2720 N2721 K2722


Y2723 A2724 E2725 H2726 S2727 H2728 D2729 K2730 W2731 S2732 M2733 D2734 K2735 L2736 A2737 N2738 G2739 W2740 I2741 Y2742 G2743 E2744 I2745 Y2746 S2747 D2748 S2749 S2750 K2751 I2752 Q2753 P2754 L2755 M2756 LYS PRO TYR LYS L2761 L2762 S2763 E2764 K2765 E2766 K2767 E2768 I2769 Y2770 R2771 W2772 P2773 I2774 K2775 E2776 S2777 L2778 K2779 T2780 M2781 L2782
A2783 W2784 GLY TRP ARG ILE GLU ARG THR ARG GLU GLY ASP SER MET ALA LEU TYR ASN ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER ILE ASP ALA ALA HIS GLY TYR SER PRO ARG ALA ILE ASP MET SER ASN VAL THR LEU SER ARG D2835 L2836 H2837 A2838 M2839 A2840 E2841 M2842
M2843 A2844 E2845 N2846 Y2847 H2848 N2849 I2850 W2851 A2852 K2853 K2854 K2855 K2856 L2857 E2858 L2859 E2860 S2861 K2862 G2863 G2864 G2865 N2866 H2867 P2868 L2869 L2870 V2871 P2872 Y2873 D2874 T2875 L2876 T2877 A2878 K2879 E2880 K2881 A2882 K2883 D2884 R2885 E2886 K2887 A2888 Q2889 D2890 I2891 F2892 K2893 F2894 L2895 Q2896 I2897 S2898 G2899 Y2900 V2901 V2902
S2903 R2904 G2905 PHE LYS ASP LEU ASP LEU ASP THR PRO SER X2916 X2917 X2918 X2919 X2920 X2921 X2922 X2923 X2924 X2925 X2930 X2935 X2936 X2937 X2938 X2939 X2940 X2941 X2942 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK X2961 X2962 X2963 X2964 X2965 X2966 X2967 X2968
X2969 X2970 X2971 X2972 X2973 X2974 X2975 X2976 X2977 X2978 X2979 X2980 X2981 X2982 X2983 X2984 X2985 X2986 X2987 X2988 X2989 X2990 X2991 X2992 X2993 X2994 X2995 X2996 X2997 X2998 X2999 X3000 X3001 X3002 X3003 X3004 X3005 X3006 X3007 X3008 X3009 X3010 X3011 X3012 X3013 X3014 X3015 X3016 X3017 X3018 X3019 X3020 X3021 X3022 X3023 X3024 X3025 X3026 X3027 X3028
X3029 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK
UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK X3104 X3105 X3106 X3107 X3108 X3109 X3110 X3111 X3112 X3113 X3114 X3115 X3116 X3117 X3118 X3119 X3120 X3121 X3122 X3123 X3124 X3125 X3126 X3127 X3128 X3129 UNK UNK UNK UNK UNK UNK X3136 X3137 X3138 X3139 X3140 X3141 X3142 X3143 X3144 X3145 X3146 X3147 X3148
X3149 X3150 X3151 X3152 X3153 X3154 X3155 X3156 X3157 X3158 X3159 X3160 X3161 X3162 X3163 X3164 X3165 X3166 X3167 X3168 X3169 X3170 X3171 X3172 X3173 X3174 X3175 X3176 X3177 X3178 X3179 X3180 X3181 X3182 X3183 X3184 X3185 X3186 X3187 X3188 X3189 X3190 X3191 X3192 X3193 X3194 X3195 X3196 X3197 X3198 X3199 X3200 X3201 X3202 UNK UNK UNK UNK UNK UNK
UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK X3231 X3232 X3233 X3234 X3235 X3236 X3237 X3238 X3239 X3240 X3241 X3242 X3243 X3244 X3245 X3246 X3247 X3248 X3249 X3250 X3251 X3252 X3253 X3254 X3255 X3256 X3257 X3258 X3259 X3260 X3261 X3262 X3263 X3264 X3265 X3266 X3267 X3268
X3269 X3270 X3271 X3272 X3273 X3274 X3275 X3276 X3277 X3278 X3279 X3280 X3281 X3282 X3283 X3284 X3285 X3286 X3287 X3288 X3289 X3290 X3291 X3292 X3293 X3294 X3295 X3296 X3297 X3298 X3299 X3300 X3301 X3302 X3303 X3304 X3305 X3306 X3307 X3308 X3309 X3310 X3311 X3312 X3313 X3314 X3315 X3316 X3317 X3318 X3319 X3320 X3321 X3322 X3323 X3324 X3325 X3326 X3327 X3328
X3329 X3330 X3331 X3332 X3333 X3334 X3335 X3336 X3337 X3338 X3339 X3340 X3341 X3342 X3343 X3344 X3345 X3346 X3347 X3348 X3349 X3350 X3351 X3352 X3353 X3354 X3355 X3356 X3357 X3358 X3359 X3360 X3361 X3362 X3363 X3364 X3365 X3366 X3367 X3368 X3369 X3370 X3371 X3372 X3373 X3374 X3375 X3376 X3377 X3378 X3379 X3380 X3381 X3382 X3383 X3384 X3385 X3386 X3387 X3388
X3389 X3390 X3391 X3392 X3393 X3394 X3395 X3396 X3397 X3398 X3399 X3400 X3401 X3402 X3403 X3404 X3405 X3406 X3407 X3408 X3409 X3410 X3411 X3412 X3413 X3414 X3415 X3416 X3417 X3418 X3419 X3420 X3421 X3422 X3423 X3424 X3425 X3426 X3427 X3428 X3429 X3430 X3431 X3432 X3433 X3434 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK
UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK X3477 X3478 X3479 X3480 X3481 X3482 X3483 X3484 X3485 X3486 X3487 X3488 X3489 X3490 X3491 X3492 X3493 X3494 X3495 X3496 X3497 X3498 X3499 X3500 X3501 X3502 X3503 X3504 X3505 X3506 X3507 X3508

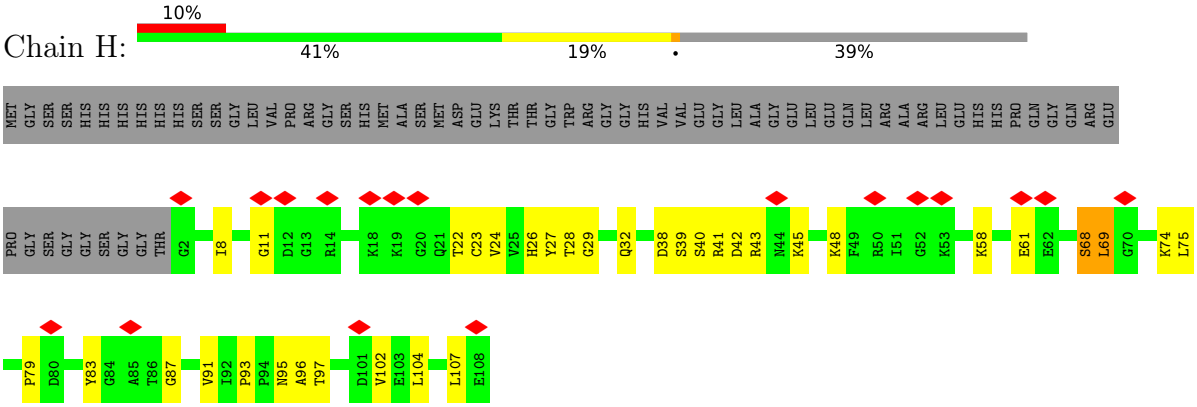

X3509 X3510 X3511 X3512 X3513 X3514 X3515 X3516 X3517 X3518 X3519 X3520 X3521 X3522 X3523 X3524 X3525 X3526 X3527 X3528 X3529 X3530 X3531 X3532 X3533 X3534 X3535 X3536 X3537 X3538 X3539 X3540 X3541 X3542 X3543 X3544 X3545 X3546 X3547 X3548 X3549 X3550 X3551 X3552 X3553 X3554 X3555 X3556 X3557 X3558 X3559 X3560 X3561 X3562 X3563 X3564 X3565 X3566 X3567 X3568
X3569 X3570 X3571 X3572 X3573 X3574 X3575 X3576 X3577 X3578 X3579 UNK P3611 R3612 H3613 R3614 A3615 V3616 N3617 L3618 F3619 L3620 E3624 T3630 E3631 L3639
A3648 GLU LEU PRO GLU GLU ASP GLU ALA MET LYS R3659 L3666 E3682 L3686 Y3690 A3691 D3692 I3693 C3698 H3699 ASP GLU GLU ASP ASP GLY GLU GLU GLU VAL LYS S3712 F3713 E3714 E3715 K3716 E3717 Q3727 A3728 R3729 L3730 H3731 D3732 R3733 G3761 I3762 A3763 I3764 L3765 N3766
N3769 V3772 Q3773 V3786 Q3790 S3800 V3801 L3802 D3803 L3804 N3805 A3806 E3814 G3815 L3816 G3817 M3818 V3819 T3820 E3821 E3822 G3823 S3824 G3825 E3826 K3827 Q3830 F3839 R3840 Q3843 L3844 N3850 Q3860 N3864 T3865 T3866 V3867 N3868 I3871 S3872 T3873 Y3876 L3877 L3878 R3879 S3885
Y3890 Y3891 I3896 I3897 D3898 E3899 Q3900 F3905 A3908 I3909 T3920 E3921 Y3922 I3923 T3928 L3934 S3937 R3938 L3939 W3940 D3941 A3942 V3943 V3949 F3950 L3957 S3961 S3962 E3965 L3966 E3969 L3970 M3971 D3972 L3973 Q3974 K3975 M3980 L3981 L3982 S3983 M3984 V3989 V3990
V4009 I4012 L4013 D4017 M4018 K4023 D4024 L4025 T4026 S4027 S4028 D4029 T4030 F4031 K4032 E4033 Y4034 D4035 P4036 D4037 G4038 K4039 G4040 V4041 I4042 S4043 K4044 R4045 D4046 F4047 H4048 K4049 A4050 M4051 E4052 S4053 H4054 K4055 H4056 Y4057 T4058 Q4059 S4060 E4061 T4062 E4063 F4064 L4065 L4066 A4069 E4070 T4071 D4072 E4073 N4074 E4075
T4076 L4077 D4078 Y4079 E4080 E4081 F4082 V4083 K4084 R4085 F4086 H4087 E4088 I4093 A4098 V4099 L4100 E4106 H4107 M4108 P4109 N4110 D4111 T4412 Q4115 T4416 E4119 L4120 A4121 E4122 S4123 V4124 L4125 R4134 I4137 K4142 Y4148 S4152 E4153 S4154 Q4158 S4167 E4178 G4179 G4180 E4181 K4182
V4189 E4193 D4194 T4195 I4196 F4197 I4205 SER GLU SER ASP LEU ASN GLU ARG LEU ALA ASN LYS GLU GLU SER GLU LYS GLU ARG PRO GLU GLU GLN ALA PRO ARG MET GLY PHE PHE SER LEU LEU THR ILE GLN SER ALA LEU PHE ALA LEU ARG TYR ASN VAL LEU THR LEU VAL
ARG MET LEU SER LEU LYS SER LEU LYS LYS GLN MET LYS ARG MET LYS LYS MET THR VAL LYS ASP MET VAL LEU ALA PHE PHE SER SER TYR TRP SER VAL PHE VAL THR LEU LEU HIS PHE SER VAL ALA LEU PHE PHE ARG ILE VAL SER SER LEU LEU LEU GLY GLY
SER LEU VAL GLU GLY ALA LYS LYS ILE LYS VAL ALA GLU LEU LEU ALA ASN MET PRO ASP PRO THR GLN ASP GLU VAL ARG GLY ASP GLU GLU GLU GLY GLU ARG LYS PRO LEU GLU SER ALA LEU PRO SER GLU ASP LEU THR GLU LEU LYS GLU LEU THR GLU GLU SER ASP LEU LEU
SER ASP ILE PHE GLY LEU ASP LEU LYS ARG GLU GLY GLY GLN TYR LYS LEU ILE PRO HIS ASN PRO ASN ALA GLY LEU SER ASP LEU MET THR ASN PRO VAL PRO VAL PRO GLU VAL GLN GLU LYS PHE GLN GLU GLN LYS ALA LYS GLU GLU LYS GLU GLU LYS LYS GLU GLU SER THR LYS SER
GLU PRO GLU LYS ALA GLU GLY GLU GLU LYS GLU GLU LYS ALA LYS ASP GLU LYS SER LYS GLN LYS LEU ARG GLN LEU HIS THR HIS ARG TYR GLY GLU PRO GLU VAL PRO GLU SER ALA F4478 W4479 K4480 K4481 I4482 N4496 N4499 Y4518 K4519 V4520 S4521 THR SER SER VAL
VAL GLU GLY LYS GLU LEU PRO THR ARG THR SER SER ASP THR ALA LYS VAL THR ASN SER LEU ASP SER SER PRO HIS ARG ILE ILE ALA V4556 H4557 Y4558 V4559 L4560 E4561 E4562 S4563 S4564 G4565 Y4566 R4572 I4586 L4596 F4599 K4600 R4601 R4607 D4612 Y4615 E4618
S4621 E4622 D4623 D4624 Q4628 W4629 D4630 R4631 L4632 V4633 I4634 P4640 W4644 D4645 K4646 K4649 R4650 E4658 F4659 Y4660 G4661 R4662 D4663 R4664 E4667 L4668 L4669 G4670 M4671 D4672 K4673 A4674 A4675 L4676 D4677 F4678 S4679 D4680 A4681 R4682 E4683 K4684 K4685 K4686 P4687 K4688 K4689 D4690 S4691 S4692 L4693 S4694 A4695 V4696



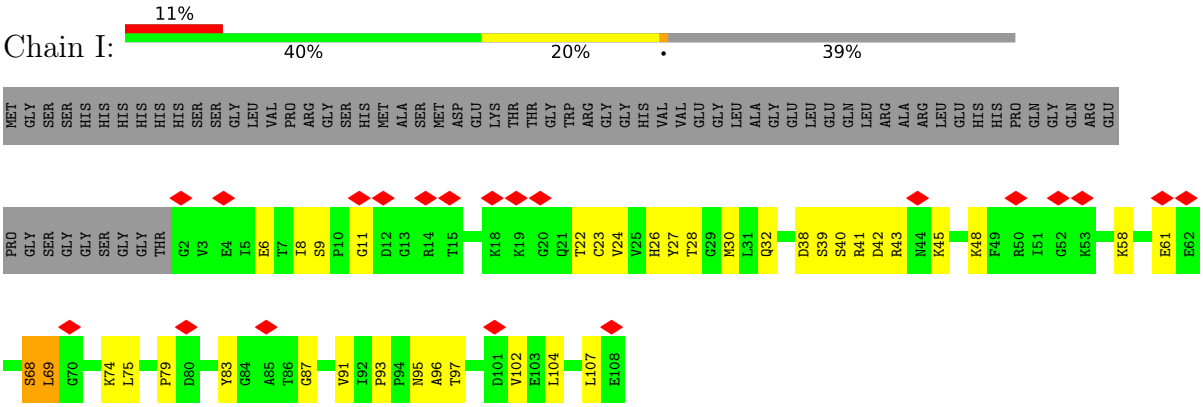
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

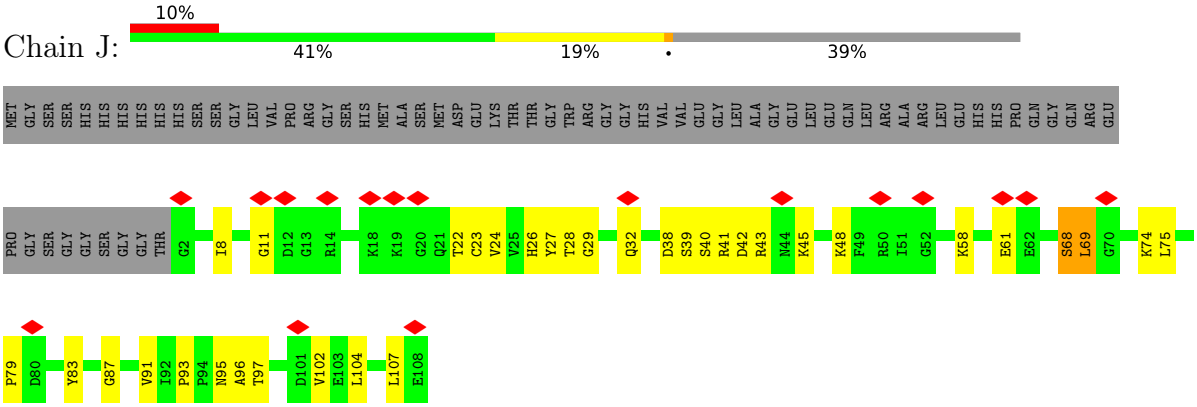


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J:


10%
41%
19%
39%
MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA SER MET ASP GLU LYS THR THR GLY TRP ARG GLY GLY HIS VAL VAL GLU GLY LEU ALA GLY GLU LEU GLU GLN LEU ARG ALA ARG LEU GLU HIS HIS PRO GLN GLY GLN ARG GLU
PRO GLY SER GLY GLY SER GLY GLY THR G2 I8 G11 D12 G13 R14 K18 K19 G20 G21 T22 C23 V24 V25 H26 Y27 T28 G29 Q32 D38 S39 S40 R41 D42 R43 N44 K45 K48 F49 R50 I51 G52 K58 E61 E62 S68 L69 G70 K74 L75
P79 D80 Y83 G87 V91 I92 P93 P94 N95 A96 T97 D101 V102 E103 L104 L107 E108

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42375	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.165	Depositor
Minimum map value	-0.096	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.021	Depositor
Map size (Å)	421.25998, 421.25998, 421.25998	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.239, 1.239, 1.239	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.26	0/26573	0.45	4/35881 (0.0%)
1	B	0.26	0/26573	0.45	4/35881 (0.0%)
1	C	0.26	0/26573	0.45	4/35881 (0.0%)
1	D	0.26	0/26573	0.45	4/35881 (0.0%)
2	G	0.26	0/835	0.49	0/1123
2	H	0.26	0/835	0.49	0/1123
2	I	0.26	0/835	0.49	0/1123
2	J	0.26	0/835	0.49	0/1123
All	All	0.26	0/109632	0.45	16/148016 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1170	GLU	CA-CB-CG	5.88	126.33	113.40
1	D	1170	GLU	CA-CB-CG	5.88	126.33	113.40
1	A	1170	GLU	CA-CB-CG	5.86	126.29	113.40
1	B	1170	GLU	CA-CB-CG	5.86	126.28	113.40
1	A	1838	GLU	CA-CB-CG	5.66	125.85	113.40
1	C	1838	GLU	CA-CB-CG	5.66	125.85	113.40
1	B	1838	GLU	CA-CB-CG	5.65	125.83	113.40
1	D	1838	GLU	CA-CB-CG	5.65	125.83	113.40
1	C	944	LEU	CA-CB-CG	5.34	127.57	115.30
1	A	944	LEU	CA-CB-CG	5.33	127.55	115.30
1	D	944	LEU	CA-CB-CG	5.32	127.53	115.30
1	B	944	LEU	CA-CB-CG	5.30	127.49	115.30
1	A	2725	GLU	CA-CB-CG	5.14	124.71	113.40
1	D	2725	GLU	CA-CB-CG	5.13	124.70	113.40
1	B	2725	GLU	CA-CB-CG	5.12	124.66	113.40
1	C	2725	GLU	CA-CB-CG	5.12	124.66	113.40

There are no chirality outliers.

There are no planarity outliers.

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	29688	0	26383	563	0
1	B	29688	0	26383	564	0
1	C	29688	0	26383	563	0
1	D	29688	0	26383	571	0
2	G	819	0	821	22	0
2	H	819	0	821	22	0
2	I	819	0	821	25	0
2	J	819	0	821	22	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	122036	0	108816	2307	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 10.

All (2307) 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:1687:LEU:O	1:A:1691:GLU:HB3	1.78	0.84
1:B:1687:LEU:O	1:B:1691:GLU:HB3	1.78	0.84
1:A:1170:GLU:OE1	1:A:1170:GLU:N	2.11	0.84
1:C:1687:LEU:O	1:C:1691:GLU:HB3	1.78	0.84
1:D:1687:LEU:O	1:D:1691:GLU:HB3	1.78	0.84
1:B:1170:GLU:OE1	1:B:1170:GLU:N	2.11	0.83
1:D:760:ASP:HB3	1:D:764:PRO:HG2	1.61	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1170:GLU:N	1:C:1170:GLU:OE1	2.11	0.83
1:C:748:LEU:HD23	2:I:8:ILE:HG23	1.59	0.83
1:A:760:ASP:HB3	1:A:764:PRO:HG2	1.61	0.83
1:D:1170:GLU:OE1	1:D:1170:GLU:N	2.11	0.82
1:C:760:ASP:HB3	1:C:764:PRO:HG2	1.61	0.82
1:B:760:ASP:HB3	1:B:764:PRO:HG2	1.61	0.81
1:A:3843:GLN:HG3	1:A:3921:GLU:HG3	1.65	0.79
1:C:4833:PRO:HD3	1:C:4842:ARG:HE	1.48	0.79
1:B:3843:GLN:HG3	1:B:3921:GLU:HG3	1.65	0.78
1:A:4833:PRO:HD3	1:A:4842:ARG:HE	1.48	0.78
1:B:4833:PRO:HD3	1:B:4842:ARG:HE	1.48	0.78
1:D:4833:PRO:HD3	1:D:4842:ARG:HE	1.48	0.78
1:D:3843:GLN:HG3	1:D:3921:GLU:HG3	1.65	0.77
1:C:3843:GLN:HG3	1:C:3921:GLU:HG3	1.65	0.76
1:C:156:GLU:HG2	1:C:187:SER:HB3	1.68	0.75
1:B:156:GLU:HG2	1:B:187:SER:HB3	1.68	0.74
1:D:4844:ILE:HD12	1:D:4847:ILE:HD11	1.70	0.74
1:D:156:GLU:HG2	1:D:187:SER:HB3	1.68	0.74
1:B:189:GLU:OE2	1:C:2321:ARG:NH1	2.21	0.73
1:A:156:GLU:HG2	1:A:187:SER:HB3	1.68	0.73
1:A:4844:ILE:HD12	1:A:4847:ILE:HD11	1.70	0.73
1:C:4844:ILE:HD12	1:C:4847:ILE:HD11	1.70	0.72
1:B:719:GLY:H	1:B:724:SER:HB3	1.54	0.72
1:C:2740:TRP:HD1	1:C:2751:LYS:HE3	1.55	0.72
1:A:3773:GLN:OE1	1:A:3850:ASN:ND2	2.23	0.72
1:C:719:GLY:H	1:C:724:SER:HB3	1.54	0.72
1:A:719:GLY:H	1:A:724:SER:HB3	1.54	0.72
1:B:1060:TYR:HD1	1:B:1060:TYR:H	1.38	0.72
1:A:2765:LYS:O	1:A:2769:ILE:HG23	1.90	0.71
1:B:4844:ILE:HD12	1:B:4847:ILE:HD11	1.70	0.71
1:C:1060:TYR:H	1:C:1060:TYR:HD1	1.38	0.71
1:B:2765:LYS:O	1:B:2769:ILE:HG23	1.90	0.71
1:C:3773:GLN:OE1	1:C:3850:ASN:ND2	2.23	0.71
1:D:1060:TYR:HD1	1:D:1060:TYR:H	1.38	0.71
1:D:2765:LYS:O	1:D:2769:ILE:HG23	1.90	0.71
1:A:1681:VAL:HG23	1:A:1682:ASP:H	1.55	0.71
1:C:1700:ARG:NH1	1:C:1817:PHE:O	2.24	0.71
1:A:1060:TYR:H	1:A:1060:TYR:HD1	1.38	0.71
1:B:924:LEU:HG	1:B:925:PRO:HD2	1.73	0.71
1:A:924:LEU:HG	1:A:925:PRO:HD2	1.73	0.71
1:B:3773:GLN:OE1	1:B:3850:ASN:ND2	2.23	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1700:ARG:NH1	1:D:1817:PHE:O	2.24	0.71
1:C:1681:VAL:HG23	1:C:1682:ASP:H	1.56	0.70
1:D:3773:GLN:OE1	1:D:3850:ASN:ND2	2.23	0.70
1:B:2740:TRP:HD1	1:B:2751:LYS:HE3	1.54	0.70
1:A:4866:ILE:HD11	1:D:4859:ALA:HB1	1.74	0.70
1:B:1700:ARG:NH1	1:B:1817:PHE:O	2.24	0.70
1:D:719:GLY:H	1:D:724:SER:HB3	1.54	0.70
2:G:75:LEU:HD22	2:G:102:VAL:HG21	1.74	0.70
1:B:1681:VAL:HG23	1:B:1682:ASP:H	1.56	0.70
1:D:924:LEU:HG	1:D:925:PRO:HD2	1.73	0.70
1:A:2740:TRP:HD1	1:A:2751:LYS:HE3	1.54	0.69
1:D:2740:TRP:HD1	1:D:2751:LYS:HE3	1.54	0.69
2:H:75:LEU:HD22	2:H:102:VAL:HG21	1.74	0.69
1:C:924:LEU:HG	1:C:925:PRO:HD2	1.73	0.69
1:C:1684:PRO:HD3	2:I:42:ASP:HB3	1.73	0.69
1:C:2765:LYS:O	1:C:2769:ILE:HG23	1.90	0.69
1:A:1700:ARG:NH1	1:A:1817:PHE:O	2.24	0.69
2:J:75:LEU:HD22	2:J:102:VAL:HG21	1.74	0.69
1:D:1681:VAL:HG23	1:D:1682:ASP:H	1.56	0.69
2:I:75:LEU:HD22	2:I:102:VAL:HG21	1.74	0.69
1:D:1262:PRO:HG2	1:D:1265:HIS:HB2	1.75	0.69
1:B:1970:GLU:HA	1:B:1973:ASN:HB2	1.75	0.68
1:C:3802:LEU:HD11	1:C:3908:ALA:HB2	1.76	0.68
1:A:2406:HIS:HA	1:A:2409:HIS:HB3	1.76	0.68
1:B:2406:HIS:HA	1:B:2409:HIS:HB3	1.76	0.68
1:C:1262:PRO:HG2	1:C:1265:HIS:HB2	1.75	0.68
1:B:191:TYR:OH	1:C:2325:ARG:NH1	2.26	0.68
1:A:1262:PRO:HG2	1:A:1265:HIS:HB2	1.75	0.68
1:C:1970:GLU:HA	1:C:1973:ASN:HB2	1.75	0.68
1:C:4830:ILE:HG13	1:C:4842:ARG:HH22	1.59	0.67
1:A:3802:LEU:HD11	1:A:3908:ALA:HB2	1.76	0.67
1:A:759:LEU:HD13	1:A:766:ILE:HG22	1.77	0.67
1:A:970:TYR:HE2	1:A:977:LYS:HG2	1.60	0.67
1:A:1682:ASP:HB2	1:A:1685:GLN:HB3	1.76	0.67
1:B:1682:ASP:HB2	1:B:1685:GLN:HB3	1.76	0.67
1:B:4830:ILE:HG13	1:B:4842:ARG:HH22	1.59	0.67
1:C:970:TYR:HE2	1:C:977:LYS:HG2	1.60	0.67
1:C:1682:ASP:HB2	1:C:1685:GLN:HB3	1.75	0.67
1:D:3802:LEU:HD11	1:D:3908:ALA:HB2	1.76	0.67
1:B:759:LEU:HD13	1:B:766:ILE:HG22	1.77	0.67
1:D:1970:GLU:HA	1:D:1973:ASN:HB2	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LEU:HD12	1:A:201:TRP:HB3	1.77	0.67
1:A:4830:ILE:HG13	1:A:4842:ARG:HH22	1.60	0.67
1:C:759:LEU:HD13	1:C:766:ILE:HG22	1.77	0.67
1:D:759:LEU:HD13	1:D:766:ILE:HG22	1.77	0.67
1:B:3802:LEU:HD11	1:B:3908:ALA:HB2	1.76	0.67
1:D:1682:ASP:HB2	1:D:1685:GLN:HB3	1.76	0.67
1:D:2406:HIS:HA	1:D:2409:HIS:HB3	1.76	0.67
1:A:1970:GLU:HA	1:A:1973:ASN:HB2	1.75	0.66
1:B:1262:PRO:HG2	1:B:1265:HIS:HB2	1.75	0.66
1:C:748:LEU:CD2	2:I:8:ILE:HG23	2.25	0.66
1:D:970:TYR:HE2	1:D:977:LYS:HG2	1.60	0.66
1:C:2081:ARG:HG3	1:C:3686:LEU:HD22	1.76	0.66
1:D:654:SER:H	1:D:841:LYS:NZ	1.93	0.66
1:C:2406:HIS:HA	1:C:2409:HIS:HB3	1.76	0.66
1:C:2893:LYS:O	1:C:2897:ILE:HG13	1.96	0.66
1:A:804:LEU:HD22	1:A:822:CYS:HB2	1.78	0.66
1:A:2081:ARG:HG3	1:A:3686:LEU:HD22	1.76	0.66
1:B:970:TYR:HE2	1:B:977:LYS:HG2	1.60	0.66
1:C:654:SER:H	1:C:841:LYS:NZ	1.93	0.66
1:C:1720:LEU:HD21	1:C:1831:ILE:HD13	1.78	0.66
2:I:104:LEU:HD21	2:I:107:LEU:HD21	1.78	0.66
1:B:49:LEU:HD12	1:B:201:TRP:HB3	1.77	0.66
1:C:804:LEU:HD22	1:C:822:CYS:HB2	1.78	0.66
1:D:4830:ILE:HG13	1:D:4842:ARG:HH22	1.59	0.66
1:A:2893:LYS:O	1:A:2897:ILE:HG13	1.96	0.66
1:D:49:LEU:HD12	1:D:201:TRP:HB3	1.77	0.66
1:D:804:LEU:HD22	1:D:822:CYS:HB2	1.78	0.66
2:G:104:LEU:HD21	2:G:107:LEU:HD21	1.78	0.66
1:B:1720:LEU:HD21	1:B:1831:ILE:HD13	1.78	0.66
1:D:2081:ARG:HG3	1:D:3686:LEU:HD22	1.76	0.66
1:D:2893:LYS:O	1:D:2897:ILE:HG13	1.96	0.66
1:B:2893:LYS:O	1:B:2897:ILE:HG13	1.95	0.66
1:D:590:LYS:H	1:D:593:HIS:HD2	1.44	0.66
1:A:654:SER:H	1:A:841:LYS:NZ	1.93	0.65
1:B:412:GLU:HG3	1:B:488:LEU:HD11	1.78	0.65
1:D:412:GLU:HG3	1:D:488:LEU:HD11	1.79	0.65
1:A:1266:GLU:O	1:A:1267:HIS:ND1	2.29	0.65
1:B:1266:GLU:O	1:B:1267:HIS:ND1	2.29	0.65
1:D:1266:GLU:O	1:D:1267:HIS:ND1	2.29	0.65
1:D:3786:VAL:O	1:D:3790:GLN:HG3	1.97	0.65
1:B:2081:ARG:HG3	1:B:3686:LEU:HD22	1.76	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3826:GLU:HG2	1:B:3827:LYS:H	1.62	0.65
1:B:804:LEU:HD22	1:B:822:CYS:HB2	1.78	0.65
1:B:3786:VAL:O	1:B:3790:GLN:HG3	1.97	0.65
1:C:49:LEU:HD12	1:C:201:TRP:HB3	1.77	0.65
1:C:1719:ARG:O	1:C:1723:ASN:HB2	1.97	0.65
1:C:1985:CYS:SG	1:C:1992:ARG:NH1	2.70	0.65
1:C:3786:VAL:O	1:C:3790:GLN:HG3	1.96	0.65
1:C:3826:GLU:HG2	1:C:3827:LYS:H	1.62	0.65
1:D:4840:ILE:HD12	1:D:4843:ILE:HD11	1.78	0.65
2:J:104:LEU:HD21	2:J:107:LEU:HD21	1.78	0.65
1:A:1985:CYS:SG	1:A:1992:ARG:NH1	2.70	0.65
1:B:654:SER:H	1:B:841:LYS:NZ	1.93	0.65
1:C:590:LYS:H	1:C:593:HIS:HD2	1.44	0.65
1:C:1266:GLU:O	1:C:1267:HIS:ND1	2.29	0.65
1:A:412:GLU:HG3	1:A:488:LEU:HD11	1.78	0.65
1:B:1985:CYS:SG	1:B:1992:ARG:NH1	2.70	0.65
2:I:28:THR:HA	2:I:39:SER:HA	1.79	0.65
1:A:3826:GLU:HG2	1:A:3827:LYS:H	1.62	0.65
1:B:1793:ILE:HG12	1:B:1843:ILE:HD11	1.79	0.65
1:C:412:GLU:HG3	1:C:488:LEU:HD11	1.78	0.65
1:C:1793:ILE:HG12	1:C:1843:ILE:HD11	1.79	0.65
1:D:1720:LEU:HD21	1:D:1831:ILE:HD13	1.78	0.65
1:A:4840:ILE:HD12	1:A:4843:ILE:HD11	1.78	0.64
1:D:1688:TYR:HA	1:D:1691:GLU:HG2	1.79	0.64
1:C:2844:ALA:HB1	1:C:2884:ASP:HB3	1.78	0.64
1:D:1719:ARG:O	1:D:1723:ASN:HB2	1.97	0.64
1:D:3826:GLU:HG2	1:D:3827:LYS:H	1.62	0.64
1:C:3611:PRO:HD2	1:C:3614:ARG:HD3	1.79	0.64
1:A:1720:LEU:HD21	1:A:1831:ILE:HD13	1.78	0.64
1:B:1719:ARG:O	1:B:1723:ASN:HB2	1.97	0.64
1:B:4840:ILE:HD12	1:B:4843:ILE:HD11	1.78	0.64
2:H:28:THR:HA	2:H:39:SER:HA	1.79	0.64
2:H:104:LEU:HD21	2:H:107:LEU:HD21	1.78	0.64
1:A:3786:VAL:O	1:A:3790:GLN:HG3	1.97	0.64
1:B:2844:ALA:HB1	1:B:2884:ASP:HB3	1.78	0.64
1:D:1985:CYS:SG	1:D:1992:ARG:NH1	2.70	0.64
2:G:28:THR:HA	2:G:39:SER:HA	1.79	0.64
1:A:590:LYS:H	1:A:593:HIS:HD2	1.44	0.64
1:A:2844:ALA:HB1	1:A:2884:ASP:HB3	1.78	0.64
1:A:3611:PRO:HD2	1:A:3614:ARG:HD3	1.79	0.64
1:D:943:LEU:HG	1:D:999:LEU:HD13	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:943:LEU:HG	1:A:999:LEU:HD13	1.80	0.64
1:D:2844:ALA:HB1	1:D:2884:ASP:HB3	1.78	0.64
1:A:1719:ARG:O	1:A:1723:ASN:HB2	1.97	0.63
1:B:3611:PRO:HD2	1:B:3614:ARG:HD3	1.79	0.63
1:C:1257:GLN:HA	1:C:1384:LEU:HD23	1.81	0.63
1:D:1793:ILE:HG12	1:D:1843:ILE:HD11	1.79	0.63
1:D:3727:GLN:OE1	1:D:3769:ASN:ND2	2.31	0.63
1:C:1688:TYR:HA	1:C:1691:GLU:HG2	1.79	0.63
1:C:4840:ILE:HD12	1:C:4843:ILE:HD11	1.78	0.63
1:D:3611:PRO:HD2	1:D:3614:ARG:HD3	1.79	0.63
1:A:644:LEU:HD13	1:A:1631:LEU:HD21	1.81	0.63
1:A:1793:ILE:HG12	1:A:1843:ILE:HD11	1.79	0.63
1:C:943:LEU:HG	1:C:999:LEU:HD13	1.80	0.63
1:D:644:LEU:HD13	1:D:1631:LEU:HD21	1.81	0.63
1:A:1688:TYR:HA	1:A:1691:GLU:HG2	1.79	0.63
1:D:3613:HIS:O	1:D:3617:ASN:ND2	2.32	0.63
1:B:2485:HIS:O	1:B:2489:VAL:HG22	1.99	0.63
1:C:3613:HIS:O	1:C:3617:ASN:ND2	2.32	0.63
1:B:590:LYS:H	1:B:593:HIS:HD2	1.44	0.63
1:C:4624:ASP:O	1:C:4628:GLN:NE2	2.32	0.63
1:D:1257:GLN:HA	1:D:1384:LEU:HD23	1.81	0.63
1:D:2485:HIS:O	1:D:2489:VAL:HG22	1.99	0.63
2:J:28:THR:HA	2:J:39:SER:HA	1.79	0.63
1:A:3727:GLN:OE1	1:A:3769:ASN:ND2	2.31	0.63
1:A:2414:GLU:OE1	1:A:2414:GLU:N	2.32	0.63
1:B:2414:GLU:OE1	1:B:2414:GLU:N	2.32	0.63
1:B:4624:ASP:O	1:B:4628:GLN:NE2	2.32	0.63
1:D:1166:VAL:HG22	1:D:1173:MET:HG2	1.80	0.63
1:B:207:PHE:CE1	1:C:2324:ILE:HD12	2.34	0.62
1:B:2442:PRO:HG2	1:B:2506:LEU:HD21	1.81	0.62
1:B:1257:GLN:HA	1:B:1384:LEU:HD23	1.81	0.62
1:C:4042:ILE:HG22	1:C:4044:LYS:H	1.64	0.62
1:D:4624:ASP:O	1:D:4628:GLN:NE2	2.32	0.62
1:A:2485:HIS:O	1:A:2489:VAL:HG22	1.99	0.62
1:B:1166:VAL:HG22	1:B:1173:MET:HG2	1.81	0.62
1:C:2414:GLU:N	1:C:2414:GLU:OE1	2.32	0.62
1:B:943:LEU:HG	1:B:999:LEU:HD13	1.80	0.62
1:C:2485:HIS:O	1:C:2489:VAL:HG22	1.99	0.62
2:J:11:GLY:O	2:J:68:SER:OG	2.18	0.62
1:B:1663:SER:OG	1:B:1709:ASP:OD2	2.17	0.62
1:C:1789:LYS:HG3	1:C:1835:PHE:HE1	1.65	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2442:PRO:HG2	1:D:2506:LEU:HD21	1.81	0.62
1:B:4042:ILE:HG22	1:B:4044:LYS:H	1.64	0.62
1:A:2442:PRO:HG2	1:A:2506:LEU:HD21	1.82	0.62
1:A:4624:ASP:O	1:A:4628:GLN:NE2	2.32	0.62
1:A:1257:GLN:HA	1:A:1384:LEU:HD23	1.81	0.62
1:B:644:LEU:HD13	1:B:1631:LEU:HD21	1.81	0.62
1:B:1688:TYR:HA	1:B:1691:GLU:HG2	1.79	0.62
1:D:2414:GLU:OE1	1:D:2414:GLU:N	2.32	0.62
1:A:276:ARG:NE	1:A:278:GLU:OE2	2.31	0.62
1:A:1663:SER:OG	1:A:1709:ASP:OD2	2.17	0.62
1:A:4660:TYR:HB3	1:A:4664:ARG:HH21	1.65	0.62
1:C:676:GLU:HB2	1:C:803:LEU:HB2	1.81	0.62
1:C:2442:PRO:HG2	1:C:2506:LEU:HD21	1.81	0.62
1:B:4660:TYR:HB3	1:B:4664:ARG:HH21	1.65	0.61
1:A:35:LEU:HD13	1:A:49:LEU:HD13	1.82	0.61
1:B:676:GLU:HB2	1:B:803:LEU:HB2	1.81	0.61
1:C:644:LEU:HD13	1:C:1631:LEU:HD21	1.81	0.61
1:C:1294:ASN:ND2	1:C:1296:ASN:O	2.33	0.61
1:D:258:ARG:NH1	1:D:316:LEU:O	2.33	0.61
1:D:1789:LYS:HG3	1:D:1835:PHE:HE1	1.65	0.61
2:G:11:GLY:O	2:G:68:SER:OG	2.18	0.61
1:B:732:LEU:HD23	1:B:779:PHE:CZ	2.35	0.61
1:D:35:LEU:HD13	1:D:49:LEU:HD13	1.82	0.61
1:A:4042:ILE:HG22	1:A:4044:LYS:H	1.64	0.61
1:B:1839:ASP:O	1:B:1843:ILE:HG12	2.01	0.61
1:C:1166:VAL:HG22	1:C:1173:MET:HG2	1.81	0.61
1:D:1839:ASP:O	1:D:1843:ILE:HG12	2.01	0.61
1:D:4042:ILE:HG22	1:D:4044:LYS:H	1.65	0.61
1:D:4842:ARG:NH1	1:D:4846:ASP:OD2	2.34	0.61
1:A:671:LYS:HA	1:A:761:LEU:HD12	1.82	0.61
1:A:1166:VAL:HG22	1:A:1173:MET:HG2	1.81	0.61
1:A:732:LEU:HD23	1:A:779:PHE:CZ	2.35	0.61
1:C:4779:LEU:O	1:C:4783:VAL:HG23	2.01	0.61
1:D:676:GLU:HB2	1:D:803:LEU:HB2	1.81	0.61
1:A:601:LEU:HB2	1:A:610:VAL:HG11	1.83	0.61
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.82	0.61
1:B:258:ARG:NH1	1:B:316:LEU:O	2.33	0.61
1:B:1095:ALA:HB1	1:B:1200:GLY:HA3	1.82	0.61
1:C:732:LEU:HD23	1:C:779:PHE:CZ	2.35	0.61
1:C:1741:PRO:HB3	1:C:1746:LYS:HE3	1.83	0.61
1:C:3727:GLN:OE1	1:C:3769:ASN:ND2	2.31	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1095:ALA:HB1	1:D:1200:GLY:HA3	1.82	0.61
1:D:2880:GLU:HA	1:D:2883:LYS:HB2	1.83	0.61
1:A:4842:ARG:NH1	1:A:4846:ASP:OD2	2.34	0.61
1:B:601:LEU:HB2	1:B:610:VAL:HG11	1.83	0.61
1:B:1789:LYS:HG3	1:B:1835:PHE:HE1	1.65	0.61
2:I:11:GLY:O	2:I:68:SER:OG	2.18	0.61
1:D:601:LEU:HB2	1:D:610:VAL:HG11	1.83	0.61
1:D:732:LEU:HD23	1:D:779:PHE:CZ	2.35	0.61
1:D:1294:ASN:ND2	1:D:1296:ASN:O	2.33	0.61
1:D:4779:LEU:O	1:D:4783:VAL:HG23	2.01	0.61
1:A:1839:ASP:O	1:A:1843:ILE:HG12	2.01	0.61
1:B:247:VAL:O	1:B:272:ARG:NH1	2.34	0.61
1:B:4772:LEU:O	1:B:4776:VAL:HG22	2.01	0.61
2:H:11:GLY:O	2:H:68:SER:OG	2.18	0.61
1:A:62:LEU:HA	1:A:65:CYS:HB2	1.82	0.61
1:A:676:GLU:HB2	1:A:803:LEU:HB2	1.81	0.61
1:A:4779:LEU:O	1:A:4783:VAL:HG23	2.01	0.61
1:B:2880:GLU:HA	1:B:2883:LYS:HB2	1.83	0.61
1:B:4018:MET:HB3	1:B:4065:LEU:HD21	1.83	0.61
1:C:1663:SER:OG	1:C:1709:ASP:OD2	2.17	0.61
1:C:4660:TYR:HB3	1:C:4664:ARG:HH21	1.65	0.61
1:D:1663:SER:OG	1:D:1709:ASP:OD2	2.17	0.61
1:D:1741:PRO:HB3	1:D:1746:LYS:HE3	1.83	0.61
1:A:1741:PRO:HB3	1:A:1746:LYS:HE3	1.83	0.60
1:A:4772:LEU:O	1:A:4776:VAL:HG22	2.01	0.60
1:D:4660:TYR:HB3	1:D:4664:ARG:HH21	1.65	0.60
1:D:4772:LEU:O	1:D:4776:VAL:HG22	2.01	0.60
1:B:2003:MET:HB3	1:B:2008:ILE:HD11	1.83	0.60
1:B:3613:HIS:O	1:B:3617:ASN:ND2	2.32	0.60
1:C:247:VAL:O	1:C:272:ARG:NH1	2.34	0.60
1:C:258:ARG:NH1	1:C:316:LEU:O	2.33	0.60
1:C:276:ARG:NE	1:C:278:GLU:OE2	2.31	0.60
1:C:601:LEU:HB2	1:C:610:VAL:HG11	1.83	0.60
1:C:2385:ASN:O	1:C:2389:THR:HG22	2.01	0.60
1:A:258:ARG:NH1	1:A:316:LEU:O	2.33	0.60
1:A:2003:MET:HB3	1:A:2008:ILE:HD11	1.83	0.60
1:A:4018:MET:HB3	1:A:4065:LEU:HD21	1.83	0.60
1:B:4779:LEU:O	1:B:4783:VAL:HG23	2.01	0.60
1:D:247:VAL:O	1:D:272:ARG:NH1	2.34	0.60
1:D:276:ARG:NE	1:D:278:GLU:OE2	2.31	0.60
1:A:1294:ASN:ND2	1:A:1296:ASN:O	2.33	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2385:ASN:O	1:A:2389:THR:HG22	2.01	0.60
1:B:4046:ASP:HA	1:B:4049:LYS:HG2	1.84	0.60
1:C:671:LYS:HA	1:C:761:LEU:HD12	1.82	0.60
1:C:3891:TYR:OH	1:C:3898:ASP:OD2	2.19	0.60
1:C:4046:ASP:HA	1:C:4049:LYS:HG2	1.84	0.60
1:B:62:LEU:HA	1:B:65:CYS:HB2	1.82	0.60
1:D:3891:TYR:OH	1:D:3898:ASP:OD2	2.19	0.60
1:A:1095:ALA:HB1	1:A:1200:GLY:HA3	1.82	0.60
1:B:671:LYS:HA	1:B:761:LEU:HD12	1.83	0.60
1:C:1839:ASP:O	1:C:1843:ILE:HG12	2.01	0.60
1:C:1962:ARG:O	1:C:1966:SER:OG	2.20	0.60
1:B:3727:GLN:OE1	1:B:3769:ASN:ND2	2.31	0.60
1:C:35:LEU:HD13	1:C:49:LEU:HD13	1.82	0.60
1:C:62:LEU:HA	1:C:65:CYS:HB2	1.82	0.60
1:C:1095:ALA:HB1	1:C:1200:GLY:HA3	1.82	0.60
1:C:4842:ARG:NH1	1:C:4846:ASP:OD2	2.34	0.60
1:D:4046:ASP:HA	1:D:4049:LYS:HG2	1.84	0.60
1:A:262:TYR:HB2	1:A:389:ARG:HG3	1.84	0.60
1:A:708:GLY:O	1:A:838:ARG:NH1	2.35	0.60
1:A:1789:LYS:HG3	1:A:1835:PHE:HE1	1.65	0.60
1:A:2880:GLU:HA	1:A:2883:LYS:HB2	1.83	0.60
1:B:1294:ASN:ND2	1:B:1296:ASN:O	2.33	0.60
1:C:262:TYR:HB2	1:C:389:ARG:HG3	1.84	0.60
1:C:2880:GLU:HA	1:C:2883:LYS:HB2	1.83	0.60
1:D:671:LYS:HA	1:D:761:LEU:HD12	1.82	0.60
1:D:1962:ARG:O	1:D:1966:SER:OG	2.20	0.60
1:A:1962:ARG:O	1:A:1966:SER:OG	2.20	0.60
1:C:4111:ASP:O	1:C:4115:GLN:N	2.35	0.60
1:A:247:VAL:O	1:A:272:ARG:NH1	2.34	0.60
1:B:708:GLY:O	1:B:838:ARG:NH1	2.35	0.60
1:B:1741:PRO:HB3	1:B:1746:LYS:HE3	1.83	0.60
1:B:4842:ARG:NH1	1:B:4846:ASP:OD2	2.34	0.59
1:C:2003:MET:HB3	1:C:2008:ILE:HD11	1.83	0.59
1:D:2385:ASN:O	1:D:2389:THR:HG22	2.01	0.59
1:D:4111:ASP:O	1:D:4115:GLN:N	2.35	0.59
1:A:4046:ASP:HA	1:A:4049:LYS:HG2	1.84	0.59
1:B:262:TYR:HB2	1:B:389:ARG:HG3	1.84	0.59
1:B:1609:VAL:HA	1:B:1620:VAL:HA	1.84	0.59
1:B:2385:ASN:O	1:B:2389:THR:HG22	2.01	0.59
1:D:62:LEU:HA	1:D:65:CYS:HB2	1.82	0.59
1:D:360:ILE:HG23	1:D:402:GLY:HA2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:32:GLN:NE2	2:H:97:THR:OG1	2.35	0.59
1:C:360:ILE:HG23	1:C:402:GLY:HA2	1.84	0.59
1:C:4018:MET:HB3	1:C:4065:LEU:HD21	1.83	0.59
1:C:4772:LEU:O	1:C:4776:VAL:HG22	2.01	0.59
1:D:708:GLY:O	1:D:838:ARG:NH1	2.35	0.59
1:A:890:HIS:O	1:A:894:VAL:HG22	2.03	0.59
1:C:708:GLY:O	1:C:838:ARG:NH1	2.35	0.59
1:D:28:ILE:HG12	1:D:29:HIS:ND1	2.17	0.59
1:D:2003:MET:HB3	1:D:2008:ILE:HD11	1.83	0.59
1:D:2732:SER:HA	1:D:2735:LYS:HD2	1.84	0.59
2:J:32:GLN:NE2	2:J:97:THR:OG1	2.36	0.59
1:A:3613:HIS:O	1:A:3617:ASN:ND2	2.32	0.59
1:A:4813:MET:HG3	1:D:4843:ILE:HD13	1.84	0.59
1:B:28:ILE:HG12	1:B:29:HIS:ND1	2.17	0.59
1:B:4111:ASP:O	1:B:4115:GLN:N	2.35	0.59
1:C:1144:ARG:NH1	1:C:1191:ALA:O	2.36	0.59
1:A:1144:ARG:NH1	1:A:1191:ALA:O	2.36	0.59
1:A:1684:PRO:HD3	2:G:42:ASP:HB3	1.84	0.59
1:B:1962:ARG:O	1:B:1966:SER:OG	2.20	0.59
2:I:32:GLN:NE2	2:I:97:THR:OG1	2.35	0.59
1:D:262:TYR:HB2	1:D:389:ARG:HG3	1.84	0.59
1:D:2261:LEU:O	1:D:2265:VAL:HG22	2.03	0.59
1:D:4018:MET:HB3	1:D:4065:LEU:HD21	1.83	0.59
1:B:123:HIS:HD2	1:B:126:SER:H	1.51	0.59
1:B:3891:TYR:OH	1:B:3898:ASP:OD2	2.19	0.59
1:D:1144:ARG:NH1	1:D:1191:ALA:O	2.36	0.59
1:A:946:LEU:HD13	1:A:995:MET:HG2	1.85	0.59
1:A:2732:SER:HA	1:A:2735:LYS:HD2	1.84	0.59
1:B:946:LEU:HD13	1:B:995:MET:HG2	1.85	0.59
1:B:1607:VAL:HG23	1:B:1622:CYS:HB2	1.85	0.59
1:B:2413:GLY:HA2	1:B:2416:ILE:HD12	1.85	0.59
1:B:2732:SER:HA	1:B:2735:LYS:HD2	1.84	0.59
1:C:890:HIS:O	1:C:894:VAL:HG22	2.03	0.59
1:D:881:ILE:O	1:D:884:ARG:HG3	2.03	0.59
1:D:4633:VAL:HG12	1:D:4703:LYS:HG2	1.85	0.59
2:G:32:GLN:NE2	2:G:97:THR:OG1	2.35	0.58
1:B:1144:ARG:NH1	1:B:1191:ALA:O	2.36	0.58
1:C:28:ILE:HG12	1:C:29:HIS:ND1	2.17	0.58
1:C:4633:VAL:HG12	1:C:4703:LYS:HG2	1.85	0.58
1:D:1607:VAL:HG23	1:D:1622:CYS:HB2	1.85	0.58
1:A:881:ILE:O	1:A:884:ARG:HG3	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4111:ASP:O	1:A:4115:GLN:N	2.35	0.58
1:C:946:LEU:HD13	1:C:995:MET:HG2	1.85	0.58
1:C:2413:GLY:HA2	1:C:2416:ILE:HD12	1.85	0.58
1:D:946:LEU:HD13	1:D:995:MET:HG2	1.85	0.58
1:D:2314:GLU:O	1:D:2318:VAL:HG22	2.03	0.58
1:A:4478:PHE:HA	1:A:4481:LYS:HE2	1.84	0.58
1:B:360:ILE:HG23	1:B:402:GLY:HA2	1.84	0.58
1:C:4797:ASP:OD1	1:C:4797:ASP:N	2.36	0.58
1:D:1989:GLU:HG2	1:D:1992:ARG:HD3	1.85	0.58
1:D:4478:PHE:HA	1:D:4481:LYS:HE2	1.84	0.58
1:A:123:HIS:HD2	1:A:126:SER:H	1.51	0.58
1:A:360:ILE:HG23	1:A:402:GLY:HA2	1.84	0.58
1:A:2261:LEU:O	1:A:2265:VAL:HG22	2.03	0.58
1:A:2314:GLU:O	1:A:2318:VAL:HG22	2.03	0.58
1:A:2413:GLY:HA2	1:A:2416:ILE:HD12	1.85	0.58
1:B:890:HIS:O	1:B:894:VAL:HG22	2.03	0.58
1:B:2314:GLU:O	1:B:2318:VAL:HG22	2.03	0.58
1:C:2732:SER:HA	1:C:2735:LYS:HD2	1.84	0.58
1:A:1607:VAL:HG23	1:A:1622:CYS:HB2	1.85	0.58
1:B:2261:LEU:O	1:B:2265:VAL:HG22	2.03	0.58
1:B:2348:GLU:O	1:B:2352:ILE:HG13	2.04	0.58
1:C:332:ARG:NH1	1:C:364:GLN:OE1	2.37	0.58
1:C:881:ILE:O	1:C:884:ARG:HG3	2.03	0.58
1:C:2261:LEU:O	1:C:2265:VAL:HG22	2.03	0.58
1:D:890:HIS:O	1:D:894:VAL:HG22	2.03	0.58
1:A:28:ILE:HG12	1:A:29:HIS:ND1	2.17	0.58
1:B:4633:VAL:HG12	1:B:4703:LYS:HG2	1.85	0.58
1:B:881:ILE:O	1:B:884:ARG:HG3	2.03	0.58
1:C:2314:GLU:O	1:C:2318:VAL:HG22	2.04	0.58
1:D:1723:ASN:O	1:D:1918:ARG:NH2	2.36	0.58
1:D:3909:ILE:HG21	1:D:3969:GLU:HB3	1.86	0.58
1:A:671:LYS:HB3	1:A:761:LEU:HB2	1.86	0.58
1:A:1609:VAL:HA	1:A:1620:VAL:HA	1.84	0.58
1:A:1723:ASN:O	1:A:1918:ARG:NH2	2.36	0.58
1:A:4923:TYR:O	1:A:4927:LYS:HB2	2.03	0.58
1:C:1272:ARG:NH2	1:C:1584:PRO:O	2.37	0.58
1:C:1607:VAL:HG23	1:C:1622:CYS:HB2	1.85	0.58
1:C:1723:ASN:O	1:C:1918:ARG:NH2	2.36	0.58
1:C:2348:GLU:O	1:C:2352:ILE:HG13	2.04	0.58
1:D:2127:SER:O	1:D:2131:VAL:HG23	2.04	0.58
1:B:332:ARG:NH1	1:B:364:GLN:OE1	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4478:PHE:HA	1:B:4481:LYS:HE2	1.84	0.58
1:C:1989:GLU:HG2	1:C:1992:ARG:HD3	1.85	0.58
1:A:400:ASP:OD1	1:A:400:ASP:N	2.37	0.58
1:B:1253:LYS:HB3	1:B:1598:SER:HB2	1.86	0.58
1:B:1723:ASN:O	1:B:1918:ARG:NH2	2.36	0.58
1:B:1989:GLU:HA	1:B:1992:ARG:HD3	1.86	0.58
1:B:1989:GLU:HG2	1:B:1992:ARG:HD3	1.85	0.58
1:B:4923:TYR:O	1:B:4927:LYS:HB2	2.03	0.58
1:C:400:ASP:OD1	1:C:400:ASP:N	2.37	0.58
1:D:1609:VAL:HA	1:D:1620:VAL:HA	1.85	0.58
1:B:2127:SER:O	1:B:2131:VAL:HG23	2.04	0.57
1:C:1609:VAL:HA	1:C:1620:VAL:HA	1.84	0.57
1:C:2127:SER:O	1:C:2131:VAL:HG23	2.04	0.57
1:C:4923:TYR:O	1:C:4927:LYS:HB2	2.03	0.57
1:A:4797:ASP:OD1	1:A:4797:ASP:N	2.36	0.57
1:D:655:MET:SD	1:D:836:HIS:ND1	2.77	0.57
1:D:2413:GLY:HA2	1:D:2416:ILE:HD12	1.85	0.57
1:D:4923:TYR:O	1:D:4927:LYS:HB2	2.03	0.57
1:A:332:ARG:NH1	1:A:364:GLN:OE1	2.37	0.57
1:A:1989:GLU:HA	1:A:1992:ARG:HD3	1.86	0.57
1:A:4633:VAL:HG12	1:A:4703:LYS:HG2	1.86	0.57
1:B:276:ARG:NE	1:B:278:GLU:OE2	2.31	0.57
1:B:1272:ARG:NH2	1:B:1584:PRO:O	2.37	0.57
1:B:1684:PRO:HD3	2:H:42:ASP:HB3	1.85	0.57
1:C:1609:VAL:HG23	1:C:1610:SER:H	1.70	0.57
1:C:4478:PHE:HA	1:C:4481:LYS:HE2	1.84	0.57
1:D:1253:LYS:HB3	1:D:1598:SER:HB2	1.86	0.57
1:A:987:LYS:HD2	1:A:988:LEU:N	2.20	0.57
1:A:3891:TYR:OH	1:A:3898:ASP:OD2	2.19	0.57
1:D:332:ARG:NH1	1:D:364:GLN:OE1	2.37	0.57
1:D:671:LYS:HB3	1:D:761:LEU:HB2	1.86	0.57
1:D:1989:GLU:HA	1:D:1992:ARG:HD3	1.86	0.57
1:A:1989:GLU:HG2	1:A:1992:ARG:HD3	1.85	0.57
1:A:2145:LEU:HD23	1:A:2148:ILE:HD11	1.87	0.57
1:B:2145:LEU:HD23	1:B:2148:ILE:HD11	1.87	0.57
1:C:1929:ASP:OD1	1:C:3612:ARG:NH2	2.38	0.57
1:C:1989:GLU:HA	1:C:1992:ARG:HD3	1.86	0.57
1:C:3909:ILE:HG21	1:C:3969:GLU:HB3	1.86	0.57
1:A:1929:ASP:OD1	1:A:3612:ARG:NH2	2.38	0.57
1:B:1929:ASP:OD1	1:B:3612:ARG:NH2	2.38	0.57
1:C:671:LYS:HB3	1:C:761:LEU:HB2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1054:VAL:HA	1:C:1057:LEU:HB2	1.87	0.57
1:D:400:ASP:N	1:D:400:ASP:OD1	2.37	0.57
1:D:853:PRO:HG2	1:D:1209:VAL:HA	1.87	0.57
1:A:655:MET:SD	1:A:836:HIS:ND1	2.77	0.57
1:A:853:PRO:HG2	1:A:1209:VAL:HA	1.87	0.57
1:A:2197:ARG:HB2	1:A:2236:SER:HB3	1.86	0.57
1:A:2348:GLU:O	1:A:2352:ILE:HG13	2.04	0.57
1:B:400:ASP:N	1:B:400:ASP:OD1	2.37	0.57
1:B:1353:HIS:CE1	1:B:1367:LYS:HB3	2.40	0.57
1:C:1353:HIS:CE1	1:C:1367:LYS:HB3	2.40	0.57
1:B:3909:ILE:HG21	1:B:3969:GLU:HB3	1.86	0.57
1:B:4797:ASP:OD1	1:B:4797:ASP:N	2.36	0.57
1:C:123:HIS:HD2	1:C:126:SER:H	1.51	0.57
1:C:498:VAL:HG13	1:C:533:LEU:HD22	1.87	0.57
1:C:1253:LYS:HB3	1:C:1598:SER:HB2	1.86	0.57
1:D:123:HIS:HD2	1:D:126:SER:H	1.51	0.57
1:A:1353:HIS:CE1	1:A:1367:LYS:HB3	2.40	0.57
1:B:989:THR:HG23	1:B:992:GLN:H	1.70	0.57
1:B:1054:VAL:HA	1:B:1057:LEU:HB2	1.87	0.57
1:D:987:LYS:HD2	1:D:988:LEU:N	2.20	0.57
1:A:498:VAL:HG13	1:A:533:LEU:HD22	1.87	0.56
1:A:989:THR:HG23	1:A:992:GLN:H	1.70	0.56
1:A:1272:ARG:NH2	1:A:1584:PRO:O	2.37	0.56
1:B:655:MET:SD	1:B:836:HIS:ND1	2.77	0.56
1:C:655:MET:SD	1:C:836:HIS:ND1	2.77	0.56
1:C:987:LYS:HD2	1:C:988:LEU:N	2.20	0.56
1:D:1353:HIS:CE1	1:D:1367:LYS:HB3	2.40	0.56
1:A:1253:LYS:HB3	1:A:1598:SER:HB2	1.86	0.56
1:A:2127:SER:O	1:A:2131:VAL:HG23	2.04	0.56
1:B:498:VAL:HG13	1:B:533:LEU:HD22	1.87	0.56
1:B:4662:ARG:NH2	1:B:4675:ALA:O	2.38	0.56
1:D:989:THR:HG23	1:D:992:GLN:H	1.70	0.56
1:D:2348:GLU:O	1:D:2352:ILE:HG13	2.04	0.56
1:A:1609:VAL:HG23	1:A:1610:SER:H	1.70	0.56
1:A:2881:LYS:O	1:A:2885:ARG:HD3	2.06	0.56
1:B:671:LYS:HB3	1:B:761:LEU:HB2	1.86	0.56
1:B:987:LYS:HD2	1:B:988:LEU:N	2.20	0.56
1:B:1609:VAL:HG23	1:B:1610:SER:H	1.70	0.56
1:B:2197:ARG:HB2	1:B:2236:SER:HB3	1.86	0.56
1:C:853:PRO:HG2	1:C:1209:VAL:HA	1.87	0.56
1:C:4662:ARG:NH2	1:C:4675:ALA:O	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1929:ASP:OD1	1:D:3612:ARG:NH2	2.38	0.56
1:D:4195:THR:HB	1:D:4918:LEU:HD11	1.88	0.56
1:A:1054:VAL:HA	1:A:1057:LEU:HB2	1.87	0.56
1:A:1715:TYR:CZ	1:A:1762:MET:HB3	2.41	0.56
1:A:4026:THR:HG21	1:A:4083:VAL:HG11	1.88	0.56
1:B:4137:ILE:HG23	1:B:4950:PHE:HB2	1.88	0.56
1:C:2145:LEU:HD23	1:C:2148:ILE:HD11	1.87	0.56
1:D:4026:THR:HG21	1:D:4083:VAL:HG11	1.88	0.56
1:A:1952:MET:HA	1:A:1956:LEU:HD12	1.87	0.56
1:A:4662:ARG:NH2	1:A:4675:ALA:O	2.38	0.56
1:C:2197:ARG:HB2	1:C:2236:SER:HB3	1.86	0.56
1:C:4137:ILE:HG23	1:C:4950:PHE:HB2	1.88	0.56
1:D:1609:VAL:HG23	1:D:1610:SER:H	1.70	0.56
1:D:4662:ARG:NH2	1:D:4675:ALA:O	2.38	0.56
1:A:1789:LYS:HG3	1:A:1835:PHE:CE1	2.40	0.56
1:A:3909:ILE:HG21	1:A:3969:GLU:HB3	1.86	0.56
1:A:4195:THR:HB	1:A:4918:LEU:HD11	1.88	0.56
1:D:1715:TYR:CZ	1:D:1762:MET:HB3	2.41	0.56
1:C:1060:TYR:N	1:C:1060:TYR:CD1	2.74	0.56
1:D:1054:VAL:HA	1:D:1057:LEU:HB2	1.87	0.56
1:D:2145:LEU:HD23	1:D:2148:ILE:HD11	1.87	0.56
1:B:853:PRO:HG2	1:B:1209:VAL:HA	1.87	0.56
1:B:2881:LYS:O	1:B:2885:ARG:HD3	2.06	0.56
1:B:4195:THR:HB	1:B:4918:LEU:HD11	1.88	0.56
1:D:1952:MET:HA	1:D:1956:LEU:HD12	1.86	0.56
1:B:748:LEU:HD23	2:H:8:ILE:HG23	1.88	0.56
1:B:1060:TYR:N	1:B:1060:TYR:CD1	2.74	0.56
1:C:3974:GLN:HE22	1:C:4012:ILE:HG21	1.71	0.56
1:C:4195:THR:HB	1:C:4918:LEU:HD11	1.88	0.56
1:D:503:ASP:HA	1:D:561:ARG:HH12	1.71	0.56
1:B:226:GLY:O	1:B:356:TYR:N	2.35	0.56
1:B:3864:ASN:OD1	1:B:3865:THR:N	2.39	0.56
1:B:3974:GLN:HE22	1:B:4012:ILE:HG21	1.71	0.56
1:C:503:ASP:HA	1:C:561:ARG:HH12	1.71	0.56
1:A:857:LEU:HB3	1:A:859:GLN:HG3	1.88	0.55
1:A:1810:PRO:HB3	1:A:1818:LEU:HD22	1.88	0.55
1:B:857:LEU:HB3	1:B:859:GLN:HG3	1.88	0.55
1:B:1715:TYR:CZ	1:B:1762:MET:HB3	2.41	0.55
1:B:1789:LYS:HG3	1:B:1835:PHE:CE1	2.40	0.55
1:D:694:ARG:HG2	1:D:728:ASP:HB3	1.88	0.55
1:D:1272:ARG:NH2	1:D:1584:PRO:O	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:989:THR:HG23	1:C:992:GLN:H	1.70	0.55
1:C:2723:TYR:O	1:C:2727:SER:OG	2.23	0.55
1:D:411:GLU:O	1:D:415:THR:OG1	2.25	0.55
1:D:878:LEU:HG	1:D:881:ILE:HB	1.88	0.55
1:D:1060:TYR:N	1:D:1060:TYR:CD1	2.74	0.55
1:A:1708:ILE:HD12	1:A:1828:THR:HG21	1.89	0.55
1:B:207:PHE:CZ	1:C:2324:ILE:HD12	2.41	0.55
1:B:1631:LEU:HD22	1:B:1645:LEU:HD11	1.89	0.55
1:C:857:LEU:HB3	1:C:859:GLN:HG3	1.88	0.55
1:C:878:LEU:HG	1:C:881:ILE:HB	1.88	0.55
1:C:1715:TYR:CZ	1:C:1762:MET:HB3	2.41	0.55
1:D:498:VAL:HG13	1:D:533:LEU:HD22	1.87	0.55
1:D:2881:LYS:O	1:D:2885:ARG:HD3	2.06	0.55
1:B:411:GLU:O	1:B:415:THR:OG1	2.25	0.55
1:B:1810:PRO:HB3	1:B:1818:LEU:HD22	1.88	0.55
1:D:857:LEU:HB3	1:D:859:GLN:HG3	1.88	0.55
1:D:2197:ARG:HB2	1:D:2236:SER:HB3	1.86	0.55
1:A:4862:GLN:HG3	1:D:4855:VAL:O	2.06	0.55
1:B:878:LEU:HG	1:B:881:ILE:HB	1.88	0.55
1:D:119:ILE:N	1:D:160:TRP:O	2.39	0.55
1:D:1972:ILE:HA	1:D:1975:LEU:HG	1.89	0.55
1:D:2723:TYR:O	1:D:2727:SER:OG	2.23	0.55
1:D:3840:ARG:HH21	1:D:3844:LEU:HD21	1.72	0.55
1:D:3864:ASN:OD1	1:D:3865:THR:N	2.39	0.55
1:A:411:GLU:O	1:A:415:THR:OG1	2.25	0.55
1:A:1631:LEU:HD22	1:A:1645:LEU:HD11	1.89	0.55
1:A:1956:LEU:O	1:A:1960:LYS:HG2	2.07	0.55
1:B:503:ASP:HA	1:B:561:ARG:HH12	1.71	0.55
1:B:1118:SER:HB3	1:B:1204:VAL:HG11	1.89	0.55
1:B:1952:MET:HA	1:B:1956:LEU:HD12	1.87	0.55
1:C:2881:LYS:O	1:C:2885:ARG:HD3	2.06	0.55
1:D:1789:LYS:HG3	1:D:1835:PHE:CE1	2.40	0.55
1:A:119:ILE:N	1:A:160:TRP:O	2.39	0.55
1:A:902:TRP:HE3	1:A:915:HIS:HB2	1.72	0.55
1:A:1060:TYR:N	1:A:1060:TYR:CD1	2.74	0.55
1:A:2723:TYR:O	1:A:2727:SER:OG	2.23	0.55
1:A:4137:ILE:HG23	1:A:4950:PHE:HB2	1.88	0.55
1:B:1968:PRO:HB2	1:B:3618:LEU:HD13	1.89	0.55
1:C:119:ILE:N	1:C:160:TRP:O	2.39	0.55
1:D:1631:LEU:HD22	1:D:1645:LEU:HD11	1.89	0.55
1:D:3974:GLN:HE22	1:D:4012:ILE:HG21	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:GLY:O	1:C:356:TYR:N	2.35	0.55
1:C:694:ARG:HG2	1:C:728:ASP:HB3	1.88	0.55
1:C:902:TRP:HE3	1:C:915:HIS:HB2	1.72	0.55
1:C:1708:ILE:HD12	1:C:1828:THR:HG21	1.89	0.55
1:C:1952:MET:HA	1:C:1956:LEU:HD12	1.87	0.55
1:A:503:ASP:HA	1:A:561:ARG:HH12	1.71	0.55
1:B:4026:THR:HG21	1:B:4083:VAL:HG11	1.88	0.55
1:C:1956:LEU:O	1:C:1960:LYS:HG2	2.07	0.55
1:D:1118:SER:HB3	1:D:1204:VAL:HG11	1.89	0.55
1:D:1176:THR:HG22	1:D:1181:ILE:HG12	1.89	0.55
1:D:1265:HIS:HD2	1:D:1268:ILE:HB	1.72	0.55
1:D:2099:ARG:O	1:D:2103:LYS:NZ	2.36	0.55
1:A:1176:THR:HG22	1:A:1181:ILE:HG12	1.89	0.55
1:D:4797:ASP:OD1	1:D:4797:ASP:N	2.36	0.55
1:A:878:LEU:HG	1:A:881:ILE:HB	1.89	0.54
1:A:1118:SER:HB3	1:A:1204:VAL:HG11	1.89	0.54
1:A:3860:GLN:HE22	1:A:3867:VAL:H	1.55	0.54
1:B:3840:ARG:HH21	1:B:3844:LEU:HD21	1.72	0.54
1:C:1030:PRO:O	1:C:1033:VAL:HG12	2.07	0.54
1:C:1176:THR:HG22	1:C:1181:ILE:HG12	1.89	0.54
1:C:1789:LYS:HG3	1:C:1835:PHE:CE1	2.40	0.54
1:C:1986:PRO:HB2	1:C:1988:PRO:HD2	1.89	0.54
1:D:1221:VAL:HA	1:D:1224:LEU:HB2	1.89	0.54
1:D:1683:GLU:HB3	2:J:42:ASP:HB3	1.88	0.54
1:D:1956:LEU:O	1:D:1960:LYS:HG2	2.07	0.54
1:D:2851:TRP:CZ3	1:D:2855:LYS:HG2	2.42	0.54
1:D:3860:GLN:HE22	1:D:3867:VAL:H	1.55	0.54
1:B:188:SER:HB3	1:B:190:ARG:HD2	1.89	0.54
1:B:694:ARG:HG2	1:B:728:ASP:HB3	1.88	0.54
1:C:1118:SER:HB3	1:C:1204:VAL:HG11	1.89	0.54
1:C:1631:LEU:HD22	1:C:1645:LEU:HD11	1.89	0.54
1:C:1968:PRO:HB2	1:C:3618:LEU:HD13	1.89	0.54
1:C:2858:GLU:O	1:C:2862:LYS:HG2	2.08	0.54
1:C:4026:THR:HG21	1:C:4083:VAL:HG11	1.88	0.54
1:A:992:GLN:HE22	1:A:1058:LEU:HD13	1.73	0.54
1:A:1030:PRO:O	1:A:1033:VAL:HG12	2.07	0.54
1:A:1682:ASP:HB3	1:A:1684:PRO:HD2	1.89	0.54
1:B:756:SER:OG	1:B:769:ARG:HB2	2.08	0.54
1:C:4859:ALA:HB1	1:D:4866:ILE:HD11	1.88	0.54
1:D:756:SER:OG	1:D:769:ARG:HB2	2.07	0.54
1:D:3975:LYS:HB2	1:D:4093:ILE:HG13	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4137:ILE:HG23	1:D:4950:PHE:HB2	1.88	0.54
1:A:1968:PRO:HB2	1:A:3618:LEU:HD13	1.89	0.54
1:C:1810:PRO:HB3	1:C:1818:LEU:HD22	1.88	0.54
1:C:3864:ASN:OD1	1:C:3865:THR:N	2.39	0.54
1:D:992:GLN:HE22	1:D:1058:LEU:HD13	1.73	0.54
1:A:756:SER:OG	1:A:769:ARG:HB2	2.07	0.54
1:A:2851:TRP:CZ3	1:A:2855:LYS:HG2	2.43	0.54
1:A:2858:GLU:O	1:A:2862:LYS:HG2	2.08	0.54
1:A:3840:ARG:HH21	1:A:3844:LEU:HD21	1.72	0.54
1:B:1708:ILE:HD12	1:B:1828:THR:HG21	1.89	0.54
1:D:1091:GLU:OE1	1:D:1093:THR:OG1	2.25	0.54
1:D:1810:PRO:HB3	1:D:1818:LEU:HD22	1.88	0.54
1:D:1968:PRO:HB2	1:D:3618:LEU:HD13	1.89	0.54
1:D:2738:ASN:N	1:D:2738:ASN:OD1	2.41	0.54
1:A:1265:HIS:HD2	1:A:1268:ILE:HB	1.72	0.54
1:A:1972:ILE:HA	1:A:1975:LEU:HG	1.89	0.54
1:A:1986:PRO:HB2	1:A:1988:PRO:HD2	1.89	0.54
1:B:988:LEU:HD22	1:B:1055:ARG:HG2	1.90	0.54
1:B:1176:THR:HG22	1:B:1181:ILE:HG12	1.89	0.54
1:D:678:MET:HG3	1:D:801:ARG:HB3	1.90	0.54
1:D:988:LEU:HD22	1:D:1055:ARG:HG2	1.90	0.54
1:D:1030:PRO:O	1:D:1033:VAL:HG12	2.07	0.54
1:A:694:ARG:HG2	1:A:728:ASP:HB3	1.88	0.54
1:A:3974:GLN:HE22	1:A:4012:ILE:HG21	1.71	0.54
1:B:1956:LEU:O	1:B:1960:LYS:HG2	2.07	0.54
1:C:1982:LYS:NZ	1:C:1983:SER:O	2.29	0.54
1:D:1682:ASP:HB3	1:D:1684:PRO:HD2	1.89	0.54
1:A:226:GLY:O	1:A:356:TYR:N	2.35	0.54
1:A:1221:VAL:HA	1:A:1224:LEU:HB2	1.90	0.54
1:A:1829:LEU:HB3	1:A:1834:ILE:HD11	1.90	0.54
1:A:3975:LYS:HB2	1:A:4093:ILE:HG13	1.89	0.54
1:B:902:TRP:HE3	1:B:915:HIS:HB2	1.72	0.54
1:B:992:GLN:HE22	1:B:1058:LEU:HD13	1.73	0.54
1:B:1030:PRO:O	1:B:1033:VAL:HG12	2.07	0.54
1:B:1972:ILE:HA	1:B:1975:LEU:HG	1.89	0.54
1:B:2851:TRP:CZ3	1:B:2855:LYS:HG2	2.42	0.54
1:C:2851:TRP:CZ3	1:C:2855:LYS:HG2	2.42	0.54
1:D:1708:ILE:HD12	1:D:1828:THR:HG21	1.89	0.54
1:B:55:SER:O	1:B:296:ARG:NH2	2.34	0.54
1:B:1682:ASP:HB3	1:B:1684:PRO:HD2	1.89	0.54
1:B:1986:PRO:HB2	1:B:1988:PRO:HD2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:TYR:HE1	1:C:414:ARG:HA	1.73	0.54
1:D:1608:ASP:HB2	1:D:1611:ARG:HD3	1.90	0.54
1:A:988:LEU:HD22	1:A:1055:ARG:HG2	1.90	0.54
1:A:1608:ASP:HB2	1:A:1611:ARG:HD3	1.90	0.54
1:A:4106:GLU:OE2	1:A:4148:TYR:OH	2.19	0.54
1:B:1265:HIS:HD2	1:B:1268:ILE:HB	1.72	0.54
1:C:678:MET:HG3	1:C:801:ARG:HB3	1.90	0.54
1:C:1265:HIS:HD2	1:C:1268:ILE:HB	1.72	0.54
1:C:2257:ARG:NH1	1:C:3806:ALA:HB2	2.24	0.54
1:D:188:SER:HB3	1:D:190:ARG:HD2	1.89	0.54
1:D:970:TYR:CE2	1:D:977:LYS:HG2	2.43	0.54
1:D:2858:GLU:O	1:D:2862:LYS:HG2	2.08	0.54
1:A:188:SER:HB3	1:A:190:ARG:HD2	1.89	0.53
1:B:2723:TYR:O	1:B:2727:SER:OG	2.23	0.53
1:B:2858:GLU:O	1:B:2862:LYS:HG2	2.08	0.53
1:C:1221:VAL:HA	1:C:1224:LEU:HB2	1.90	0.53
1:C:2738:ASN:N	1:C:2738:ASN:OD1	2.41	0.53
1:C:3860:GLN:HE22	1:C:3867:VAL:H	1.55	0.53
1:A:363:ILE:HD11	1:A:372:LEU:HB3	1.90	0.53
1:A:2099:ARG:O	1:A:2103:LYS:NZ	2.36	0.53
1:A:2257:ARG:NH1	1:A:3806:ALA:HB2	2.23	0.53
1:A:3864:ASN:OD1	1:A:3865:THR:N	2.39	0.53
1:B:2738:ASN:OD1	1:B:2738:ASN:N	2.41	0.53
1:B:3860:GLN:HE22	1:B:3867:VAL:H	1.55	0.53
1:C:188:SER:HB3	1:C:190:ARG:HD2	1.89	0.53
1:C:1012:ILE:HG13	1:C:1013:ARG:HD2	1.90	0.53
1:D:902:TRP:HE3	1:D:915:HIS:HB2	1.72	0.53
1:A:2738:ASN:N	1:A:2738:ASN:OD1	2.41	0.53
1:B:1829:LEU:HB3	1:B:1834:ILE:HD11	1.90	0.53
1:B:2099:ARG:O	1:B:2103:LYS:NZ	2.36	0.53
1:B:4731:GLY:HA2	1:B:4737:PHE:HB2	1.91	0.53
1:C:411:GLU:O	1:C:415:THR:OG1	2.25	0.53
1:C:756:SER:OG	1:C:769:ARG:HB2	2.07	0.53
1:C:1682:ASP:HB3	1:C:1684:PRO:HD2	1.89	0.53
1:C:3840:ARG:HH21	1:C:3844:LEU:HD21	1.72	0.53
1:D:125:TYR:HE1	1:D:414:ARG:HA	1.73	0.53
1:A:748:LEU:HD23	2:G:8:ILE:HG23	1.89	0.53
1:A:2107:ILE:HG13	1:A:2108:ASN:H	1.74	0.53
1:B:125:TYR:HE1	1:B:414:ARG:HA	1.73	0.53
1:A:1012:ILE:HG13	1:A:1013:ARG:HD2	1.90	0.53
1:D:78:LEU:HD11	1:D:159:TRP:CG	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:878:LEU:HD23	1:D:882:ARG:HG3	1.91	0.53
1:A:125:TYR:HE1	1:A:414:ARG:HA	1.73	0.53
1:A:4731:GLY:HA2	1:A:4737:PHE:HB2	1.91	0.53
1:C:653:SER:O	1:C:793:SER:HA	2.09	0.53
1:C:1972:ILE:HA	1:C:1975:LEU:HG	1.89	0.53
1:D:653:SER:O	1:D:793:SER:HA	2.09	0.53
1:B:119:ILE:N	1:B:160:TRP:O	2.39	0.53
1:C:363:ILE:HD11	1:C:372:LEU:HB3	1.90	0.53
1:C:988:LEU:HD22	1:C:1055:ARG:HG2	1.90	0.53
1:C:3975:LYS:HB2	1:C:4093:ILE:HG13	1.89	0.53
1:D:1709:ASP:HA	1:D:1713:SER:HB3	1.91	0.53
1:D:2107:ILE:HG13	1:D:2108:ASN:H	1.74	0.53
2:J:43:ARG:HG3	2:J:45:LYS:HG2	1.91	0.53
1:A:653:SER:O	1:A:793:SER:HA	2.09	0.53
1:B:363:ILE:HD11	1:B:372:LEU:HB3	1.90	0.53
1:B:2257:ARG:NH1	1:B:3806:ALA:HB2	2.24	0.53
1:B:4042:ILE:H	1:B:4076:THR:HG23	1.74	0.53
1:C:992:GLN:HE22	1:C:1058:LEU:HD13	1.73	0.53
1:C:2859:LEU:HD12	1:C:2867:HIS:CE1	2.44	0.53
1:A:678:MET:HG3	1:A:801:ARG:HB3	1.90	0.53
1:B:1221:VAL:HA	1:B:1224:LEU:HB2	1.89	0.53
1:B:3975:LYS:HB2	1:B:4093:ILE:HG13	1.90	0.53
1:D:799:LYS:HG2	1:D:1621:GLN:HG3	1.91	0.53
1:D:1986:PRO:HB2	1:D:1988:PRO:HD2	1.89	0.53
1:D:2722:LYS:NZ	1:D:2726:HIS:HB2	2.24	0.53
1:A:78:LEU:HD11	1:A:159:TRP:CG	2.44	0.53
1:B:1608:ASP:HB2	1:B:1611:ARG:HD3	1.90	0.53
1:C:799:LYS:HG2	1:C:1621:GLN:HG3	1.91	0.53
1:C:878:LEU:HD23	1:C:882:ARG:HG3	1.91	0.53
1:C:4042:ILE:H	1:C:4076:THR:HG23	1.74	0.53
1:D:363:ILE:HD11	1:D:372:LEU:HB3	1.90	0.53
1:D:2257:ARG:NH1	1:D:3806:ALA:HB2	2.24	0.53
1:A:4042:ILE:H	1:A:4076:THR:HG23	1.74	0.52
1:B:878:LEU:HD23	1:B:882:ARG:HG3	1.91	0.52
1:B:2859:LEU:HD12	1:B:2867:HIS:CE1	2.44	0.52
1:C:763:ALA:HB3	1:C:764:PRO:HD3	1.91	0.52
1:C:1091:GLU:OE1	1:C:1093:THR:OG1	2.25	0.52
1:C:1608:ASP:HB2	1:C:1611:ARG:HD3	1.90	0.52
2:I:8:ILE:HD11	2:I:74:LYS:HB2	1.91	0.52
1:D:226:GLY:O	1:D:356:TYR:N	2.35	0.52
1:D:763:ALA:HB3	1:D:764:PRO:HD3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4042:ILE:H	1:D:4076:THR:HG23	1.74	0.52
1:B:1012:ILE:HG13	1:B:1013:ARG:HD2	1.90	0.52
1:B:2084:PHE:O	1:B:3690:TYR:OH	2.25	0.52
2:H:43:ARG:HG3	2:H:45:LYS:HG2	1.91	0.52
1:C:4059:GLN:O	1:C:4063:GLU:HG3	2.10	0.52
1:D:4059:GLN:O	1:D:4063:GLU:HG3	2.10	0.52
1:A:799:LYS:HG2	1:A:1621:GLN:HG3	1.91	0.52
1:B:678:MET:HG3	1:B:801:ARG:HB3	1.90	0.52
1:B:2107:ILE:HG13	1:B:2108:ASN:H	1.74	0.52
1:C:1207:LEU:HB3	1:C:1211:GLN:HB2	1.92	0.52
1:C:4106:GLU:OE1	1:C:4134:ARG:NH1	2.43	0.52
1:D:1012:ILE:HG13	1:D:1013:ARG:HD2	1.90	0.52
1:A:878:LEU:HD23	1:A:882:ARG:HG3	1.91	0.52
1:C:1829:LEU:HB3	1:C:1834:ILE:HD11	1.90	0.52
1:C:2722:LYS:NZ	1:C:2726:HIS:HB2	2.24	0.52
1:C:4884:GLU:HA	1:C:4884:GLU:OE2	2.10	0.52
1:D:1829:LEU:HB3	1:D:1834:ILE:HD11	1.90	0.52
1:A:271:ALA:O	1:A:301:THR:OG1	2.28	0.52
1:A:2722:LYS:NZ	1:A:2726:HIS:HB2	2.24	0.52
1:B:78:LEU:HD11	1:B:159:TRP:CG	2.44	0.52
1:D:1982:LYS:NZ	1:D:1983:SER:O	2.29	0.52
1:D:4106:GLU:OE1	1:D:4134:ARG:NH1	2.43	0.52
1:B:1207:LEU:HB3	1:B:1211:GLN:HB2	1.92	0.52
1:C:78:LEU:HD11	1:C:159:TRP:CG	2.44	0.52
1:C:1680:HIS:CE1	2:I:91:VAL:HA	2.44	0.52
1:C:3639:LEU:HD23	1:C:3693:ILE:HG21	1.92	0.52
1:C:4731:GLY:HA2	1:C:4737:PHE:HB2	1.91	0.52
1:A:763:ALA:HB3	1:A:764:PRO:HD3	1.91	0.52
1:B:1709:ASP:HA	1:B:1713:SER:HB3	1.91	0.52
1:B:1727:ILE:HD12	1:B:2119:LEU:HD11	1.91	0.52
1:C:2107:ILE:HG13	1:C:2108:ASN:H	1.74	0.52
1:D:4046:ASP:OD1	1:D:4046:ASP:N	2.43	0.52
1:B:653:SER:O	1:B:793:SER:HA	2.09	0.52
1:B:2722:LYS:NZ	1:B:2726:HIS:HB2	2.24	0.52
1:C:620:CYS:SG	1:C:621:HIS:N	2.83	0.52
1:C:1727:ILE:HD12	1:C:2119:LEU:HD11	1.91	0.52
1:D:56:LYS:HD2	1:D:56:LYS:C	2.30	0.52
1:D:706:TYR:OH	1:D:852:GLY:O	2.28	0.52
1:D:2859:LEU:HD12	1:D:2867:HIS:CE1	2.44	0.52
1:A:56:LYS:HD2	1:A:56:LYS:C	2.31	0.52
1:A:620:CYS:SG	1:A:621:HIS:N	2.83	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1709:ASP:HA	1:A:1713:SER:HB3	1.91	0.52
1:B:56:LYS:HD2	1:B:56:LYS:C	2.31	0.52
1:C:271:ALA:O	1:C:301:THR:OG1	2.28	0.52
1:C:1683:GLU:HB3	2:I:42:ASP:HB3	1.92	0.52
1:C:2091:TYR:CD2	1:C:3639:LEU:HD13	2.45	0.52
1:D:2091:TYR:CD2	1:D:3639:LEU:HD13	2.45	0.52
1:D:4884:GLU:HA	1:D:4884:GLU:OE2	2.10	0.52
2:J:8:ILE:HD11	2:J:74:LYS:HB2	1.91	0.52
1:A:2859:LEU:HD12	1:A:2867:HIS:CE1	2.44	0.52
1:A:4050:ALA:O	1:A:4054:HIS:ND1	2.43	0.52
2:G:43:ARG:HG3	2:G:45:LYS:HG2	1.91	0.52
1:B:970:TYR:CE2	1:B:977:LYS:HG2	2.43	0.52
1:C:1709:ASP:HA	1:C:1713:SER:HB3	1.91	0.52
2:I:43:ARG:HG3	2:I:45:LYS:HG2	1.91	0.52
1:D:4731:GLY:HA2	1:D:4737:PHE:HB2	1.91	0.52
1:A:1609:VAL:H	1:A:1611:ARG:NH1	2.08	0.51
1:A:1677:LEU:O	1:A:1681:VAL:HG22	2.10	0.51
1:A:4106:GLU:OE1	1:A:4134:ARG:NH1	2.43	0.51
1:B:763:ALA:HB3	1:B:764:PRO:HD3	1.91	0.51
1:A:2118:LEU:HD12	1:A:2148:ILE:HG22	1.93	0.51
1:A:4046:ASP:OD1	1:A:4046:ASP:N	2.43	0.51
1:A:4884:GLU:HA	1:A:4884:GLU:OE2	2.10	0.51
2:G:8:ILE:HD11	2:G:74:LYS:HB2	1.91	0.51
1:B:620:CYS:SG	1:B:621:HIS:N	2.83	0.51
1:B:1090:ALA:HB3	1:B:1202:ILE:HG23	1.92	0.51
1:A:37:LEU:HD22	1:A:192:LEU:HD21	1.92	0.51
1:A:1090:ALA:HB3	1:A:1202:ILE:HG23	1.92	0.51
1:A:1165:MET:HE1	1:A:1231:GLY:HA3	1.91	0.51
1:A:3639:LEU:HD23	1:A:3693:ILE:HG21	1.92	0.51
1:B:4050:ALA:O	1:B:4054:HIS:ND1	2.43	0.51
1:B:4059:GLN:O	1:B:4063:GLU:HG3	2.10	0.51
1:D:271:ALA:O	1:D:301:THR:OG1	2.28	0.51
1:D:754:VAL:HG13	1:D:771:ASN:HA	1.93	0.51
1:D:1245:ARG:NH1	1:D:1809:ASP:O	2.44	0.51
1:D:1731:THR:O	1:D:1734:THR:OG1	2.27	0.51
1:A:1091:GLU:OE1	1:A:1093:THR:OG1	2.25	0.51
1:A:2487:LEU:O	1:A:2492:LEU:HG	2.11	0.51
1:A:3712:SER:HG	1:A:3716:LYS:HZ3	1.58	0.51
1:B:2118:LEU:HD12	1:B:2148:ILE:HG22	1.93	0.51
1:B:4836:ASP:OD1	1:B:4836:ASP:N	2.42	0.51
1:C:1609:VAL:H	1:C:1611:ARG:NH1	2.08	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1207:LEU:HB3	1:D:1211:GLN:HB2	1.92	0.51
1:B:2487:LEU:O	1:B:2492:LEU:HG	2.11	0.51
1:B:4106:GLU:OE1	1:B:4134:ARG:NH1	2.43	0.51
1:C:1786:ASP:OD1	1:C:1786:ASP:N	2.44	0.51
1:C:4929:GLU:HG2	1:C:4930:THR:N	2.26	0.51
1:D:1609:VAL:H	1:D:1611:ARG:NH1	2.08	0.51
1:D:1677:LEU:O	1:D:1681:VAL:HG22	2.10	0.51
1:D:1769:PHE:O	2:J:83:TYR:OH	2.27	0.51
1:A:942:THR:HB	1:A:999:LEU:HD12	1.93	0.51
1:A:1727:ILE:HD12	1:A:2119:LEU:HD11	1.91	0.51
1:A:4929:GLU:HG2	1:A:4930:THR:N	2.26	0.51
1:B:1677:LEU:O	1:B:1681:VAL:HG22	2.10	0.51
1:B:3639:LEU:HD23	1:B:3693:ILE:HG21	1.92	0.51
1:B:4884:GLU:OE2	1:B:4884:GLU:HA	2.10	0.51
2:H:8:ILE:HD11	2:H:74:LYS:HB2	1.91	0.51
1:C:754:VAL:HG13	1:C:771:ASN:HA	1.93	0.51
1:C:4050:ALA:O	1:C:4054:HIS:ND1	2.43	0.51
1:D:942:THR:HB	1:D:999:LEU:HD12	1.93	0.51
1:A:754:VAL:HG13	1:A:771:ASN:HA	1.93	0.51
1:B:37:LEU:HD22	1:B:192:LEU:HD21	1.92	0.51
1:B:1165:MET:HE1	1:B:1231:GLY:HA3	1.91	0.51
1:C:37:LEU:HD22	1:C:192:LEU:HD21	1.92	0.51
1:D:721:ASP:N	1:D:721:ASP:OD1	2.44	0.51
1:D:1786:ASP:OD1	1:D:1786:ASP:N	2.44	0.51
2:J:69:LEU:HD12	2:J:107:LEU:HD23	1.93	0.51
1:A:706:TYR:OH	1:A:852:GLY:O	2.28	0.51
1:B:2342:LEU:HD21	1:B:2467:MET:HE3	1.92	0.51
1:C:1677:LEU:O	1:C:1681:VAL:HG22	2.11	0.51
1:C:2118:LEU:HD12	1:C:2148:ILE:HG22	1.93	0.51
1:D:620:CYS:SG	1:D:621:HIS:N	2.83	0.51
1:D:699:SER:OG	1:D:700:THR:N	2.44	0.51
1:D:1727:ILE:HD12	1:D:2119:LEU:HD11	1.91	0.51
1:A:970:TYR:CE2	1:A:977:LYS:HG2	2.43	0.51
1:B:2091:TYR:CD2	1:B:3639:LEU:HD13	2.45	0.51
1:B:4063:GLU:HA	1:B:4066:LEU:HG	1.93	0.51
1:B:4929:GLU:HG2	1:B:4930:THR:N	2.26	0.51
1:D:37:LEU:HD22	1:D:192:LEU:HD21	1.92	0.51
1:D:1086:ARG:HH21	1:D:1251:LEU:HD13	1.76	0.51
1:D:4106:GLU:OE2	1:D:4148:TYR:OH	2.19	0.51
1:A:1245:ARG:NH1	1:A:1809:ASP:O	2.44	0.51
2:G:69:LEU:HD12	2:G:107:LEU:HD23	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:699:SER:OG	1:B:700:THR:N	2.44	0.51
1:B:799:LYS:HG2	1:B:1621:GLN:HG3	1.91	0.51
1:B:2471:LEU:HD11	1:B:2482:PHE:HZ	1.76	0.51
1:D:1655:HIS:HA	1:D:1658:THR:HG22	1.93	0.51
1:D:2118:LEU:HD12	1:D:2148:ILE:HG22	1.93	0.51
1:A:1207:LEU:HB3	1:A:1211:GLN:HB2	1.92	0.50
1:A:4059:GLN:O	1:A:4063:GLU:HG3	2.10	0.50
1:C:706:TYR:OH	1:C:852:GLY:O	2.28	0.50
1:C:1090:ALA:HB3	1:C:1202:ILE:HG23	1.92	0.50
1:D:1090:ALA:HB3	1:D:1202:ILE:HG23	1.92	0.50
1:D:4050:ALA:O	1:D:4054:HIS:ND1	2.43	0.50
1:A:54:ASN:ND2	1:A:57:ASN:OD1	2.45	0.50
1:A:4063:GLU:HA	1:A:4066:LEU:HG	1.93	0.50
1:B:754:VAL:HG13	1:B:771:ASN:HA	1.93	0.50
1:B:1245:ARG:NH1	1:B:1809:ASP:O	2.44	0.50
1:B:1972:ILE:HD13	1:B:1975:LEU:HD21	1.93	0.50
1:B:4640:PRO:HG2	1:B:4646:LYS:HA	1.93	0.50
1:B:4781:THR:HG21	1:B:4812:TYR:HB2	1.94	0.50
1:D:677:LEU:HD23	1:D:755:ILE:HD13	1.94	0.50
1:A:721:ASP:N	1:A:721:ASP:OD1	2.44	0.50
1:A:1086:ARG:HH21	1:A:1251:LEU:HD13	1.76	0.50
1:A:2471:LEU:HD11	1:A:2482:PHE:HZ	1.76	0.50
1:A:4781:THR:HG21	1:A:4812:TYR:HB2	1.94	0.50
1:B:706:TYR:OH	1:B:852:GLY:O	2.28	0.50
1:B:1588:HIS:HE1	1:B:1590:GLN:HE21	1.59	0.50
1:B:1609:VAL:H	1:B:1611:ARG:NH1	2.08	0.50
1:C:674:TYR:CE1	1:C:756:SER:HB2	2.47	0.50
1:C:1972:ILE:HD13	1:C:1975:LEU:HD21	1.93	0.50
1:C:2471:LEU:HD11	1:C:2482:PHE:HZ	1.77	0.50
1:D:3639:LEU:HD23	1:D:3693:ILE:HG21	1.92	0.50
1:A:1731:THR:O	1:A:1734:THR:OG1	2.27	0.50
1:A:2330:PHE:HD1	1:A:2394:LEU:HD21	1.76	0.50
1:B:4023:LYS:HG3	1:B:4087:HIS:CD2	2.47	0.50
1:C:54:ASN:ND2	1:C:57:ASN:OD1	2.45	0.50
1:C:970:TYR:CE2	1:C:977:LYS:HG2	2.43	0.50
1:C:4640:PRO:HG2	1:C:4646:LYS:HA	1.93	0.50
1:D:55:SER:O	1:D:296:ARG:NH2	2.34	0.50
1:A:1595:VAL:O	1:A:1595:VAL:HG23	2.12	0.50
1:A:1655:HIS:HA	1:A:1658:THR:HG22	1.93	0.50
1:A:4640:PRO:HG2	1:A:4646:LYS:HA	1.93	0.50
1:C:2342:LEU:HD21	1:C:2467:MET:HE3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2084:PHE:O	1:D:3690:TYR:OH	2.25	0.50
1:D:2442:PRO:HG3	1:D:2454:ASP:HB2	1.94	0.50
1:A:893:TRP:CE3	1:A:893:TRP:HA	2.47	0.50
1:A:4836:ASP:OD1	1:A:4836:ASP:N	2.42	0.50
1:A:4858:LEU:HD21	1:D:4855:VAL:HG11	1.93	0.50
1:B:271:ALA:O	1:B:301:THR:OG1	2.28	0.50
1:B:1048:ASP:O	1:B:1052:GLU:HG3	2.12	0.50
1:B:1595:VAL:HG23	1:B:1595:VAL:O	2.12	0.50
1:C:56:LYS:HD2	1:C:56:LYS:C	2.30	0.50
1:C:677:LEU:HD23	1:C:755:ILE:HD13	1.94	0.50
1:C:1086:ARG:HH21	1:C:1251:LEU:HD13	1.76	0.50
1:C:1588:HIS:HE1	1:C:1590:GLN:HE21	1.59	0.50
1:C:4046:ASP:OD1	1:C:4046:ASP:N	2.43	0.50
1:B:54:ASN:ND2	1:B:57:ASN:OD1	2.45	0.50
1:C:1655:HIS:HA	1:C:1658:THR:HG22	1.93	0.50
1:C:2099:ARG:O	1:C:2103:LYS:NZ	2.36	0.50
1:C:4023:LYS:HG3	1:C:4087:HIS:CD2	2.47	0.50
1:D:54:ASN:ND2	1:D:57:ASN:OD1	2.45	0.50
1:D:2220:LEU:HD11	1:D:2242:ALA:HB2	1.94	0.50
1:A:1102:TYR:HD1	1:A:1165:MET:HG2	1.76	0.50
1:B:674:TYR:CE1	1:B:756:SER:HB2	2.47	0.50
1:B:942:THR:HB	1:B:999:LEU:HD12	1.93	0.50
1:B:1086:ARG:HH21	1:B:1251:LEU:HD13	1.76	0.50
1:B:1102:TYR:HD1	1:B:1165:MET:HG2	1.76	0.50
1:C:2487:LEU:O	1:C:2492:LEU:HG	2.11	0.50
1:D:893:TRP:CE3	1:D:893:TRP:HA	2.47	0.50
1:D:2487:LEU:O	1:D:2492:LEU:HG	2.11	0.50
1:A:1750:PRO:HG3	1:A:2057:LEU:HD22	1.94	0.50
1:A:4023:LYS:HG3	1:A:4087:HIS:CD2	2.47	0.50
1:B:4046:ASP:N	1:B:4046:ASP:OD1	2.43	0.50
1:A:3989:VAL:HG12	1:A:3990:VAL:H	1.77	0.49
1:B:1950:LEU:O	1:B:1956:LEU:HD11	2.12	0.49
1:B:3971:MET:HB3	1:B:4093:ILE:HD13	1.94	0.49
1:C:699:SER:OG	1:C:700:THR:N	2.44	0.49
1:C:4009:VAL:HA	1:C:4012:ILE:HD12	1.94	0.49
1:D:674:TYR:CE1	1:D:756:SER:HB2	2.47	0.49
1:D:1595:VAL:O	1:D:1595:VAL:HG23	2.12	0.49
1:D:3989:VAL:HG12	1:D:3990:VAL:H	1.76	0.49
1:D:4063:GLU:HA	1:D:4066:LEU:HG	1.93	0.49
1:D:4781:THR:HG21	1:D:4812:TYR:HB2	1.94	0.49
1:A:982:ASP:OD1	1:A:985:PHE:HB3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2220:LEU:HD11	1:A:2242:ALA:HB2	1.93	0.49
1:A:3698:CYS:SG	1:A:3730:LEU:HD21	2.52	0.49
1:B:624:ALA:HB3	1:B:2131:VAL:HG13	1.94	0.49
1:B:759:LEU:HD11	1:B:761:LEU:HD23	1.94	0.49
1:B:2076:ASP:HB3	1:B:2079:LEU:HB3	1.94	0.49
1:B:3989:VAL:HG12	1:B:3990:VAL:H	1.76	0.49
1:C:942:THR:HB	1:C:999:LEU:HD12	1.93	0.49
1:C:1102:TYR:HD1	1:C:1165:MET:HG2	1.76	0.49
1:C:3989:VAL:HG12	1:C:3990:VAL:H	1.77	0.49
1:C:4063:GLU:HA	1:C:4066:LEU:HG	1.93	0.49
1:C:4836:ASP:OD1	1:C:4836:ASP:N	2.42	0.49
1:D:1048:ASP:O	1:D:1052:GLU:HG3	2.12	0.49
1:D:1972:ILE:HD13	1:D:1975:LEU:HD21	1.93	0.49
1:D:4929:GLU:HG2	1:D:4930:THR:N	2.26	0.49
1:A:1827:TYR:CZ	1:A:1831:ILE:HD11	2.48	0.49
1:A:1924:ILE:HA	1:A:1998:PHE:HZ	1.78	0.49
1:A:1950:LEU:O	1:A:1956:LEU:HD11	2.12	0.49
1:A:2091:TYR:CD2	1:A:3639:LEU:HD13	2.45	0.49
1:B:721:ASP:OD1	1:B:721:ASP:N	2.44	0.49
1:B:1655:HIS:HA	1:B:1658:THR:HG22	1.93	0.49
1:B:1683:GLU:HB3	2:H:42:ASP:HB3	1.93	0.49
1:B:1715:TYR:CE2	1:B:1719:ARG:HD2	2.48	0.49
1:B:1719:ARG:NE	1:B:1831:ILE:O	2.46	0.49
1:B:4106:GLU:OE2	1:B:4148:TYR:OH	2.19	0.49
1:C:3728:ALA:HA	1:C:3731:HIS:CE1	2.48	0.49
1:C:4808:MET:HB2	1:D:4518:TYR:HD2	1.78	0.49
1:A:1048:ASP:O	1:A:1052:GLU:HG3	2.12	0.49
1:B:893:TRP:HA	1:B:893:TRP:CE3	2.47	0.49
1:B:2442:PRO:HG3	1:B:2454:ASP:HB2	1.94	0.49
1:C:340:VAL:HG23	1:C:341:GLY:H	1.78	0.49
1:C:2220:LEU:HD11	1:C:2242:ALA:HB2	1.93	0.49
2:I:69:LEU:HD12	2:I:107:LEU:HD23	1.93	0.49
1:D:1924:ILE:HA	1:D:1998:PHE:HZ	1.78	0.49
1:D:3698:CYS:SG	1:D:3730:LEU:HD21	2.52	0.49
1:D:3971:MET:HB3	1:D:4093:ILE:HD13	1.94	0.49
1:D:4023:LYS:HG3	1:D:4087:HIS:CD2	2.47	0.49
1:C:624:ALA:HB3	1:C:2131:VAL:HG13	1.94	0.49
1:C:721:ASP:OD1	1:C:721:ASP:N	2.44	0.49
1:C:1595:VAL:HG23	1:C:1595:VAL:O	2.12	0.49
1:C:1950:LEU:O	1:C:1956:LEU:HD11	2.12	0.49
1:C:4781:THR:HG21	1:C:4812:TYR:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1102:TYR:HD1	1:D:1165:MET:HG2	1.76	0.49
1:D:1750:PRO:HG3	1:D:2057:LEU:HD22	1.94	0.49
1:A:674:TYR:CE1	1:A:756:SER:HB2	2.47	0.49
1:A:1588:HIS:HE1	1:A:1590:GLN:HE21	1.59	0.49
1:A:4009:VAL:HA	1:A:4012:ILE:HD12	1.94	0.49
1:B:909:ASP:OD1	1:B:910:ASP:N	2.45	0.49
1:B:1750:PRO:HG3	1:B:2057:LEU:HD22	1.94	0.49
1:C:794:PHE:CD1	1:C:798:ILE:HG21	2.48	0.49
1:C:1048:ASP:O	1:C:1052:GLU:HG3	2.12	0.49
1:C:1257:GLN:HB2	1:C:1596:LEU:HD11	1.95	0.49
1:C:1924:ILE:HA	1:C:1998:PHE:HZ	1.78	0.49
1:C:2343:LEU:O	1:C:2347:GLU:HG2	2.13	0.49
1:D:1588:HIS:HE1	1:D:1590:GLN:HE21	1.59	0.49
1:A:794:PHE:CD1	1:A:798:ILE:HG21	2.48	0.49
1:A:1715:TYR:CE2	1:A:1719:ARG:HD2	2.48	0.49
1:A:1786:ASP:OD1	1:A:1786:ASP:N	2.44	0.49
1:A:1972:ILE:HD13	1:A:1975:LEU:HD21	1.93	0.49
1:B:730:LEU:HD22	1:B:731:HIS:CE1	2.48	0.49
2:H:38:ASP:OD1	2:H:39:SER:N	2.46	0.49
1:C:606:ARG:NH1	1:C:1635:GLU:OE2	2.46	0.49
1:D:982:ASP:OD1	1:D:985:PHE:HB3	2.12	0.49
1:D:2076:ASP:HB3	1:D:2079:LEU:HB3	1.94	0.49
1:A:2442:PRO:HG3	1:A:2454:ASP:HB2	1.94	0.49
1:A:3786:VAL:HG11	1:A:3865:THR:HG23	1.95	0.49
1:B:1827:TYR:CZ	1:B:1831:ILE:HD11	2.48	0.49
1:B:3698:CYS:SG	1:B:3730:LEU:HD21	2.53	0.49
1:C:730:LEU:HD22	1:C:731:HIS:CE1	2.48	0.49
2:I:38:ASP:OD1	2:I:39:SER:N	2.46	0.49
1:D:624:ALA:HB3	1:D:2131:VAL:HG13	1.94	0.49
1:D:730:LEU:HD22	1:D:731:HIS:CE1	2.48	0.49
1:D:759:LEU:HD11	1:D:761:LEU:HD23	1.94	0.49
1:D:1257:GLN:HB2	1:D:1596:LEU:HD11	1.95	0.49
1:D:2471:LEU:HD11	1:D:2482:PHE:HZ	1.76	0.49
1:D:4836:ASP:OD1	1:D:4836:ASP:N	2.42	0.49
1:A:125:TYR:OH	1:A:417:ARG:HB3	2.13	0.49
1:A:699:SER:OG	1:A:700:THR:N	2.44	0.49
1:A:759:LEU:HD11	1:A:761:LEU:HD23	1.94	0.49
1:A:2076:ASP:HB3	1:A:2079:LEU:HB3	1.94	0.49
1:A:2343:LEU:O	1:A:2347:GLU:HG2	2.13	0.49
1:C:125:TYR:OH	1:C:417:ARG:HB3	2.13	0.49
1:C:2442:PRO:HG3	1:C:2454:ASP:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4806:ASP:O	1:D:4520:VAL:HG12	2.13	0.49
1:D:225:GLN:OE1	1:D:225:GLN:HA	2.13	0.49
1:D:893:TRP:HA	1:D:893:TRP:HE3	1.78	0.49
1:D:1950:LEU:O	1:D:1956:LEU:HD11	2.12	0.49
1:D:2330:PHE:HD1	1:D:2394:LEU:HD21	1.76	0.49
1:A:235:ARG:HB2	1:A:406:SER:OG	2.13	0.49
1:A:340:VAL:HG23	1:A:341:GLY:H	1.78	0.49
1:A:677:LEU:HD23	1:A:755:ILE:HD13	1.94	0.49
1:B:982:ASP:OD1	1:B:985:PHE:HB3	2.12	0.49
1:B:1932:VAL:HG11	1:B:3616:VAL:HB	1.95	0.49
1:B:2220:LEU:HD11	1:B:2242:ALA:HB2	1.93	0.49
1:C:28:ILE:HG12	1:C:29:HIS:CE1	2.48	0.49
1:C:1165:MET:HE1	1:C:1231:GLY:HA3	1.94	0.49
1:C:1715:TYR:CE2	1:C:1719:ARG:HD2	2.48	0.49
1:C:2265:VAL:HG21	1:C:2322:LEU:HB3	1.95	0.49
1:C:2317:ASN:O	1:C:2321:ARG:HG2	2.13	0.49
1:C:2330:PHE:HD1	1:C:2394:LEU:HD21	1.77	0.49
1:C:3971:MET:HB3	1:C:4093:ILE:HD13	1.94	0.49
1:D:416:ALA:HA	1:D:419:ILE:HD12	1.95	0.49
1:D:1715:TYR:CE2	1:D:1719:ARG:HD2	2.48	0.49
1:D:4009:VAL:HA	1:D:4012:ILE:HD12	1.94	0.49
1:A:477:ASN:OD1	1:A:480:ARG:NH2	2.45	0.48
1:A:893:TRP:HA	1:A:893:TRP:HE3	1.78	0.48
1:B:2265:VAL:HG21	1:B:2322:LEU:HB3	1.95	0.48
1:B:2343:LEU:O	1:B:2347:GLU:HG2	2.13	0.48
1:B:3905:PHE:O	1:B:3909:ILE:HG12	2.13	0.48
1:B:4009:VAL:HA	1:B:4012:ILE:HD12	1.94	0.48
1:B:4029:ASP:OD2	1:B:4054:HIS:NE2	2.46	0.48
1:B:4671:MET:HG2	1:B:4674:ALA:HB3	1.95	0.48
1:C:759:LEU:HD11	1:C:761:LEU:HD23	1.94	0.48
1:C:1719:ARG:NE	1:C:1831:ILE:O	2.46	0.48
1:C:2076:ASP:HB3	1:C:2079:LEU:HB3	1.94	0.48
1:D:28:ILE:HG12	1:D:29:HIS:CE1	2.48	0.48
1:D:3957:LEU:HG	1:D:3966:LEU:HD22	1.95	0.48
1:D:4640:PRO:HG2	1:D:4646:LYS:HA	1.93	0.48
1:D:4671:MET:HG2	1:D:4674:ALA:HB3	1.95	0.48
1:A:28:ILE:HG12	1:A:29:HIS:CE1	2.48	0.48
1:A:624:ALA:HB3	1:A:2131:VAL:HG13	1.94	0.48
1:A:4671:MET:HG2	1:A:4674:ALA:HB3	1.95	0.48
2:G:38:ASP:OD1	2:G:39:SER:N	2.46	0.48
1:B:125:TYR:OH	1:B:417:ARG:HB3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:LEU:HD23	1:B:755:ILE:HD13	1.94	0.48
1:B:1924:ILE:HA	1:B:1998:PHE:HZ	1.78	0.48
1:B:2888:ALA:O	1:B:2892:PHE:HD1	1.96	0.48
1:B:3728:ALA:HA	1:B:3731:HIS:CE1	2.48	0.48
2:H:69:LEU:HD12	2:H:107:LEU:HD23	1.93	0.48
1:C:1685:GLN:NE2	1:C:1703:TYR:OH	2.46	0.48
1:C:1750:PRO:HG3	1:C:2057:LEU:HD22	1.94	0.48
1:D:340:VAL:HG23	1:D:341:GLY:H	1.78	0.48
1:D:1165:MET:HE1	1:D:1231:GLY:HA3	1.94	0.48
1:D:2478:GLU:HG2	1:D:2479:VAL:HG22	1.95	0.48
1:D:3728:ALA:HA	1:D:3731:HIS:CE1	2.48	0.48
2:J:38:ASP:OD1	2:J:39:SER:N	2.46	0.48
1:A:225:GLN:OE1	1:A:225:GLN:HA	2.13	0.48
1:A:730:LEU:HD22	1:A:731:HIS:CE1	2.48	0.48
1:A:909:ASP:OD1	1:A:910:ASP:N	2.45	0.48
1:A:2253:ALA:O	1:A:2315:ASN:ND2	2.40	0.48
1:A:2777:SER:OG	1:A:2843:MET:SD	2.68	0.48
1:A:2888:ALA:O	1:A:2892:PHE:HD1	1.96	0.48
1:A:3905:PHE:O	1:A:3909:ILE:HG12	2.13	0.48
1:A:3971:MET:HB3	1:A:4093:ILE:HD13	1.94	0.48
1:B:416:ALA:HA	1:B:419:ILE:HD12	1.95	0.48
1:B:794:PHE:CD1	1:B:798:ILE:HG21	2.48	0.48
1:C:982:ASP:OD1	1:C:985:PHE:HB3	2.13	0.48
1:C:1827:TYR:CZ	1:C:1831:ILE:HD11	2.48	0.48
1:D:1827:TYR:CZ	1:D:1831:ILE:HD11	2.47	0.48
1:D:2522:UNK:C	1:D:2524:UNK:H	2.27	0.48
1:D:4596:LEU:HG	1:D:4600:LYS:HE3	1.95	0.48
1:A:3728:ALA:HA	1:A:3731:HIS:CE1	2.48	0.48
1:A:3957:LEU:HG	1:A:3966:LEU:HD22	1.95	0.48
1:A:4722:ALA:O	1:A:4726:THR:HG23	2.13	0.48
1:B:606:ARG:NH1	1:B:1635:GLU:OE2	2.46	0.48
1:B:893:TRP:HA	1:B:893:TRP:HE3	1.78	0.48
1:B:3786:VAL:HG11	1:B:3865:THR:HG23	1.95	0.48
1:C:235:ARG:HB2	1:C:406:SER:OG	2.13	0.48
1:C:416:ALA:HA	1:C:419:ILE:HD12	1.95	0.48
1:C:893:TRP:HE3	1:C:893:TRP:HA	1.78	0.48
1:C:1245:ARG:NH1	1:C:1809:ASP:O	2.44	0.48
1:C:1704:TYR:O	1:C:1708:ILE:HG12	2.14	0.48
1:C:1932:VAL:HG11	1:C:3616:VAL:HB	1.95	0.48
1:C:3698:CYS:SG	1:C:3730:LEU:HD21	2.52	0.48
1:C:4194:ASP:HA	1:C:4599:PHE:HE2	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:ARG:NH1	1:A:1635:GLU:OE2	2.46	0.48
1:A:3420:UNK:HA	1:A:3421:UNK:HA	1.66	0.48
1:A:4112:THR:HA	1:A:4115:GLN:HB2	1.96	0.48
1:B:340:VAL:HG23	1:B:341:GLY:H	1.78	0.48
1:B:2330:PHE:HD1	1:B:2394:LEU:HD21	1.76	0.48
1:B:2405:MET:H	1:B:2405:MET:HG3	1.48	0.48
1:B:2722:LYS:HZ1	1:B:2726:HIS:HB2	1.78	0.48
1:B:4112:THR:HA	1:B:4115:GLN:HB2	1.96	0.48
1:C:125:TYR:CE1	1:C:414:ARG:HA	2.49	0.48
1:C:2742:TYR:HD1	1:C:2756:MET:H	1.60	0.48
1:C:4596:LEU:HG	1:C:4600:LYS:HE3	1.95	0.48
1:D:235:ARG:HB2	1:D:406:SER:OG	2.13	0.48
1:D:794:PHE:CD1	1:D:798:ILE:HG21	2.48	0.48
1:D:1685:GLN:NE2	1:D:1703:TYR:OH	2.46	0.48
1:D:2317:ASN:O	1:D:2321:ARG:HG2	2.13	0.48
1:A:769:ARG:HA	1:A:774:PRO:HA	1.96	0.48
1:A:1935:LEU:HD11	1:A:1975:LEU:HD13	1.96	0.48
1:A:2735:LYS:HD3	1:A:2756:MET:SD	2.54	0.48
1:A:4029:ASP:OD2	1:A:4054:HIS:NE2	2.46	0.48
1:B:4194:ASP:HA	1:B:4599:PHE:HE2	1.79	0.48
1:D:313:ASN:ND2	1:D:391:ALA:O	2.45	0.48
1:D:1704:TYR:O	1:D:1708:ILE:HG12	2.14	0.48
1:D:1719:ARG:NE	1:D:1831:ILE:O	2.46	0.48
1:D:2735:LYS:HD3	1:D:2756:MET:SD	2.54	0.48
1:D:2742:TYR:HD1	1:D:2756:MET:H	1.60	0.48
1:D:3611:PRO:HD2	1:D:3614:ARG:HH21	1.79	0.48
1:A:1257:GLN:HB2	1:A:1596:LEU:HD11	1.95	0.48
1:A:1704:TYR:O	1:A:1708:ILE:HG12	2.14	0.48
1:A:2342:LEU:HD21	1:A:2467:MET:HE3	1.95	0.48
1:B:1786:ASP:OD1	1:B:1786:ASP:N	2.44	0.48
1:B:2522:UNK:C	1:B:2524:UNK:H	2.27	0.48
1:B:4722:ALA:O	1:B:4726:THR:HG23	2.13	0.48
1:B:4920:PHE:HE2	1:B:4939:VAL:HG11	1.79	0.48
1:C:439:LYS:HE2	1:C:439:LYS:HB3	1.59	0.48
1:C:876:PRO:HA	1:C:879:GLU:HG2	1.95	0.48
1:C:893:TRP:HA	1:C:893:TRP:CE3	2.47	0.48
1:C:2888:ALA:O	1:C:2892:PHE:HD1	1.96	0.48
1:D:318:ASP:OD1	1:D:318:ASP:N	2.47	0.48
1:D:876:PRO:HA	1:D:879:GLU:HG2	1.95	0.48
1:A:4920:PHE:HE2	1:A:4939:VAL:HG11	1.79	0.48
1:B:225:GLN:OE1	1:B:225:GLN:HA	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2478:GLU:HG2	1:B:2479:VAL:HG22	1.95	0.48
1:B:2735:LYS:HD3	1:B:2756:MET:SD	2.54	0.48
1:C:3905:PHE:O	1:C:3909:ILE:HG12	2.13	0.48
1:D:606:ARG:NH1	1:D:1635:GLU:OE2	2.46	0.48
1:D:1730:MET:SD	1:D:2106:THR:OG1	2.69	0.48
1:A:2742:TYR:HD1	1:A:2756:MET:H	1.60	0.48
1:B:235:ARG:HB2	1:B:406:SER:OG	2.13	0.48
1:B:1685:GLN:NE2	1:B:1703:TYR:OH	2.46	0.48
1:B:2742:TYR:HD1	1:B:2756:MET:H	1.60	0.48
1:B:3420:UNK:HA	1:B:3421:UNK:HA	1.66	0.48
1:C:4722:ALA:O	1:C:4726:THR:HG23	2.13	0.48
1:D:606:ARG:HH22	1:D:1633:ILE:HG23	1.79	0.48
1:D:986:ILE:HG13	1:D:987:LYS:N	2.29	0.48
1:A:416:ALA:HA	1:A:419:ILE:HD12	1.95	0.48
1:A:606:ARG:HH22	1:A:1633:ILE:HG23	1.79	0.48
1:A:2217:LEU:HA	1:A:2220:LEU:HG	1.96	0.48
1:A:4013:LEU:HD22	1:A:4124:VAL:HG21	1.96	0.48
1:B:1257:GLN:HB2	1:B:1596:LEU:HD11	1.95	0.48
1:C:1120:PRO:HG3	1:C:1202:ILE:HD11	1.96	0.48
1:C:2522:UNK:C	1:C:2524:UNK:H	2.27	0.48
1:C:3712:SER:OG	1:C:3716:LYS:NZ	2.35	0.48
1:C:3786:VAL:HG11	1:C:3865:THR:HG23	1.95	0.48
1:D:125:TYR:OH	1:D:417:ARG:HB3	2.13	0.48
1:D:4029:ASP:OD2	1:D:4054:HIS:NE2	2.46	0.48
1:B:28:ILE:HG12	1:B:29:HIS:CE1	2.48	0.47
1:B:125:TYR:CE1	1:B:414:ARG:HA	2.49	0.47
1:C:503:ASP:O	1:C:507:VAL:HG13	2.14	0.47
1:C:4029:ASP:OD2	1:C:4054:HIS:NE2	2.46	0.47
1:D:769:ARG:HA	1:D:774:PRO:HA	1.96	0.47
1:D:2217:LEU:HA	1:D:2220:LEU:HG	1.96	0.47
1:D:2343:LEU:O	1:D:2347:GLU:HG2	2.13	0.47
1:D:2888:ALA:O	1:D:2892:PHE:HD1	1.96	0.47
1:D:3786:VAL:HG11	1:D:3865:THR:HG23	1.95	0.47
1:D:4722:ALA:O	1:D:4726:THR:HG23	2.13	0.47
1:A:1719:ARG:NE	1:A:1831:ILE:O	2.46	0.47
1:A:2478:GLU:HG2	1:A:2479:VAL:HG22	1.95	0.47
1:A:3611:PRO:HD2	1:A:3614:ARG:HH21	1.79	0.47
1:B:162:ILE:HG23	1:B:181:LEU:HB2	1.97	0.47
1:B:1935:LEU:HD11	1:B:1975:LEU:HD13	1.96	0.47
1:B:3611:PRO:HD2	1:B:3614:ARG:HH21	1.79	0.47
1:C:4027:SER:HA	1:C:4032:LYS:HG2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1935:LEU:HD11	1:D:1975:LEU:HD13	1.96	0.47
1:D:3905:PHE:O	1:D:3909:ILE:HG12	2.13	0.47
1:A:125:TYR:CE1	1:A:414:ARG:HA	2.49	0.47
1:A:313:ASN:ND2	1:A:391:ALA:O	2.45	0.47
1:A:2522:UNK:C	1:A:2524:UNK:H	2.27	0.47
1:A:4189:VAL:HG21	1:A:4948:TRP:CD1	2.49	0.47
1:C:647:ARG:HH22	2:I:30:MET:HE2	1.80	0.47
1:C:4920:PHE:HE2	1:C:4939:VAL:HG11	1.79	0.47
1:D:125:TYR:CE1	1:D:414:ARG:HA	2.49	0.47
1:D:1932:VAL:HG11	1:D:3616:VAL:HB	1.95	0.47
1:D:4112:THR:HA	1:D:4115:GLN:HB2	1.96	0.47
1:A:2265:VAL:HG21	1:A:2322:LEU:HB3	1.95	0.47
1:A:2317:ASN:O	1:A:2321:ARG:HG2	2.13	0.47
1:C:606:ARG:HH22	1:C:1633:ILE:HG23	1.79	0.47
1:C:2217:LEU:HA	1:C:2220:LEU:HG	1.96	0.47
1:C:2777:SER:OG	1:C:2843:MET:SD	2.68	0.47
1:C:3611:PRO:HD2	1:C:3614:ARG:HH21	1.79	0.47
1:D:3839:PHE:HE1	1:D:3873:THR:HG23	1.80	0.47
1:D:4189:VAL:HG21	1:D:4948:TRP:CD1	2.49	0.47
1:A:1932:VAL:HG11	1:A:3616:VAL:HB	1.95	0.47
1:A:2850:ILE:O	1:A:2854:LYS:HG2	2.15	0.47
1:B:503:ASP:O	1:B:507:VAL:HG13	2.14	0.47
1:B:1120:PRO:HG3	1:B:1202:ILE:HD11	1.96	0.47
1:B:2217:LEU:HA	1:B:2220:LEU:HG	1.96	0.47
1:B:3839:PHE:HE1	1:B:3873:THR:HG23	1.80	0.47
1:B:4189:VAL:HG21	1:B:4948:TRP:CD1	2.50	0.47
1:C:4112:THR:HA	1:C:4115:GLN:HB2	1.96	0.47
1:C:4671:MET:HG2	1:C:4674:ALA:HB3	1.95	0.47
1:A:162:ILE:HG23	1:A:181:LEU:HB2	1.97	0.47
1:A:423:VAL:HG23	1:A:497:LEU:HD22	1.97	0.47
1:A:2779:LYS:HE3	1:A:2779:LYS:HB3	1.72	0.47
2:G:24:VAL:HG22	2:G:48:LYS:HG2	1.97	0.47
1:B:318:ASP:OD1	1:B:318:ASP:N	2.47	0.47
1:B:2779:LYS:HE3	1:B:2779:LYS:HB3	1.72	0.47
1:B:3957:LEU:HG	1:B:3966:LEU:HD22	1.95	0.47
1:B:4142:LYS:HD3	1:B:4142:LYS:HA	1.71	0.47
1:C:225:GLN:HA	1:C:225:GLN:OE1	2.13	0.47
1:C:2735:LYS:HD3	1:C:2756:MET:SD	2.54	0.47
1:D:162:ILE:HG23	1:D:181:LEU:HB2	1.97	0.47
1:D:1120:PRO:HG3	1:D:1202:ILE:HD11	1.96	0.47
1:D:2265:VAL:HG21	1:D:2322:LEU:HB3	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4194:ASP:HA	1:D:4599:PHE:HE2	1.79	0.47
1:D:4920:PHE:HE2	1:D:4939:VAL:HG11	1.79	0.47
1:A:167:LYS:HB2	1:A:167:LYS:HE2	1.48	0.47
1:A:503:ASP:O	1:A:507:VAL:HG13	2.14	0.47
1:A:686:VAL:HG13	1:A:687:THR:H	1.80	0.47
1:A:1224:LEU:HB3	1:A:1227:PHE:HB3	1.97	0.47
1:A:1685:GLN:NE2	1:A:1703:TYR:OH	2.46	0.47
1:B:769:ARG:HA	1:B:774:PRO:HA	1.96	0.47
1:B:876:PRO:HA	1:B:879:GLU:HG2	1.95	0.47
1:B:1174:MET:HG2	1:B:1190:LEU:HA	1.96	0.47
1:B:1224:LEU:HB3	1:B:1227:PHE:HB3	1.97	0.47
1:B:2723:TYR:CE1	1:B:2770:TYR:HE2	2.33	0.47
1:B:4029:ASP:OD1	1:B:4029:ASP:N	2.48	0.47
1:C:909:ASP:OD1	1:C:910:ASP:N	2.45	0.47
1:C:986:ILE:HG13	1:C:987:LYS:N	2.29	0.47
1:C:4044:LYS:HZ1	1:C:4071:THR:H	1.62	0.47
1:C:4601:ARG:HD3	1:C:4707:TRP:CZ2	2.50	0.47
1:D:909:ASP:OD1	1:D:910:ASP:N	2.45	0.47
1:D:2764:GLU:O	1:D:2768:GLU:HG2	2.15	0.47
1:D:4027:SER:HA	1:D:4032:LYS:HG2	1.96	0.47
1:A:4033:GLU:OE1	1:A:4033:GLU:N	2.48	0.47
1:B:606:ARG:HH22	1:B:1633:ILE:HG23	1.79	0.47
1:B:2317:ASN:O	1:B:2321:ARG:HG2	2.13	0.47
1:B:2777:SER:OG	1:B:2843:MET:SD	2.68	0.47
1:C:55:SER:O	1:C:296:ARG:NH2	2.34	0.47
1:C:162:ILE:HG23	1:C:181:LEU:HB2	1.97	0.47
1:C:3712:SER:HG	1:C:3716:LYS:HZ3	1.59	0.47
1:C:3839:PHE:HE1	1:C:3873:THR:HG23	1.80	0.47
1:D:423:VAL:HG23	1:D:497:LEU:HD22	1.97	0.47
1:D:748:LEU:HD13	1:D:748:LEU:HA	1.77	0.47
1:A:207:PHE:CZ	1:B:2324:ILE:HD12	2.50	0.47
1:A:1174:MET:HG2	1:A:1190:LEU:HA	1.96	0.47
1:A:1311:ALA:HA	1:A:1312:UNK:HA	1.50	0.47
1:A:3839:PHE:HE1	1:A:3873:THR:HG23	1.80	0.47
1:B:423:VAL:HG23	1:B:497:LEU:HD22	1.97	0.47
1:B:4596:LEU:HG	1:B:4600:LYS:HE3	1.95	0.47
1:C:2723:TYR:CE1	1:C:2770:TYR:HE2	2.33	0.47
1:D:4601:ARG:HD3	1:D:4707:TRP:CZ2	2.50	0.47
1:A:4596:LEU:HG	1:A:4600:LYS:HE3	1.96	0.47
1:B:816:PRO:HB2	1:B:819:TYR:CD1	2.50	0.47
1:B:1704:TYR:O	1:B:1708:ILE:HG12	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2478:GLU:HG2	1:C:2479:VAL:HG22	1.95	0.47
1:C:3957:LEU:HG	1:C:3966:LEU:HD22	1.95	0.47
1:C:4013:LEU:HD22	1:C:4124:VAL:HG21	1.96	0.47
1:C:4033:GLU:N	1:C:4033:GLU:OE1	2.48	0.47
1:C:4785:PHE:CZ	1:D:4518:TYR:HE2	2.33	0.47
1:C:4789:ARG:NH1	1:D:4558:TYR:OH	2.48	0.47
1:D:662:GLY:O	1:D:669:GLN:NE2	2.48	0.47
1:D:686:VAL:HG13	1:D:687:THR:H	1.80	0.47
1:D:1174:MET:HG2	1:D:1190:LEU:HA	1.97	0.47
1:D:2101:LEU:HA	1:D:2104:THR:HG22	1.97	0.47
1:D:2777:SER:OG	1:D:2843:MET:SD	2.68	0.47
1:D:2850:ILE:O	1:D:2854:LYS:HG2	2.15	0.47
1:A:986:ILE:HG13	1:A:987:LYS:N	2.29	0.46
1:A:2722:LYS:HZ1	1:A:2726:HIS:HB2	1.78	0.46
1:A:2723:TYR:CE1	1:A:2770:TYR:HE2	2.33	0.46
1:B:2850:ILE:O	1:B:2854:LYS:HG2	2.15	0.46
1:C:686:VAL:HG13	1:C:687:THR:H	1.80	0.46
1:C:1358:ARG:HB2	1:C:1567:LEU:HD21	1.97	0.46
1:C:1361:LYS:HA	1:C:1566:PRO:HA	1.98	0.46
1:C:1935:LEU:HD11	1:C:1975:LEU:HD13	1.96	0.46
1:C:2101:LEU:HA	1:C:2104:THR:HG22	1.97	0.46
1:D:503:ASP:O	1:D:507:VAL:HG13	2.14	0.46
1:D:4029:ASP:OD1	1:D:4029:ASP:N	2.48	0.46
1:A:876:PRO:HA	1:A:879:GLU:HG2	1.95	0.46
1:A:4601:ARG:HD3	1:A:4707:TRP:CZ2	2.50	0.46
1:B:1358:ARG:HB2	1:B:1567:LEU:HD21	1.98	0.46
1:B:1362:ASP:N	1:B:1362:ASP:OD1	2.49	0.46
1:B:3729:ARG:O	1:B:3733:ARG:NH1	2.48	0.46
1:C:313:ASN:ND2	1:C:391:ALA:O	2.45	0.46
1:C:423:VAL:HG23	1:C:497:LEU:HD22	1.97	0.46
1:C:692:HIS:HB3	1:C:795:SER:HB3	1.97	0.46
1:C:769:ARG:HA	1:C:774:PRO:HA	1.96	0.46
1:C:4106:GLU:OE2	1:C:4148:TYR:OH	2.19	0.46
1:C:4189:VAL:HG21	1:C:4948:TRP:CD1	2.50	0.46
1:D:1362:ASP:OD1	1:D:1362:ASP:N	2.49	0.46
1:D:1982:LYS:HD2	1:D:1983:SER:H	1.81	0.46
1:D:4033:GLU:OE1	1:D:4033:GLU:N	2.48	0.46
1:A:1120:PRO:HG3	1:A:1202:ILE:HD11	1.96	0.46
1:A:1936:GLN:O	1:A:1939:GLN:HG3	2.16	0.46
1:A:3899:GLU:OE2	1:A:3900:GLN:HG2	2.15	0.46
1:B:686:VAL:HG13	1:B:687:THR:H	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2771:ARG:O	1:B:2775:LYS:HD3	2.15	0.46
1:C:816:PRO:HB2	1:C:819:TYR:CD1	2.50	0.46
1:C:2405:MET:H	1:C:2405:MET:HG3	1.48	0.46
1:C:2764:GLU:O	1:C:2768:GLU:HG2	2.15	0.46
1:D:1733:GLU:O	1:D:1736:SER:OG	2.30	0.46
1:D:4013:LEU:HD22	1:D:4124:VAL:HG21	1.96	0.46
1:B:662:GLY:O	1:B:669:GLN:NE2	2.48	0.46
1:B:4013:LEU:HD22	1:B:4124:VAL:HG21	1.96	0.46
1:B:4033:GLU:OE1	1:B:4033:GLU:N	2.48	0.46
1:C:23:GLN:HG3	1:C:213:SER:HB2	1.98	0.46
1:C:1677:LEU:HA	1:C:1680:HIS:HB2	1.97	0.46
1:C:3420:UNK:HA	1:C:3421:UNK:HA	1.65	0.46
2:J:24:VAL:HG22	2:J:48:LYS:HG2	1.97	0.46
1:A:816:PRO:HB2	1:A:819:TYR:CD1	2.50	0.46
1:A:1677:LEU:HA	1:A:1680:HIS:HB2	1.97	0.46
1:A:2231:PRO:HG3	1:A:2381:ILE:HG12	1.98	0.46
1:A:4154:SER:O	1:A:4158:GLN:HG2	2.16	0.46
1:A:4194:ASP:HA	1:A:4599:PHE:HE2	1.79	0.46
1:B:646:THR:HG21	1:B:1685:GLN:NE2	2.31	0.46
1:B:1361:LYS:HA	1:B:1566:PRO:HA	1.98	0.46
1:B:4154:SER:O	1:B:4158:GLN:HG2	2.16	0.46
1:C:646:THR:HG21	1:C:1685:GLN:NE2	2.31	0.46
1:C:1224:LEU:HB3	1:C:1227:PHE:HB3	1.97	0.46
1:C:4154:SER:O	1:C:4158:GLN:HG2	2.16	0.46
1:D:1358:ARG:HB2	1:D:1567:LEU:HD21	1.97	0.46
1:A:750:ARG:NH2	2:G:9:SER:OG	2.47	0.46
1:A:1362:ASP:OD1	1:A:1362:ASP:N	2.49	0.46
1:B:1091:GLU:OE1	1:B:1093:THR:OG1	2.25	0.46
1:B:1936:GLN:O	1:B:1939:GLN:HG3	2.16	0.46
1:B:4601:ARG:HD3	1:B:4707:TRP:CZ2	2.50	0.46
1:C:2228:LEU:HD22	1:C:2296:ARG:HG3	1.98	0.46
1:C:2850:ILE:O	1:C:2854:LYS:HG2	2.15	0.46
1:D:23:GLN:HG3	1:D:213:SER:HB2	1.98	0.46
1:D:281:ARG:NH1	1:D:346:VAL:O	2.38	0.46
1:A:662:GLY:O	1:A:669:GLN:NE2	2.48	0.46
1:A:2477:ILE:O	1:A:2477:ILE:HG13	2.16	0.46
1:A:2740:TRP:CD1	1:A:2751:LYS:HE3	2.43	0.46
1:A:2764:GLU:O	1:A:2768:GLU:HG2	2.15	0.46
1:B:943:LEU:HG	1:B:999:LEU:CD1	2.46	0.46
1:B:986:ILE:HG13	1:B:987:LYS:N	2.29	0.46
1:B:1004:HIS:HB3	1:B:1035:TYR:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3899:GLU:OE2	1:B:3900:GLN:HG2	2.15	0.46
2:H:24:VAL:HG22	2:H:48:LYS:HG2	1.97	0.46
1:C:1174:MET:HG2	1:C:1190:LEU:HA	1.96	0.46
1:C:1311:ALA:HA	1:C:1312:UNK:HA	1.50	0.46
1:C:2325:ARG:HA	1:C:2325:ARG:HD3	1.82	0.46
1:C:4601:ARG:HD2	1:C:4711:VAL:HG21	1.98	0.46
1:D:646:THR:HG21	1:D:1685:GLN:NE2	2.31	0.46
1:A:934:GLN:O	1:A:938:GLU:HG2	2.16	0.46
1:A:999:LEU:HD23	1:A:1050:LEU:HG	1.98	0.46
1:A:4027:SER:HA	1:A:4032:LYS:HG2	1.96	0.46
1:B:1677:LEU:HA	1:B:1680:HIS:HB2	1.97	0.46
1:B:4027:SER:HA	1:B:4032:LYS:HG2	1.96	0.46
1:C:1004:HIS:HB3	1:C:1035:TYR:HB2	1.98	0.46
1:C:2771:ARG:O	1:C:2775:LYS:HD3	2.15	0.46
1:D:1677:LEU:HA	1:D:1680:HIS:HB2	1.97	0.46
1:D:2228:LEU:HD22	1:D:2296:ARG:HG3	1.98	0.46
1:D:2771:ARG:O	1:D:2775:LYS:HD3	2.15	0.46
1:D:4142:LYS:HA	1:D:4142:LYS:HD3	1.71	0.46
1:A:23:GLN:HG3	1:A:213:SER:HB2	1.98	0.46
1:A:1982:LYS:HD2	1:A:1983:SER:H	1.80	0.46
1:A:4601:ARG:HD2	1:A:4711:VAL:HG21	1.98	0.46
1:B:692:HIS:HB3	1:B:795:SER:HB3	1.98	0.46
1:B:895:MET:O	1:B:899:GLU:HG3	2.16	0.46
1:B:1733:GLU:O	1:B:1736:SER:OG	2.30	0.46
1:B:2477:ILE:HG13	1:B:2477:ILE:O	2.16	0.46
1:C:662:GLY:O	1:C:669:GLN:NE2	2.48	0.46
1:C:1731:THR:O	1:C:1734:THR:OG1	2.27	0.46
1:C:3729:ARG:O	1:C:3733:ARG:NH1	2.48	0.46
1:D:1224:LEU:HB3	1:D:1227:PHE:HB3	1.97	0.46
1:D:3729:ARG:O	1:D:3733:ARG:NH1	2.48	0.46
1:A:1358:ARG:HB2	1:A:1567:LEU:HD21	1.98	0.46
1:A:2228:LEU:HD22	1:A:2296:ARG:HG3	1.98	0.46
1:A:4029:ASP:N	1:A:4029:ASP:OD1	2.48	0.46
1:B:555:LEU:HD11	1:B:585:ALA:HB1	1.98	0.46
1:C:934:GLN:O	1:C:938:GLU:HG2	2.16	0.46
1:C:943:LEU:HG	1:C:999:LEU:CD1	2.46	0.46
1:C:2722:LYS:HZ1	1:C:2726:HIS:HB2	1.80	0.46
1:C:3899:GLU:OE2	1:C:3900:GLN:HG2	2.15	0.46
1:C:4121:ALA:O	1:C:4125:LEU:HG	2.16	0.46
2:I:24:VAL:HG22	2:I:48:LYS:HG2	1.97	0.46
1:D:3899:GLU:OE2	1:D:3900:GLN:HG2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4121:ALA:O	1:D:4125:LEU:HG	2.16	0.46
1:A:895:MET:O	1:A:899:GLU:HG3	2.16	0.45
1:A:2771:ARG:O	1:A:2775:LYS:HD3	2.15	0.45
1:B:1038:LEU:O	1:B:1043:LYS:HE3	2.16	0.45
1:B:1982:LYS:HD2	1:B:1983:SER:H	1.81	0.45
1:B:2764:GLU:O	1:B:2768:GLU:HG2	2.15	0.45
1:B:4586:ILE:HD11	1:B:4718:PHE:CE2	2.51	0.45
1:B:4852:PHE:HA	1:B:4856:ILE:HD12	1.99	0.45
1:C:318:ASP:N	1:C:318:ASP:OD1	2.47	0.45
1:C:2231:PRO:HG3	1:C:2381:ILE:HG12	1.98	0.45
1:C:4586:ILE:HD11	1:C:4718:PHE:CE2	2.51	0.45
1:D:934:GLN:O	1:D:938:GLU:HG2	2.16	0.45
1:D:2723:TYR:CE1	1:D:2770:TYR:HE2	2.33	0.45
1:D:4586:ILE:HD11	1:D:4718:PHE:CE2	2.51	0.45
1:A:3729:ARG:O	1:A:3733:ARG:NH1	2.48	0.45
1:B:1311:ALA:HA	1:B:1312:UNK:HA	1.50	0.45
1:B:4615:TYR:CE1	1:B:4631:ARG:HB2	2.51	0.45
1:D:1361:LYS:HA	1:D:1566:PRO:HA	1.98	0.45
1:D:2740:TRP:CD1	1:D:2751:LYS:HE3	2.43	0.45
1:B:2101:LEU:HA	1:B:2104:THR:HG22	1.97	0.45
1:B:2228:LEU:HD22	1:B:2296:ARG:HG3	1.98	0.45
1:C:1936:GLN:O	1:C:1939:GLN:HG3	2.16	0.45
1:C:4824:GLY:O	1:D:4821:ARG:NH2	2.49	0.45
1:D:4615:TYR:CE1	1:D:4631:ARG:HB2	2.51	0.45
1:A:55:SER:O	1:A:296:ARG:NH2	2.34	0.45
1:A:189:GLU:OE2	1:B:2321:ARG:NH1	2.49	0.45
1:A:1730:MET:SD	1:A:2106:THR:OG1	2.69	0.45
1:A:4929:GLU:HG2	1:A:4930:THR:H	1.82	0.45
1:C:555:LEU:HD11	1:C:585:ALA:HB1	1.99	0.45
1:C:1982:LYS:HD2	1:C:1983:SER:H	1.80	0.45
1:D:477:ASN:OD1	1:D:480:ARG:NH2	2.45	0.45
1:D:710:GLY:H	1:D:716:ASN:HD22	1.64	0.45
1:D:816:PRO:HB2	1:D:819:TYR:CD1	2.50	0.45
1:D:1936:GLN:O	1:D:1939:GLN:HG3	2.16	0.45
1:D:2405:MET:H	1:D:2405:MET:HG3	1.48	0.45
1:A:836:HIS:NE2	1:A:842:GLN:OE1	2.46	0.45
1:A:1004:HIS:HB3	1:A:1035:TYR:HB2	1.97	0.45
1:A:4615:TYR:CE1	1:A:4631:ARG:HB2	2.51	0.45
1:B:23:GLN:HG3	1:B:213:SER:HB2	1.98	0.45
1:B:477:ASN:OD1	1:B:480:ARG:NH2	2.45	0.45
1:B:934:GLN:O	1:B:938:GLU:HG2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:999:LEU:HD23	1:B:1050:LEU:HG	1.98	0.45
1:B:2231:PRO:HG3	1:B:2381:ILE:HG12	1.97	0.45
1:C:895:MET:O	1:C:899:GLU:HG3	2.16	0.45
1:C:2154:PHE:CD2	1:C:2205:ILE:HD11	2.52	0.45
1:D:167:LYS:HB2	1:D:167:LYS:HE2	1.48	0.45
1:D:1586:ARG:NH2	1:D:1635:GLU:OE1	2.50	0.45
1:A:555:LEU:HD11	1:A:585:ALA:HB1	1.98	0.45
1:A:2101:LEU:HA	1:A:2104:THR:HG22	1.97	0.45
1:A:2154:PHE:CD2	1:A:2205:ILE:HD11	2.52	0.45
1:B:2507:SER:O	1:B:2507:SER:OG	2.35	0.45
1:B:4044:LYS:HZ1	1:B:4071:THR:H	1.64	0.45
1:C:2477:ILE:O	1:C:2477:ILE:HG13	2.16	0.45
1:D:439:LYS:HE2	1:D:439:LYS:HB3	1.59	0.45
1:D:1982:LYS:HD2	1:D:1983:SER:N	2.31	0.45
1:D:2342:LEU:HD21	1:D:2467:MET:HE3	1.98	0.45
1:D:3420:UNK:HA	1:D:3421:UNK:HA	1.65	0.45
1:D:4601:ARG:HD2	1:D:4711:VAL:HG21	1.98	0.45
1:D:4929:GLU:HG2	1:D:4930:THR:H	1.82	0.45
1:A:318:ASP:N	1:A:318:ASP:OD1	2.47	0.45
1:A:439:LYS:HB3	1:A:439:LYS:HE2	1.59	0.45
1:A:1982:LYS:HD2	1:A:1983:SER:N	2.31	0.45
1:A:2507:SER:O	1:A:2507:SER:OG	2.34	0.45
1:A:4586:ILE:HD11	1:A:4718:PHE:CE2	2.51	0.45
1:A:4850:PHE:CD2	1:B:4821:ARG:HG2	2.52	0.45
1:B:1730:MET:SD	1:B:2106:THR:OG1	2.69	0.45
1:B:2134:GLY:H	1:B:2137:GLU:HB2	1.82	0.45
1:B:4121:ALA:O	1:B:4125:LEU:HG	2.17	0.45
1:B:4122:GLU:HA	1:B:4125:LEU:HD12	1.99	0.45
1:C:2084:PHE:O	1:C:3690:TYR:OH	2.25	0.45
1:D:895:MET:O	1:D:899:GLU:HG3	2.16	0.45
1:D:4044:LYS:HZ2	1:D:4069:ALA:HB1	1.82	0.45
1:D:4154:SER:O	1:D:4158:GLN:HG2	2.16	0.45
1:A:710:GLY:H	1:A:716:ASN:HD22	1.64	0.45
1:A:1038:LEU:O	1:A:1043:LYS:HE3	2.16	0.45
1:A:1272:ARG:NH2	1:A:1583:CYS:SG	2.90	0.45
1:A:1361:LYS:HA	1:A:1566:PRO:HA	1.98	0.45
1:A:2091:TYR:CE2	1:A:3639:LEU:HD13	2.52	0.45
1:B:2154:PHE:CD2	1:B:2205:ILE:HD11	2.52	0.45
1:B:2414:GLU:H	1:B:2414:GLU:CD	2.20	0.45
1:B:3860:GLN:NE2	1:B:3867:VAL:H	2.15	0.45
1:C:477:ASN:OD1	1:C:480:ARG:NH2	2.45	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:661:LEU:HD22	1:C:673:TRP:NE1	2.32	0.45
1:C:1572:PHE:HZ	1:C:1587:LEU:HD11	1.82	0.45
1:C:1982:LYS:HD2	1:C:1983:SER:N	2.31	0.45
1:C:4142:LYS:HD3	1:C:4142:LYS:HA	1.71	0.45
1:D:2134:GLY:H	1:D:2137:GLU:HB2	1.82	0.45
1:A:646:THR:HG21	1:A:1685:GLN:NE2	2.31	0.45
1:A:2134:GLY:H	1:A:2137:GLU:HB2	1.82	0.45
1:A:2206:SER:HB2	1:A:2209:ASN:HD22	1.82	0.45
1:B:299:HIS:HD2	1:B:302:THR:HG22	1.82	0.45
1:C:299:HIS:HD2	1:C:302:THR:HG22	1.82	0.45
1:C:1733:GLU:O	1:C:1736:SER:OG	2.30	0.45
2:I:58:LYS:HA	2:I:61:GLU:HG3	1.99	0.45
1:D:24:CYS:HB3	1:D:212:TRP:CE3	2.52	0.45
1:D:692:HIS:HB3	1:D:795:SER:HB3	1.98	0.45
1:D:999:LEU:HD23	1:D:1050:LEU:HG	1.98	0.45
1:D:2206:SER:HB2	1:D:2209:ASN:HD22	1.82	0.45
1:D:2477:ILE:HG13	1:D:2477:ILE:O	2.16	0.45
1:A:4813:MET:HG3	1:D:4843:ILE:CD1	2.45	0.45
1:B:710:GLY:H	1:B:716:ASN:ND2	2.15	0.45
1:B:1982:LYS:HD2	1:B:1983:SER:N	2.31	0.45
1:C:1272:ARG:NH2	1:C:1583:CYS:SG	2.90	0.45
1:C:1586:ARG:NH2	1:C:1635:GLU:OE1	2.50	0.45
1:C:2206:SER:HB2	1:C:2209:ASN:HD22	1.82	0.45
1:C:4852:PHE:HA	1:C:4856:ILE:HD12	1.99	0.45
1:D:836:HIS:CG	1:D:841:LYS:HB3	2.52	0.45
1:D:1004:HIS:HB3	1:D:1035:TYR:HB2	1.98	0.45
1:D:1572:PHE:HZ	1:D:1587:LEU:HD11	1.82	0.45
1:D:2231:PRO:HG3	1:D:2381:ILE:HG12	1.98	0.45
1:D:4852:PHE:HA	1:D:4856:ILE:HD12	1.99	0.45
1:A:61:ASP:HB3	1:A:64:ILE:HG12	1.99	0.44
1:A:297:LEU:HD13	1:A:297:LEU:HA	1.81	0.44
1:A:606:ARG:HH22	1:A:1635:GLU:HG2	1.82	0.44
1:A:943:LEU:HG	1:A:999:LEU:CD1	2.46	0.44
1:A:1001:GLU:OE2	1:A:1035:TYR:HB3	2.17	0.44
1:A:2084:PHE:O	1:A:3690:TYR:OH	2.25	0.44
1:A:3920:THR:HG22	1:A:3980:MET:HA	1.99	0.44
1:B:313:ASN:ND2	1:B:391:ALA:O	2.45	0.44
1:B:1272:ARG:NH2	1:B:1583:CYS:SG	2.90	0.44
1:C:999:LEU:HD23	1:C:1050:LEU:HG	1.98	0.44
1:C:1362:ASP:N	1:C:1362:ASP:OD1	2.49	0.44
1:C:4929:GLU:HG2	1:C:4930:THR:H	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:675:TYR:CE1	1:D:790:PRO:HB3	2.52	0.44
1:D:775:VAL:HG23	1:D:777:GLY:H	1.82	0.44
1:A:14:LEU:HD11	1:A:214:VAL:HG21	1.99	0.44
1:A:836:HIS:CG	1:A:841:LYS:HB3	2.52	0.44
1:A:4121:ALA:O	1:A:4125:LEU:HG	2.16	0.44
1:A:4852:PHE:HA	1:A:4856:ILE:HD12	1.99	0.44
1:B:24:CYS:HB3	1:B:212:TRP:CE3	2.52	0.44
1:B:61:ASP:HB3	1:B:64:ILE:HG12	1.99	0.44
1:B:2741:ILE:HD12	1:B:2741:ILE:HA	1.72	0.44
1:B:3876:TYR:HD1	1:B:3879:ARG:HH21	1.66	0.44
1:C:710:GLY:H	1:C:716:ASN:ND2	2.15	0.44
1:C:775:VAL:HG23	1:C:777:GLY:H	1.82	0.44
1:C:1001:GLU:OE2	1:C:1035:TYR:HB3	2.17	0.44
1:C:1962:ARG:HH21	1:C:1963:GLU:HA	1.83	0.44
1:D:926:GLU:H	1:D:926:GLU:HG2	1.54	0.44
1:D:1038:LEU:O	1:D:1043:LYS:HE3	2.16	0.44
1:D:2091:TYR:CE2	1:D:3639:LEU:HD13	2.52	0.44
1:D:2501:LEU:HD11	1:D:2505:ALA:HB2	1.99	0.44
1:D:4079:TYR:O	1:D:4083:VAL:HG22	2.17	0.44
1:D:4116:THR:O	1:D:4119:GLU:HG2	2.17	0.44
1:A:3860:GLN:NE2	1:A:3867:VAL:H	2.15	0.44
1:B:836:HIS:CG	1:B:841:LYS:HB3	2.52	0.44
1:B:1060:TYR:HD1	1:B:1060:TYR:N	2.08	0.44
1:C:61:ASP:HB3	1:C:64:ILE:HG12	1.99	0.44
1:C:710:GLY:H	1:C:716:ASN:HD22	1.64	0.44
1:C:821:ALA:HB3	1:C:823:TYR:CE1	2.52	0.44
1:C:2091:TYR:CE2	1:C:3639:LEU:HD13	2.52	0.44
1:C:4029:ASP:OD1	1:C:4029:ASP:N	2.48	0.44
1:C:4079:TYR:O	1:C:4083:VAL:HG22	2.17	0.44
1:C:4615:TYR:CE1	1:C:4631:ARG:HB2	2.51	0.44
1:D:626:ARG:NH2	1:D:1669:GLY:O	2.51	0.44
1:D:3876:TYR:HD1	1:D:3879:ARG:HH21	1.65	0.44
1:D:3923:ILE:HD12	1:D:3984:MET:HG2	1.99	0.44
1:A:299:HIS:HD2	1:A:302:THR:HG22	1.82	0.44
1:A:1140:PHE:HD2	1:A:1141:LYS:HD2	1.83	0.44
1:B:14:LEU:HD11	1:B:214:VAL:HG21	1.99	0.44
1:B:1962:ARG:HH21	1:B:1963:GLU:HA	1.83	0.44
1:B:2206:SER:HB2	1:B:2209:ASN:HD22	1.82	0.44
1:B:4630:ASP:O	1:B:4634:ILE:HG23	2.18	0.44
1:C:24:CYS:HB3	1:C:212:TRP:CE3	2.52	0.44
1:C:675:TYR:CE1	1:C:790:PRO:HB3	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1038:LEU:O	1:C:1043:LYS:HE3	2.16	0.44
1:C:3920:THR:HG22	1:C:3980:MET:HA	1.99	0.44
1:C:3923:ILE:HD12	1:C:3984:MET:HG2	1.99	0.44
1:C:4116:THR:O	1:C:4119:GLU:HG2	2.17	0.44
1:C:4122:GLU:HA	1:C:4125:LEU:HD12	1.99	0.44
1:D:661:LEU:HD22	1:D:673:TRP:NE1	2.32	0.44
1:D:710:GLY:H	1:D:716:ASN:ND2	2.15	0.44
1:D:1001:GLU:OE2	1:D:1035:TYR:HB3	2.17	0.44
1:D:1196:ASP:OD1	1:D:1196:ASP:N	2.51	0.44
1:D:1272:ARG:NH2	1:D:1583:CYS:SG	2.90	0.44
1:D:1962:ARG:HH21	1:D:1963:GLU:HA	1.83	0.44
1:A:692:HIS:HB3	1:A:795:SER:HB3	1.98	0.44
1:A:1733:GLU:O	1:A:1736:SER:OG	2.30	0.44
1:A:4116:THR:O	1:A:4119:GLU:HG2	2.17	0.44
1:B:661:LEU:HD22	1:B:673:TRP:NE1	2.32	0.44
1:B:710:GLY:H	1:B:716:ASN:HD22	1.64	0.44
1:B:1140:PHE:HD2	1:B:1141:LYS:HD2	1.83	0.44
1:C:1190:LEU:HD11	1:C:1193:LYS:HE3	1.99	0.44
1:D:299:HIS:HD2	1:D:302:THR:HG22	1.82	0.44
1:D:1190:LEU:HD11	1:D:1193:LYS:HE3	1.99	0.44
1:D:3982:LEU:HD21	1:D:4100:LEU:HA	2.00	0.44
1:A:24:CYS:HB3	1:A:212:TRP:CE3	2.52	0.44
1:A:710:GLY:H	1:A:716:ASN:ND2	2.15	0.44
1:A:821:ALA:HB3	1:A:823:TYR:CE1	2.52	0.44
1:A:1586:ARG:NH2	1:A:1635:GLU:OE1	2.50	0.44
1:A:1680:HIS:CE1	2:G:91:VAL:HA	2.53	0.44
1:A:2501:LEU:HD11	1:A:2505:ALA:HB2	1.99	0.44
1:A:3982:LEU:HD21	1:A:4100:LEU:HA	2.00	0.44
1:A:4821:ARG:HG2	1:D:4850:PHE:CD2	2.53	0.44
1:B:626:ARG:NH2	1:B:1669:GLY:O	2.51	0.44
1:B:2091:TYR:CE2	1:B:3639:LEU:HD13	2.52	0.44
1:C:2134:GLY:H	1:C:2137:GLU:HB2	1.82	0.44
1:C:2414:GLU:H	1:C:2414:GLU:CD	2.20	0.44
1:D:555:LEU:HD11	1:D:585:ALA:HB1	1.98	0.44
1:D:1754:LEU:HD23	1:D:1754:LEU:HA	1.86	0.44
1:A:505:LEU:HD22	1:A:526:TRP:HD1	1.83	0.44
1:A:1196:ASP:OD1	1:A:1196:ASP:N	2.51	0.44
1:A:1819:PHE:O	1:A:1823:ILE:HG12	2.18	0.44
1:A:1976:LEU:HD11	1:A:3619:PHE:CE2	2.53	0.44
1:A:4122:GLU:HA	1:A:4125:LEU:HD12	1.99	0.44
1:B:4023:LYS:HG3	1:B:4087:HIS:CG	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4601:ARG:HD2	1:B:4711:VAL:HG21	1.98	0.44
2:H:58:LYS:HA	2:H:61:GLU:HG3	1.99	0.44
1:D:606:ARG:HH22	1:D:1635:GLU:HG2	1.82	0.44
1:D:821:ALA:HB3	1:D:823:TYR:CE1	2.52	0.44
1:D:2154:PHE:CD2	1:D:2205:ILE:HD11	2.52	0.44
1:D:2253:ALA:O	1:D:2315:ASN:ND2	2.40	0.44
1:D:4630:ASP:O	1:D:4634:ILE:HG23	2.18	0.44
1:A:1119:ARG:NH2	1:A:1196:ASP:OD1	2.51	0.44
1:A:1250:TRP:CH2	1:A:1644:GLU:HG3	2.53	0.44
1:A:2463:HIS:O	1:A:2467:MET:HG2	2.18	0.44
1:A:4821:ARG:HD3	1:D:4847:ILE:HA	2.00	0.44
1:B:675:TYR:CE1	1:B:790:PRO:HB3	2.52	0.44
1:B:1001:GLU:OE2	1:B:1035:TYR:HB3	2.17	0.44
1:B:1119:ARG:NH2	1:B:1196:ASP:OD1	2.51	0.44
1:B:1250:TRP:CH2	1:B:1644:GLU:HG3	2.53	0.44
1:B:1296:ASN:OD1	1:B:1296:ASN:N	2.51	0.44
1:B:1754:LEU:HD23	1:B:1754:LEU:HA	1.86	0.44
1:B:2740:TRP:CD1	1:B:2751:LYS:HE3	2.43	0.44
1:B:3923:ILE:HD12	1:B:3984:MET:HG2	1.99	0.44
1:B:4116:THR:O	1:B:4119:GLU:HG2	2.17	0.44
1:C:14:LEU:HD11	1:C:214:VAL:HG21	1.99	0.44
1:C:836:HIS:CG	1:C:841:LYS:HB3	2.53	0.44
1:C:3860:GLN:NE2	1:C:3867:VAL:H	2.15	0.44
1:C:4708:LYS:O	1:C:4712:VAL:HG13	2.18	0.44
1:D:61:ASP:HB3	1:D:64:ILE:HG12	1.99	0.44
1:D:1976:LEU:HD11	1:D:3619:PHE:CE2	2.53	0.44
1:D:2722:LYS:HZ1	1:D:2726:HIS:HB2	1.81	0.44
1:D:3712:SER:OG	1:D:3716:LYS:NZ	2.35	0.44
1:D:3920:THR:HG22	1:D:3980:MET:HA	1.99	0.44
1:A:2320:VAL:O	1:A:2324:ILE:HG12	2.18	0.44
1:A:3923:ILE:HD12	1:A:3984:MET:HG2	1.99	0.44
1:A:4023:LYS:HG3	1:A:4087:HIS:CG	2.53	0.44
1:A:4044:LYS:HZ2	1:A:4069:ALA:HB1	1.83	0.44
1:A:4821:ARG:O	1:D:4824:GLY:HA3	2.16	0.44
1:A:4833:PRO:HD3	1:A:4842:ARG:NE	2.25	0.44
2:G:58:LYS:HA	2:G:61:GLU:HG3	1.99	0.44
1:B:1346:LEU:HD23	1:B:1347:MET:O	2.18	0.44
1:B:4929:GLU:HG2	1:B:4930:THR:H	1.82	0.44
1:C:654:SER:H	1:C:841:LYS:HZ3	1.64	0.44
1:C:1196:ASP:OD1	1:C:1196:ASP:N	2.51	0.44
1:C:1250:TRP:CH2	1:C:1644:GLU:HG3	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3950:PHE:HZ	1:C:3973:LEU:HG	1.83	0.44
1:D:943:LEU:HG	1:D:999:LEU:CD1	2.46	0.44
1:D:4023:LYS:HG3	1:D:4087:HIS:CG	2.53	0.44
1:A:884:ARG:O	1:A:887:GLU:HG3	2.18	0.43
1:B:190:ARG:HB2	1:B:205:ALA:HB1	2.00	0.43
1:B:1397:UNK:HA	1:B:1412:UNK:HA	2.00	0.43
1:B:1586:ARG:NH2	1:B:1635:GLU:OE1	2.50	0.43
1:B:1680:HIS:CE1	2:H:91:VAL:HA	2.53	0.43
1:B:3982:LEU:HD21	1:B:4100:LEU:HA	2.00	0.43
1:C:626:ARG:NH2	1:C:1669:GLY:O	2.51	0.43
1:C:884:ARG:O	1:C:887:GLU:HG3	2.18	0.43
1:C:1976:LEU:HD11	1:C:3619:PHE:CE2	2.53	0.43
2:J:58:LYS:HA	2:J:61:GLU:HG3	1.99	0.43
1:A:661:LEU:HD22	1:A:673:TRP:NE1	2.32	0.43
1:A:675:TYR:CE1	1:A:790:PRO:HB3	2.52	0.43
1:A:1962:ARG:HH21	1:A:1963:GLU:HA	1.83	0.43
1:A:2741:ILE:HD12	1:A:2741:ILE:HA	1.72	0.43
1:B:20:VAL:HG22	1:B:21:VAL:N	2.33	0.43
1:B:821:ALA:HB3	1:B:823:TYR:CE1	2.52	0.43
1:B:1731:THR:O	1:B:1734:THR:OG1	2.27	0.43
1:B:1819:PHE:O	1:B:1823:ILE:HG12	2.18	0.43
1:B:2501:LEU:HD11	1:B:2505:ALA:HB2	1.99	0.43
1:C:1119:ARG:NH2	1:C:1196:ASP:OD1	2.51	0.43
1:C:2320:VAL:O	1:C:2324:ILE:HG12	2.18	0.43
1:C:2463:HIS:O	1:C:2467:MET:HG2	2.18	0.43
1:C:2501:LEU:HD11	1:C:2505:ALA:HB2	1.99	0.43
1:C:2740:TRP:CD1	1:C:2751:LYS:HE3	2.43	0.43
1:D:884:ARG:O	1:D:887:GLU:HG3	2.18	0.43
1:D:1140:PHE:HD2	1:D:1141:LYS:HD2	1.83	0.43
1:D:2463:HIS:O	1:D:2467:MET:HG2	2.18	0.43
1:D:4122:GLU:HA	1:D:4125:LEU:HD12	1.99	0.43
1:B:748:LEU:HD13	1:B:748:LEU:HA	1.77	0.43
1:B:1040:ASP:HA	1:B:1043:LYS:HD2	2.01	0.43
1:B:3920:THR:HG22	1:B:3980:MET:HA	1.99	0.43
1:C:894:VAL:O	1:C:898:ILE:HG13	2.19	0.43
1:C:4023:LYS:HG3	1:C:4087:HIS:CG	2.53	0.43
1:D:190:ARG:HB2	1:D:205:ALA:HB1	2.00	0.43
1:D:1250:TRP:CH2	1:D:1644:GLU:HG3	2.53	0.43
1:D:1346:LEU:HD23	1:D:1347:MET:O	2.18	0.43
1:D:1712:LEU:HD22	1:D:1832:MET:SD	2.58	0.43
1:D:2414:GLU:H	1:D:2414:GLU:CD	2.20	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ARG:HD3	1:A:205:ALA:O	2.19	0.43
1:A:654:SER:H	1:A:841:LYS:HZ3	1.64	0.43
1:B:1190:LEU:HD11	1:B:1193:LYS:HE3	1.99	0.43
1:B:2853:LYS:HD3	1:B:2853:LYS:HA	1.68	0.43
1:B:3712:SER:OG	1:B:3716:LYS:NZ	2.35	0.43
1:B:4079:TYR:O	1:B:4083:VAL:HG22	2.17	0.43
1:B:4197:PHE:HB2	1:B:4644:TRP:HZ3	1.83	0.43
1:C:235:ARG:NH1	1:C:412:GLU:OE2	2.51	0.43
1:C:728:ASP:O	1:C:749:LEU:HG	2.19	0.43
1:C:1730:MET:SD	1:C:2106:THR:OG1	2.69	0.43
1:D:1119:ARG:NH2	1:D:1196:ASP:OD1	2.51	0.43
1:A:626:ARG:NH2	1:A:1669:GLY:O	2.51	0.43
1:A:1190:LEU:HD11	1:A:1193:LYS:HE3	2.00	0.43
1:A:1572:PHE:HZ	1:A:1587:LEU:HD11	1.82	0.43
1:A:4079:TYR:O	1:A:4083:VAL:HG22	2.17	0.43
1:B:606:ARG:HH22	1:B:1635:GLU:HG2	1.82	0.43
1:B:687:THR:OG1	1:B:1627:GLN:NE2	2.52	0.43
1:C:62:LEU:HD11	1:C:282:VAL:HG23	2.01	0.43
1:C:1346:LEU:HD23	1:C:1347:MET:O	2.18	0.43
1:C:1819:PHE:O	1:C:1823:ILE:HG12	2.18	0.43
1:D:505:LEU:HD22	1:D:526:TRP:HD1	1.83	0.43
1:D:562:LEU:HD21	1:D:600:LEU:HD22	2.00	0.43
1:D:2321:ARG:O	1:D:2325:ARG:HG2	2.18	0.43
1:A:34:LYS:HB3	1:A:34:LYS:HE3	1.92	0.43
1:A:1712:LEU:HD22	1:A:1832:MET:SD	2.58	0.43
1:A:4197:PHE:HB2	1:A:4644:TRP:HZ3	1.83	0.43
1:B:190:ARG:HD3	1:B:205:ALA:O	2.19	0.43
1:B:775:VAL:HG23	1:B:777:GLY:H	1.82	0.43
1:C:2741:ILE:HD12	1:C:2741:ILE:HA	1.72	0.43
1:C:3982:LEU:HD21	1:C:4100:LEU:HA	2.00	0.43
1:C:4197:PHE:HB2	1:C:4644:TRP:HZ3	1.83	0.43
1:C:4630:ASP:O	1:C:4634:ILE:HG23	2.18	0.43
1:D:137:ARG:HH21	1:D:202:HIS:CD2	2.37	0.43
1:D:1040:ASP:HA	1:D:1043:LYS:HD2	2.01	0.43
1:D:2320:VAL:O	1:D:2324:ILE:HG12	2.18	0.43
1:D:2853:LYS:HA	1:D:2853:LYS:HD3	1.68	0.43
1:A:331:PHE:HE1	1:A:363:ILE:HG22	1.84	0.43
1:A:934:GLN:OE1	1:A:935:MET:N	2.52	0.43
1:A:939:THR:O	1:A:999:LEU:HD11	2.19	0.43
1:A:3876:TYR:HD1	1:A:3879:ARG:HH21	1.66	0.43
1:B:137:ARG:HH21	1:B:202:HIS:CD2	2.37	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:LEU:HD22	1:B:526:TRP:HD1	1.83	0.43
1:B:894:VAL:O	1:B:898:ILE:HG13	2.19	0.43
1:B:934:GLN:OE1	1:B:935:MET:N	2.52	0.43
1:B:2253:ALA:O	1:B:2315:ASN:ND2	2.40	0.43
1:B:3950:PHE:HZ	1:B:3973:LEU:HG	1.83	0.43
1:C:20:VAL:HG22	1:C:21:VAL:N	2.33	0.43
1:C:190:ARG:HD3	1:C:205:ALA:O	2.19	0.43
1:C:224:ALA:HB3	1:C:227:TYR:HD2	1.84	0.43
1:C:297:LEU:HD13	1:C:297:LEU:HA	1.81	0.43
1:C:669:GLN:HB3	1:C:673:TRP:HZ2	1.83	0.43
1:C:687:THR:OG1	1:C:1627:GLN:NE2	2.52	0.43
1:C:1140:PHE:HD2	1:C:1141:LYS:HD2	1.83	0.43
1:C:3763:ALA:HA	1:C:3766:ASN:ND2	2.34	0.43
1:C:3961:SER:OG	1:C:3962:SER:N	2.52	0.43
1:D:687:THR:OG1	1:D:1627:GLN:NE2	2.52	0.43
1:D:1311:ALA:HA	1:D:1312:UNK:HA	1.50	0.43
1:D:1397:UNK:HA	1:D:1412:UNK:HA	2.00	0.43
1:D:2428:LEU:HD21	1:D:2482:PHE:CE1	2.54	0.43
1:D:2507:SER:O	1:D:2507:SER:OG	2.35	0.43
1:D:4708:LYS:O	1:D:4712:VAL:HG13	2.18	0.43
1:A:137:ARG:HH21	1:A:202:HIS:CD2	2.37	0.43
1:A:235:ARG:NH1	1:A:412:GLU:OE2	2.51	0.43
1:A:669:GLN:HB3	1:A:673:TRP:HZ2	1.83	0.43
1:A:775:VAL:HG23	1:A:777:GLY:H	1.82	0.43
1:A:1826:PHE:CE1	1:A:1843:ILE:HG21	2.54	0.43
1:A:3950:PHE:HZ	1:A:3973:LEU:HG	1.83	0.43
1:A:3961:SER:OG	1:A:3962:SER:N	2.52	0.43
1:B:19:GLU:HB2	1:B:217:ILE:HB	2.01	0.43
1:B:235:ARG:NH1	1:B:412:GLU:OE2	2.51	0.43
1:B:1712:LEU:HD22	1:B:1832:MET:SD	2.58	0.43
1:B:3763:ALA:HA	1:B:3766:ASN:ND2	2.34	0.43
1:C:137:ARG:HH21	1:C:202:HIS:CD2	2.37	0.43
1:C:191:TYR:OH	1:D:2325:ARG:NH1	2.51	0.43
1:C:606:ARG:HH22	1:C:1635:GLU:HG2	1.82	0.43
1:C:1712:LEU:HD22	1:C:1832:MET:SD	2.58	0.43
1:D:331:PHE:HE1	1:D:363:ILE:HG22	1.84	0.43
1:D:728:ASP:O	1:D:749:LEU:HG	2.19	0.43
1:D:1684:PRO:HD3	2:J:42:ASP:HB3	2.00	0.43
1:D:1819:PHE:O	1:D:1823:ILE:HG12	2.18	0.43
1:D:3961:SER:OG	1:D:3962:SER:N	2.52	0.43
1:D:4841:TYR:O	1:D:4844:ILE:HG22	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:29:GLY:N	2:J:38:ASP:O	2.48	0.43
1:A:20:VAL:HG22	1:A:21:VAL:N	2.33	0.43
1:A:728:ASP:O	1:A:749:LEU:HG	2.19	0.43
1:A:1909:LEU:HD13	1:A:2061:ILE:HG12	2.01	0.43
1:A:4630:ASP:O	1:A:4634:ILE:HG23	2.18	0.43
1:A:4708:LYS:O	1:A:4712:VAL:HG13	2.18	0.43
1:B:669:GLN:HB3	1:B:673:TRP:HZ2	1.83	0.43
1:B:1196:ASP:OD1	1:B:1196:ASP:N	2.51	0.43
1:B:1572:PHE:HZ	1:B:1587:LEU:HD11	1.82	0.43
1:B:2428:LEU:HD21	1:B:2482:PHE:CE1	2.53	0.43
1:C:750:ARG:NH2	2:I:9:SER:OG	2.47	0.43
2:I:79:PRO:HB3	2:I:95:ASN:HA	2.01	0.43
2:I:93:PRO:HG2	2:I:96:ALA:HB2	2.01	0.43
1:D:14:LEU:HD11	1:D:214:VAL:HG21	1.99	0.43
1:D:62:LEU:HD11	1:D:282:VAL:HG23	2.01	0.43
1:D:1826:PHE:CE1	1:D:1843:ILE:HG21	2.54	0.43
1:D:1901:VAL:O	1:D:1905:MET:HG2	2.19	0.43
2:J:93:PRO:HG2	2:J:96:ALA:HB2	2.01	0.43
1:A:674:TYR:HE1	1:A:756:SER:HB2	1.83	0.43
1:A:1397:UNK:HA	1:A:1412:UNK:HA	2.00	0.43
1:A:1841:LYS:O	1:A:1845:GLN:HG2	2.19	0.43
2:G:83:TYR:HB3	2:G:87:GLY:HA2	2.01	0.43
1:B:62:LEU:HD11	1:B:282:VAL:HG23	2.01	0.43
1:B:167:LYS:HE2	1:B:167:LYS:HB2	1.48	0.43
1:B:562:LEU:HD21	1:B:600:LEU:HD22	2.00	0.43
1:B:884:ARG:O	1:B:887:GLU:HG3	2.18	0.43
1:B:1909:LEU:HD13	1:B:2061:ILE:HG12	2.01	0.43
1:B:1976:LEU:HD11	1:B:3619:PHE:CE2	2.53	0.43
1:C:190:ARG:HB2	1:C:205:ALA:HB1	2.00	0.43
1:C:555:LEU:HD13	1:C:589:ILE:HD11	2.01	0.43
1:C:686:VAL:HG13	1:C:687:THR:N	2.34	0.43
1:C:894:VAL:HG21	1:C:976:TYR:HE2	1.83	0.43
1:D:555:LEU:HD13	1:D:589:ILE:HD11	2.01	0.43
2:J:79:PRO:HB3	2:J:95:ASN:HA	2.00	0.43
1:A:19:GLU:HG2	1:A:68:VAL:HG22	2.01	0.42
1:A:224:ALA:HB3	1:A:227:TYR:HD2	1.84	0.42
1:A:363:ILE:HG12	1:A:372:LEU:HD22	2.01	0.42
1:A:562:LEU:HD21	1:A:600:LEU:HD22	2.00	0.42
1:A:2065:MET:SD	1:A:2083:MET:HG3	2.59	0.42
1:A:2171:MET:O	1:A:2175:VAL:HG13	2.19	0.42
1:A:2224:SER:OG	1:A:2239:LEU:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:79:PRO:HB3	2:G:95:ASN:HA	2.01	0.42
1:B:1901:VAL:O	1:B:1905:MET:HG2	2.19	0.42
1:B:2065:MET:SD	1:B:2083:MET:HG3	2.59	0.42
1:B:2113:GLU:OE1	1:B:2113:GLU:N	2.37	0.42
1:B:2320:VAL:O	1:B:2324:ILE:HG12	2.18	0.42
1:B:2463:HIS:O	1:B:2467:MET:HG2	2.18	0.42
1:B:4841:TYR:O	1:B:4844:ILE:HG22	2.19	0.42
2:H:93:PRO:HG2	2:H:96:ALA:HB2	2.01	0.42
1:C:748:LEU:HD13	1:C:748:LEU:HA	1.77	0.42
1:C:939:THR:O	1:C:999:LEU:HD11	2.19	0.42
1:C:1397:UNK:HA	1:C:1412:UNK:HA	2.00	0.42
1:C:1704:TYR:CG	1:C:1821:PRO:HB2	2.54	0.42
1:C:2321:ARG:O	1:C:2325:ARG:HG2	2.18	0.42
1:C:3728:ALA:HA	1:C:3731:HIS:ND1	2.34	0.42
1:D:20:VAL:HG22	1:D:21:VAL:N	2.33	0.42
1:D:894:VAL:HG21	1:D:976:TYR:HE2	1.83	0.42
1:D:939:THR:O	1:D:999:LEU:HD11	2.19	0.42
1:A:190:ARG:HB2	1:A:205:ALA:HB1	2.00	0.42
1:A:2223:ASN:O	1:A:2226:VAL:HG22	2.19	0.42
2:G:27:TYR:O	2:G:40:SER:N	2.53	0.42
2:G:93:PRO:HG2	2:G:96:ALA:HB2	2.01	0.42
1:B:331:PHE:HE1	1:B:363:ILE:HG22	1.84	0.42
1:B:555:LEU:HD13	1:B:589:ILE:HD11	2.01	0.42
1:B:686:VAL:HG13	1:B:687:THR:N	2.34	0.42
1:B:2102:PRO:HD3	1:B:3624:GLU:HG3	2.01	0.42
1:B:3804:LEU:HD21	1:B:3890:TYR:HB2	2.01	0.42
2:H:79:PRO:HB3	2:H:95:ASN:HA	2.00	0.42
1:C:562:LEU:HD21	1:C:600:LEU:HD22	2.00	0.42
1:C:1909:LEU:HD13	1:C:2061:ILE:HG12	2.01	0.42
1:D:19:GLU:HB2	1:D:217:ILE:HB	2.01	0.42
1:D:363:ILE:HG12	1:D:372:LEU:HD22	2.01	0.42
1:D:2223:ASN:O	1:D:2226:VAL:HG22	2.19	0.42
1:D:2741:ILE:HD12	1:D:2741:ILE:HA	1.72	0.42
1:D:3727:GLN:O	1:D:3731:HIS:ND1	2.41	0.42
1:D:4197:PHE:HB2	1:D:4644:TRP:HZ3	1.83	0.42
1:A:514:PHE:HD2	1:A:523:GLY:HA2	1.84	0.42
1:A:2414:GLU:H	1:A:2414:GLU:CD	2.20	0.42
1:B:224:ALA:HB3	1:B:227:TYR:HD2	1.84	0.42
1:B:728:ASP:O	1:B:749:LEU:HG	2.19	0.42
1:B:754:VAL:HG21	1:B:812:LYS:HD3	2.01	0.42
1:B:1704:TYR:CG	1:B:1821:PRO:HB2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1826:PHE:CE1	1:B:1843:ILE:HG21	2.54	0.42
1:B:2224:SER:OG	1:B:2239:LEU:HB2	2.19	0.42
1:B:4708:LYS:O	1:B:4712:VAL:HG13	2.18	0.42
1:B:4798:GLY:HA3	1:B:4799:ASP:HA	1.85	0.42
1:C:1353:HIS:CE1	1:C:1367:LYS:HD2	2.55	0.42
1:D:224:ALA:HB3	1:D:227:TYR:HD2	1.84	0.42
1:D:489:PHE:HD2	1:D:494:MET:HG2	1.84	0.42
1:D:882:ARG:NH2	1:D:944:LEU:HD21	2.35	0.42
1:D:3860:GLN:NE2	1:D:3867:VAL:H	2.15	0.42
1:A:489:PHE:HD2	1:A:494:MET:HG2	1.84	0.42
1:A:894:VAL:O	1:A:898:ILE:HG13	2.19	0.42
1:A:894:VAL:HG21	1:A:976:TYR:HE2	1.83	0.42
1:A:1353:HIS:CE1	1:A:1367:LYS:HD2	2.55	0.42
1:A:2321:ARG:O	1:A:2325:ARG:HG2	2.18	0.42
1:A:3728:ALA:HA	1:A:3731:HIS:ND1	2.34	0.42
1:A:3804:LEU:HD21	1:A:3890:TYR:HB2	2.02	0.42
1:B:836:HIS:NE2	1:B:842:GLN:OE1	2.46	0.42
1:B:2171:MET:O	1:B:2175:VAL:HG13	2.19	0.42
2:H:83:TYR:HB3	2:H:87:GLY:HA2	2.01	0.42
1:C:836:HIS:NE2	1:C:842:GLN:OE1	2.46	0.42
1:C:1841:LYS:O	1:C:1845:GLN:HG2	2.19	0.42
1:C:2243:ALA:O	1:C:2247:MET:HB2	2.19	0.42
1:C:4841:TYR:O	1:C:4844:ILE:HG22	2.19	0.42
1:D:654:SER:H	1:D:841:LYS:HZ1	1.63	0.42
1:D:894:VAL:O	1:D:898:ILE:HG13	2.19	0.42
1:D:2102:PRO:HD3	1:D:3624:GLU:HG3	2.01	0.42
1:D:4044:LYS:NZ	1:D:4069:ALA:HB1	2.35	0.42
1:A:687:THR:OG1	1:A:1627:GLN:NE2	2.52	0.42
1:A:1060:TYR:HD1	1:A:1060:TYR:N	2.08	0.42
1:A:1346:LEU:HD23	1:A:1347:MET:O	2.18	0.42
1:A:2279:LEU:HB3	1:A:2284:TYR:HB2	2.01	0.42
1:A:2428:LEU:HD21	1:A:2482:PHE:CE1	2.54	0.42
1:A:4044:LYS:HZ1	1:A:4071:THR:H	1.68	0.42
1:B:489:PHE:HD2	1:B:494:MET:HG2	1.84	0.42
1:B:654:SER:H	1:B:841:LYS:HZ1	1.65	0.42
1:B:2000:GLU:O	1:B:2004:THR:HG23	2.20	0.42
1:B:2321:ARG:O	1:B:2325:ARG:HG2	2.18	0.42
1:B:3933:SER:O	1:B:3937:SER:OG	2.34	0.42
2:H:26:HIS:CE1	2:H:41:ARG:HG2	2.55	0.42
1:C:495:ILE:O	1:C:499:LEU:HG	2.20	0.42
1:C:674:TYR:HE1	1:C:756:SER:HB2	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:882:ARG:NH2	1:C:944:LEU:HD21	2.35	0.42
1:C:2238:PRO:O	1:C:2241:VAL:HG12	2.20	0.42
1:C:3727:GLN:O	1:C:3731:HIS:ND1	2.41	0.42
1:C:3804:LEU:HD21	1:C:3890:TYR:HB2	2.02	0.42
2:I:26:HIS:CE1	2:I:41:ARG:HG2	2.54	0.42
1:D:190:ARG:HD3	1:D:205:ALA:O	2.19	0.42
1:D:235:ARG:NH1	1:D:412:GLU:OE2	2.51	0.42
1:D:669:GLN:HB3	1:D:673:TRP:HZ2	1.83	0.42
1:D:674:TYR:HE1	1:D:756:SER:HB2	1.83	0.42
1:D:754:VAL:HG21	1:D:812:LYS:HD3	2.01	0.42
1:D:1704:TYR:CG	1:D:1821:PRO:HB2	2.54	0.42
1:D:2238:PRO:O	1:D:2241:VAL:HG12	2.20	0.42
1:D:3763:ALA:HA	1:D:3766:ASN:ND2	2.34	0.42
1:D:3804:LEU:HD21	1:D:3890:TYR:HB2	2.02	0.42
1:D:3950:PHE:HZ	1:D:3973:LEU:HG	1.83	0.42
1:A:1040:ASP:HA	1:A:1043:LYS:HD2	2.01	0.42
1:A:1270:VAL:HG21	1:A:1589:VAL:HG21	2.02	0.42
1:A:2900:TYR:HD1	1:A:2900:TYR:HA	1.74	0.42
2:G:29:GLY:N	2:G:38:ASP:O	2.48	0.42
1:B:514:PHE:HD2	1:B:523:GLY:HA2	1.84	0.42
1:B:939:THR:O	1:B:999:LEU:HD11	2.19	0.42
1:B:1270:VAL:HG21	1:B:1589:VAL:HG21	2.02	0.42
1:B:1353:HIS:CE1	1:B:1367:LYS:HD2	2.55	0.42
1:B:4058:THR:HG22	1:B:4061:GLU:HG3	2.02	0.42
2:H:27:TYR:O	2:H:40:SER:N	2.53	0.42
1:C:19:GLU:HG2	1:C:68:VAL:HG22	2.01	0.42
1:C:331:PHE:HE1	1:C:363:ILE:HG22	1.84	0.42
1:C:363:ILE:HG12	1:C:372:LEU:HD22	2.02	0.42
1:C:934:GLN:OE1	1:C:935:MET:N	2.52	0.42
1:C:1040:ASP:HA	1:C:1043:LYS:HD2	2.01	0.42
1:C:1682:ASP:HB2	1:C:1685:GLN:CB	2.49	0.42
1:C:3876:TYR:HD1	1:C:3879:ARG:HH21	1.66	0.42
1:C:4044:LYS:NZ	1:C:4069:ALA:HB1	2.35	0.42
1:C:4193:GLU:CD	1:C:4607:ARG:HH22	2.23	0.42
1:D:19:GLU:HG2	1:D:68:VAL:HG22	2.01	0.42
1:D:1128:LEU:HG	1:D:1136:ALA:HB2	2.02	0.42
1:D:2065:MET:SD	1:D:2083:MET:HG3	2.59	0.42
1:A:2243:ALA:O	1:A:2247:MET:HB2	2.19	0.42
1:A:2290:ASN:ND2	1:A:2293:GLU:OE1	2.53	0.42
1:A:2776:GLU:O	1:A:2780:THR:HG23	2.20	0.42
1:B:363:ILE:HG12	1:B:372:LEU:HD22	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:882:ARG:NH2	1:B:944:LEU:HD21	2.35	0.42
1:B:1841:LYS:O	1:B:1845:GLN:HG2	2.19	0.42
1:B:2325:ARG:HA	1:B:2325:ARG:HD3	1.82	0.42
1:B:3961:SER:OG	1:B:3962:SER:N	2.52	0.42
1:B:4193:GLU:CD	1:B:4607:ARG:HH22	2.23	0.42
1:C:505:LEU:HD22	1:C:526:TRP:HD1	1.83	0.42
1:C:2144:GLY:O	1:C:2148:ILE:HG12	2.20	0.42
1:C:4058:THR:HG22	1:C:4061:GLU:HG3	2.02	0.42
1:D:296:ARG:HH21	1:D:324:VAL:HB	1.85	0.42
1:D:495:ILE:O	1:D:499:LEU:HG	2.20	0.42
1:D:1841:LYS:O	1:D:1845:GLN:HG2	2.19	0.42
1:D:3728:ALA:HA	1:D:3731:HIS:ND1	2.34	0.42
2:J:26:HIS:CE1	2:J:41:ARG:HG2	2.54	0.42
2:J:27:TYR:O	2:J:40:SER:N	2.53	0.42
1:A:1901:VAL:O	1:A:1905:MET:HG2	2.19	0.42
1:B:152:ASP:OD1	1:B:152:ASP:N	2.52	0.42
1:B:439:LYS:HE2	1:B:439:LYS:HB3	1.59	0.42
1:B:674:TYR:HE1	1:B:756:SER:HB2	1.83	0.42
1:B:2182:GLU:H	1:B:2184:LYS:HZ3	1.68	0.42
1:B:2238:PRO:O	1:B:2241:VAL:HG12	2.20	0.42
1:B:3728:ALA:HA	1:B:3731:HIS:ND1	2.35	0.42
1:C:514:PHE:HD2	1:C:523:GLY:HA2	1.84	0.42
1:C:654:SER:H	1:C:841:LYS:HZ1	1.67	0.42
1:C:2065:MET:SD	1:C:2083:MET:HG3	2.59	0.42
1:C:2223:ASN:O	1:C:2226:VAL:HG22	2.19	0.42
1:C:2224:SER:OG	1:C:2239:LEU:HB2	2.20	0.42
1:C:2253:ALA:O	1:C:2315:ASN:ND2	2.40	0.42
2:I:83:TYR:HB3	2:I:87:GLY:HA2	2.01	0.42
1:D:387:ILE:O	1:D:388:GLN:NE2	2.53	0.42
1:D:946:LEU:H	1:D:946:LEU:HG	1.56	0.42
1:D:1909:LEU:HD13	1:D:2061:ILE:HG12	2.01	0.42
1:D:2144:GLY:O	1:D:2148:ILE:HG12	2.20	0.42
1:A:62:LEU:HD11	1:A:282:VAL:HG23	2.01	0.42
1:A:296:ARG:HH21	1:A:324:VAL:HB	1.85	0.42
1:A:2102:PRO:HD3	1:A:3624:GLU:HG3	2.01	0.42
1:A:4841:TYR:O	1:A:4844:ILE:HG22	2.19	0.42
1:B:296:ARG:HH21	1:B:324:VAL:HB	1.85	0.42
1:B:1643:LEU:HD22	1:B:1694:TYR:O	2.20	0.42
1:B:2223:ASN:O	1:B:2226:VAL:HG22	2.19	0.42
1:C:845:THR:HG23	1:C:847:THR:H	1.85	0.42
1:C:926:GLU:H	1:C:926:GLU:HG2	1.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1270:VAL:HG21	1:C:1589:VAL:HG21	2.02	0.42
1:C:1363:LYS:HE2	1:C:1365:THR:HG22	2.01	0.42
1:C:2428:LEU:HD21	1:C:2482:PHE:CE1	2.54	0.42
1:D:2325:ARG:HA	1:D:2325:ARG:HD3	1.82	0.42
1:D:4058:THR:HG22	1:D:4061:GLU:HG3	2.02	0.42
1:D:4833:PRO:HD3	1:D:4842:ARG:NE	2.25	0.42
1:A:555:LEU:HD13	1:A:589:ILE:HD11	2.01	0.42
1:A:1643:LEU:HD22	1:A:1694:TYR:O	2.20	0.42
1:A:4633:VAL:HG11	1:A:4707:TRP:HB2	2.02	0.42
2:G:26:HIS:CE1	2:G:41:ARG:HG2	2.55	0.42
1:B:1128:LEU:HG	1:B:1136:ALA:HB2	2.02	0.42
1:B:2290:ASN:ND2	1:B:2293:GLU:OE1	2.53	0.42
1:C:19:GLU:HB2	1:C:217:ILE:HB	2.01	0.42
1:C:1395:UNK:HA	1:C:1415:UNK:HA	2.02	0.42
1:C:2000:GLU:O	1:C:2004:THR:HG23	2.20	0.42
1:C:2279:LEU:HB3	1:C:2284:TYR:HB2	2.01	0.42
1:C:2507:SER:O	1:C:2507:SER:OG	2.35	0.42
1:C:4701:ASP:OD1	1:C:4701:ASP:N	2.45	0.42
1:D:574:VAL:HA	1:D:577:CYS:SG	2.60	0.42
1:D:934:GLN:OE1	1:D:935:MET:N	2.52	0.42
1:D:1353:HIS:CE1	1:D:1367:LYS:HD2	2.55	0.42
1:D:1363:LYS:HE2	1:D:1365:THR:HG22	2.01	0.42
1:D:2243:ALA:O	1:D:2247:MET:HB2	2.19	0.42
1:D:2290:ASN:ND2	1:D:2293:GLU:OE1	2.53	0.42
1:D:4633:VAL:HG11	1:D:4707:TRP:HB2	2.02	0.42
1:A:433:LEU:HD12	1:A:433:LEU:HA	1.93	0.41
1:A:574:VAL:HA	1:A:577:CYS:SG	2.60	0.41
1:A:2238:PRO:O	1:A:2241:VAL:HG12	2.20	0.41
1:A:3763:ALA:HA	1:A:3766:ASN:ND2	2.34	0.41
1:B:19:GLU:HG2	1:B:68:VAL:HG22	2.01	0.41
1:B:113:LEU:HD23	1:B:175:VAL:HG21	2.01	0.41
1:B:1686:LEU:HD11	1:B:1710:ILE:HD11	2.02	0.41
1:B:2144:GLY:O	1:B:2148:ILE:HG12	2.20	0.41
1:C:489:PHE:HD2	1:C:494:MET:HG2	1.84	0.41
1:C:1138:ASP:OD1	1:C:1139:GLY:N	2.53	0.41
1:C:1686:LEU:HD11	1:C:1710:ILE:HD11	2.02	0.41
1:C:2102:PRO:HD3	1:C:3624:GLU:HG3	2.01	0.41
1:C:2290:ASN:ND2	1:C:2293:GLU:OE1	2.53	0.41
1:D:514:PHE:HD2	1:D:523:GLY:HA2	1.84	0.41
1:D:1092:LYS:HE3	1:D:1092:LYS:HB2	1.93	0.41
1:D:2171:MET:O	1:D:2175:VAL:HG13	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3712:SER:HG	1:D:3716:LYS:HZ3	1.59	0.41
1:D:3727:GLN:C	1:D:3731:HIS:HD1	2.23	0.41
2:J:83:TYR:HB3	2:J:87:GLY:HA2	2.01	0.41
1:A:19:GLU:HB2	1:A:217:ILE:HB	2.01	0.41
1:A:686:VAL:HG13	1:A:687:THR:N	2.34	0.41
1:A:822:CYS:HA	1:A:825:ALA:HB3	2.03	0.41
1:A:946:LEU:H	1:A:946:LEU:HG	1.56	0.41
1:A:1031:ARG:HA	1:A:1031:ARG:HD3	1.88	0.41
1:A:1138:ASP:OD1	1:A:1139:GLY:N	2.53	0.41
1:A:1704:TYR:CG	1:A:1821:PRO:HB2	2.54	0.41
1:B:894:VAL:HG21	1:B:976:TYR:HE2	1.83	0.41
1:B:1395:UNK:HA	1:B:1415:UNK:HA	2.02	0.41
1:B:2776:GLU:O	1:B:2780:THR:HG23	2.20	0.41
1:C:1901:VAL:O	1:C:1905:MET:HG2	2.19	0.41
1:C:2423:ARG:HH21	1:C:2475:TYR:HA	1.85	0.41
1:D:686:VAL:HG13	1:D:687:THR:N	2.34	0.41
1:D:1138:ASP:OD1	1:D:1139:GLY:N	2.53	0.41
1:A:18:ASP:N	1:A:18:ASP:OD1	2.54	0.41
1:A:227:TYR:CD1	1:A:352:SER:HB3	2.56	0.41
1:A:1629:MET:HB3	1:A:1629:MET:HE2	1.89	0.41
1:A:2405:MET:H	1:A:2405:MET:HG3	1.48	0.41
1:B:495:ILE:O	1:B:499:LEU:HG	2.20	0.41
1:B:1031:ARG:HA	1:B:1031:ARG:HD3	1.88	0.41
1:B:1363:LYS:HE2	1:B:1365:THR:HG22	2.01	0.41
1:B:2243:ALA:O	1:B:2247:MET:HB2	2.19	0.41
1:B:3812:LYS:HE2	1:B:3812:LYS:HB3	1.83	0.41
1:C:281:ARG:NH1	1:C:346:VAL:O	2.38	0.41
1:C:1826:PHE:CE1	1:C:1843:ILE:HG21	2.54	0.41
1:D:747:HIS:CD2	1:D:750:ARG:HG2	2.55	0.41
1:D:1270:VAL:HG21	1:D:1589:VAL:HG21	2.02	0.41
1:D:1680:HIS:CE1	2:J:91:VAL:HA	2.55	0.41
1:D:2000:GLU:O	1:D:2004:THR:HG23	2.20	0.41
1:D:2224:SER:OG	1:D:2239:LEU:HB2	2.19	0.41
1:D:2279:LEU:HB3	1:D:2284:TYR:HB2	2.01	0.41
1:A:113:LEU:HD23	1:A:175:VAL:HG21	2.01	0.41
1:A:747:HIS:CD2	1:A:750:ARG:HG2	2.55	0.41
1:A:1128:LEU:HG	1:A:1136:ALA:HB2	2.02	0.41
1:A:2000:GLU:O	1:A:2004:THR:HG23	2.20	0.41
1:B:18:ASP:N	1:B:18:ASP:OD1	2.54	0.41
1:B:227:TYR:CD1	1:B:352:SER:HB3	2.56	0.41
1:B:4633:VAL:HG11	1:B:4707:TRP: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:189:GLU:OE2	1:D:2321:ARG:NH1	2.53	0.41
1:C:754:VAL:HG21	1:C:812:LYS:HD3	2.01	0.41
1:C:822:CYS:HA	1:C:825:ALA:HB3	2.03	0.41
1:C:2171:MET:O	1:C:2175:VAL:HG13	2.19	0.41
1:C:2776:GLU:O	1:C:2780:THR:HG23	2.20	0.41
1:D:18:ASP:OD1	1:D:18:ASP:N	2.54	0.41
1:D:200:SER:O	1:D:200:SER:OG	2.36	0.41
1:D:1642:ILE:HG23	1:D:1643:LEU:HD23	2.02	0.41
1:A:387:ILE:O	1:A:388:GLN:NE2	2.53	0.41
1:A:1157:GLN:N	1:A:1160:ASP:OD2	2.41	0.41
1:A:1274:ASP:HB3	1:A:1286:THR:HA	2.03	0.41
1:A:1395:UNK:HA	1:A:1415:UNK:HA	2.02	0.41
1:A:4044:LYS:NZ	1:A:4069:ALA:HB1	2.35	0.41
1:B:200:SER:O	1:B:200:SER:OG	2.36	0.41
1:B:2159:ASN:HD22	1:B:2162:ARG:NH2	2.19	0.41
1:B:3731:HIS:CD2	1:B:3772:VAL:HG22	2.55	0.41
1:C:3731:HIS:CD2	1:C:3772:VAL:HG22	2.55	0.41
1:C:4759:VAL:HG23	1:C:4865:ILE:HD13	2.03	0.41
1:D:1035:TYR:O	1:D:1043:LYS:HE2	2.21	0.41
1:D:1395:UNK:HA	1:D:1415:UNK:HA	2.02	0.41
1:A:1092:LYS:HE3	1:A:1092:LYS:HB2	1.93	0.41
1:A:1363:LYS:HE2	1:A:1365:THR:HG22	2.01	0.41
1:A:1609:VAL:HG12	1:A:1620:VAL:HG23	2.03	0.41
1:A:1752:ILE:HA	1:A:1837:ASN:ND2	2.36	0.41
1:A:1967:PRO:HD2	1:A:1970:GLU:OE2	2.21	0.41
1:A:2159:ASN:HD22	1:A:2162:ARG:NH2	2.19	0.41
1:A:2739:GLY:O	1:A:2751:LYS:HE2	2.21	0.41
1:A:3940:TRP:HA	1:A:3943:VAL:HG12	2.02	0.41
1:A:4798:GLY:HA3	1:A:4799:ASP:HA	1.85	0.41
1:B:237:LEU:HD23	1:B:404:ASN:O	2.21	0.41
1:B:387:ILE:O	1:B:388:GLN:NE2	2.53	0.41
1:B:1752:ILE:HA	1:B:1837:ASN:ND2	2.36	0.41
1:B:2423:ARG:HH21	1:B:2475:TYR:HA	1.85	0.41
1:B:4044:LYS:NZ	1:B:4069:ALA:HB1	2.35	0.41
1:B:4759:VAL:HG23	1:B:4865:ILE:HD13	2.03	0.41
1:C:237:LEU:HD23	1:C:404:ASN:O	2.21	0.41
1:C:1060:TYR:HD1	1:C:1060:TYR:N	2.08	0.41
1:C:3802:LEU:HB2	1:C:3883:SER:HB2	2.03	0.41
1:D:297:LEU:HD13	1:D:297:LEU:HA	1.81	0.41
1:D:433:LEU:HD12	1:D:433:LEU:HA	1.93	0.41
1:D:4044:LYS:HZ1	1:D:4071:THR:H	1.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:LEU:HD23	1:A:404:ASN:O	2.21	0.41
1:B:1274:ASP:HB3	1:B:1286:THR:HA	2.03	0.41
1:B:1642:ILE:HG23	1:B:1643:LEU:HD23	2.02	0.41
1:B:3761:GLY:O	1:B:3764:ILE:HG22	2.21	0.41
1:C:296:ARG:HH21	1:C:324:VAL:HB	1.85	0.41
1:C:747:HIS:CD2	1:C:750:ARG:HG2	2.55	0.41
1:C:747:HIS:HD2	1:C:750:ARG:HG2	1.85	0.41
1:C:1967:PRO:HD2	1:C:1970:GLU:OE2	2.21	0.41
1:C:3940:TRP:HA	1:C:3943:VAL:HG12	2.02	0.41
1:C:4633:VAL:HG11	1:C:4707:TRP:HB2	2.02	0.41
1:C:4663:ASP:OD1	1:C:4663:ASP:N	2.54	0.41
1:C:4857:LEU:O	1:C:4861:ILE:HG13	2.21	0.41
1:D:822:CYS:HA	1:D:825:ALA:HB3	2.03	0.41
1:D:1967:PRO:HD2	1:D:1970:GLU:OE2	2.21	0.41
1:D:2739:GLY:O	1:D:2751:LYS:HE2	2.21	0.41
1:D:2776:GLU:O	1:D:2780:THR:HG23	2.20	0.41
1:D:3731:HIS:CD2	1:D:3772:VAL:HG22	2.55	0.41
1:D:4098:ALA:HB1	1:D:4125:LEU:HD23	2.03	0.41
1:D:4193:GLU:CD	1:D:4607:ARG:HH22	2.23	0.41
1:D:4759:VAL:HG23	1:D:4865:ILE:HD13	2.03	0.41
1:A:281:ARG:NH1	1:A:346:VAL:O	2.38	0.41
1:A:495:ILE:O	1:A:499:LEU:HG	2.20	0.41
1:A:992:GLN:HA	1:A:995:MET:SD	2.61	0.41
1:A:1209:VAL:O	1:A:1211:GLN:NE2	2.54	0.41
1:A:4496:ASN:HD22	1:A:4499:ASN:HD22	1.69	0.41
1:A:4651:LYS:HB2	1:A:4651:LYS:HE3	1.89	0.41
1:A:4759:VAL:HG23	1:A:4865:ILE:HD13	2.03	0.41
1:B:459:LEU:HD12	1:B:459:LEU:HA	1.95	0.41
1:B:747:HIS:HD2	1:B:750:ARG:HG2	1.85	0.41
1:B:1138:ASP:OD1	1:B:1139:GLY:N	2.53	0.41
1:B:4098:ALA:HB1	1:B:4125:LEU:HD23	2.03	0.41
1:C:387:ILE:O	1:C:388:GLN:NE2	2.53	0.41
1:C:1035:TYR:O	1:C:1043:LYS:HE2	2.21	0.41
1:C:1643:LEU:HD22	1:C:1694:TYR:O	2.20	0.41
1:C:1752:ILE:HA	1:C:1837:ASN:ND2	2.36	0.41
1:C:1754:LEU:HD23	1:C:1754:LEU:HA	1.86	0.41
1:C:2182:GLU:H	1:C:2184:LYS:HZ3	1.69	0.41
1:C:4601:ARG:HD3	1:C:4707:TRP:HZ2	1.86	0.41
1:D:113:LEU:HD23	1:D:175:VAL:HG21	2.01	0.41
1:D:992:GLN:HA	1:D:995:MET:SD	2.61	0.41
1:A:747:HIS:HD2	1:A:750:ARG:HG2	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:VAL:HG21	1:A:812:LYS:HD3	2.01	0.41
1:A:845:THR:HG23	1:A:847:THR:H	1.85	0.41
1:A:882:ARG:HH21	1:A:944:LEU:HD21	1.86	0.41
1:A:2144:GLY:O	1:A:2148:ILE:HG12	2.20	0.41
1:A:3765:LEU:HB3	1:A:3844:LEU:HB3	2.03	0.41
1:A:3923:ILE:HG13	1:A:3983:SER:HB3	2.03	0.41
1:A:4065:LEU:HD13	1:A:4065:LEU:HA	1.95	0.41
1:A:4193:GLU:CD	1:A:4607:ARG:HH22	2.23	0.41
1:A:4843:ILE:HG13	1:A:4844:ILE:N	2.36	0.41
2:G:68:SER:C	2:G:104:LEU:HD23	2.42	0.41
1:B:191:TYR:N	1:B:206:ALA:O	2.54	0.41
1:B:538:ALA:HB1	1:B:542:ARG:HH21	1.86	0.41
1:B:747:HIS:CD2	1:B:750:ARG:HG2	2.55	0.41
1:B:822:CYS:HA	1:B:825:ALA:HB3	2.03	0.41
1:B:845:THR:HG23	1:B:847:THR:H	1.85	0.41
1:B:1035:TYR:O	1:B:1043:LYS:HE2	2.21	0.41
1:B:2084:PHE:CZ	1:B:3666:LEU:HB2	2.56	0.41
1:B:2279:LEU:HB3	1:B:2284:TYR:HB2	2.01	0.41
1:B:4496:ASN:HD22	1:B:4499:ASN:HD22	1.69	0.41
1:C:113:LEU:HD23	1:C:175:VAL:HG21	2.01	0.41
1:C:1100:ARG:HG3	1:C:1167:ASP:CG	2.41	0.41
1:C:1128:LEU:HG	1:C:1136:ALA:HB2	2.02	0.41
1:C:1965:ARG:O	1:C:1966:SER:OG	2.35	0.41
1:C:2755:LEU:HD13	1:C:2764:GLU:OE2	2.21	0.41
1:D:306:LEU:HG	1:D:314:LEU:HD23	2.03	0.41
1:D:403:LEU:HD23	1:D:403:LEU:HA	1.90	0.41
1:D:747:HIS:HD2	1:D:750:ARG:HG2	1.85	0.41
1:D:1609:VAL:HG12	1:D:1620:VAL:HG23	2.03	0.41
1:D:2159:ASN:HD22	1:D:2162:ARG:NH2	2.19	0.41
1:D:2755:LEU:HD13	1:D:2764:GLU:OE2	2.21	0.41
1:D:3765:LEU:HB3	1:D:3844:LEU:HB3	2.03	0.41
1:D:3940:TRP:HA	1:D:3943:VAL:HG12	2.02	0.41
1:A:274:LEU:HD22	1:A:408:SER:OG	2.21	0.41
1:A:882:ARG:NH2	1:A:944:LEU:HD21	2.35	0.41
1:A:988:LEU:HD21	1:A:1054:VAL:HG23	2.03	0.41
1:B:712:GLU:OE1	1:B:838:ARG:HB3	2.21	0.41
1:B:988:LEU:HD21	1:B:1054:VAL:HG23	2.03	0.41
1:B:3765:LEU:HB3	1:B:3844:LEU:HB3	2.03	0.41
1:B:3940:TRP:HA	1:B:3943:VAL:HG12	2.02	0.41
1:B:4047:PHE:O	1:B:4051:MET:HG2	2.21	0.41
1:C:82:LEU:HD11	1:C:156:GLU:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:CYS:SG	1:C:273:SER:HB2	2.61	0.41
1:C:1609:VAL:HG12	1:C:1620:VAL:HG23	2.03	0.41
1:C:1642:ILE:HG23	1:C:1643:LEU:HD23	2.02	0.41
1:C:2159:ASN:HD22	1:C:2162:ARG:NH2	2.19	0.41
1:D:227:TYR:CD1	1:D:352:SER:HB3	2.56	0.41
1:D:237:LEU:HD23	1:D:404:ASN:O	2.21	0.41
1:D:882:ARG:NH1	1:D:937:LEU:HG	2.36	0.41
1:D:2113:GLU:OE1	1:D:2113:GLU:N	2.37	0.41
1:D:4047:PHE:O	1:D:4051:MET:HG2	2.21	0.41
1:D:4601:ARG:HD3	1:D:4707:TRP:HZ2	1.86	0.41
1:A:306:LEU:HG	1:A:314:LEU:HD23	2.03	0.40
1:A:748:LEU:HD13	1:A:748:LEU:HA	1.77	0.40
1:A:941:LYS:HA	1:A:944:LEU:HG	2.03	0.40
1:A:1035:TYR:O	1:A:1043:LYS:HE2	2.21	0.40
1:A:1686:LEU:HD11	1:A:1710:ILE:HD11	2.02	0.40
1:A:2182:GLU:H	1:A:2184:LYS:HZ3	1.69	0.40
1:A:4058:THR:HG22	1:A:4061:GLU:HG3	2.02	0.40
1:A:4098:ALA:HB1	1:A:4125:LEU:HD23	2.03	0.40
1:B:244:CYS:SG	1:B:273:SER:HB2	2.61	0.40
1:B:926:GLU:H	1:B:926:GLU:HG2	1.54	0.40
1:B:2334:LEU:HD13	1:B:2342:LEU:HB2	2.03	0.40
1:B:4833:PRO:HD3	1:B:4842:ARG:NE	2.25	0.40
2:H:29:GLY:N	2:H:38:ASP:O	2.48	0.40
1:C:227:TYR:CD1	1:C:352:SER:HB3	2.56	0.40
1:C:274:LEU:HD22	1:C:408:SER:OG	2.21	0.40
1:C:1111:GLY:HA3	1:C:1211:GLN:HE22	1.87	0.40
1:C:3765:LEU:HB3	1:C:3844:LEU:HB3	2.03	0.40
2:I:68:SER:C	2:I:104:LEU:HD23	2.42	0.40
1:D:191:TYR:N	1:D:206:ALA:O	2.54	0.40
1:D:237:LEU:HD23	1:D:237:LEU:H	1.87	0.40
1:D:314:LEU:HD11	1:D:393:MET:HG3	2.03	0.40
1:D:836:HIS:NE2	1:D:842:GLN:OE1	2.46	0.40
1:D:845:THR:HG23	1:D:847:THR:H	1.85	0.40
1:D:1274:ASP:HB3	1:D:1286:THR:HA	2.03	0.40
1:D:3761:GLY:O	1:D:3764:ILE:HG22	2.21	0.40
1:D:3923:ILE:HG13	1:D:3983:SER:HB3	2.03	0.40
1:D:4857:LEU:O	1:D:4861:ILE:HG13	2.21	0.40
1:A:1962:ARG:NH2	1:A:1963:GLU:HA	2.36	0.40
1:A:2755:LEU:HD13	1:A:2764:GLU:OE2	2.21	0.40
1:A:4649:LYS:HA	1:A:4669:LEU:HD21	2.04	0.40
1:B:2157:HIS:O	1:B:2161:MET:HG2	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:68:SER:C	2:H:104:LEU:HD23	2.42	0.40
1:C:574:VAL:HA	1:C:577:CYS:SG	2.60	0.40
1:C:730:LEU:HD21	2:I:6:GLU:OE2	2.21	0.40
1:C:882:ARG:NH1	1:C:937:LEU:HG	2.37	0.40
1:C:992:GLN:HA	1:C:995:MET:SD	2.61	0.40
1:C:1776:CYS:O	1:C:1778:GLN:HG3	2.22	0.40
1:C:2084:PHE:CZ	1:C:3666:LEU:HB2	2.56	0.40
1:C:4047:PHE:O	1:C:4051:MET:HG2	2.21	0.40
2:I:27:TYR:O	2:I:40:SER:N	2.53	0.40
1:D:274:LEU:HD22	1:D:408:SER:OG	2.21	0.40
1:D:1643:LEU:HD22	1:D:1694:TYR:O	2.20	0.40
1:D:1776:CYS:O	1:D:1778:GLN:HG3	2.22	0.40
1:D:1962:ARG:NH2	1:D:1963:GLU:HA	2.36	0.40
1:D:3934:LEU:HD23	1:D:3939:LEU:HD22	2.03	0.40
1:D:4496:ASN:HD22	1:D:4499:ASN:HD22	1.69	0.40
2:J:68:SER:C	2:J:104:LEU:HD23	2.42	0.40
1:A:882:ARG:NH1	1:A:937:LEU:HG	2.36	0.40
1:A:1719:ARG:HD3	1:A:1832:MET:HA	2.04	0.40
1:A:2325:ARG:HA	1:A:2325:ARG:HD3	1.82	0.40
1:A:3731:HIS:CD2	1:A:3772:VAL:HG22	2.55	0.40
1:A:4847:ILE:HA	1:B:4821:ARG:HD3	2.02	0.40
1:B:304:LYS:HB2	1:B:316:LEU:HD23	2.03	0.40
1:B:882:ARG:HH21	1:B:944:LEU:HD21	1.86	0.40
1:B:882:ARG:NH1	1:B:937:LEU:HG	2.36	0.40
1:B:941:LYS:HA	1:B:944:LEU:HG	2.03	0.40
1:B:1962:ARG:NH2	1:B:1963:GLU:HA	2.37	0.40
1:B:3878:LEU:HD22	1:B:3938:ARG:HE	1.86	0.40
1:B:4895:ASP:OD1	1:B:4895:ASP:N	2.54	0.40
1:B:4929:GLU:HA	1:B:4932:HIS:CD2	2.57	0.40
1:C:191:TYR:N	1:C:206:ALA:O	2.54	0.40
1:C:237:LEU:HD23	1:C:237:LEU:H	1.86	0.40
1:C:387:ILE:HD11	1:C:389:ARG:NH1	2.37	0.40
1:C:538:ALA:HB1	1:C:542:ARG:HH21	1.86	0.40
1:C:1843:ILE:O	1:C:1846:LEU:HG	2.21	0.40
1:C:2230:SER:O	1:C:2230:SER:OG	2.39	0.40
1:C:3878:LEU:HD22	1:C:3938:ARG:HE	1.85	0.40
1:C:4098:ALA:HB1	1:C:4125:LEU:HD23	2.03	0.40
1:C:4483:ILE:O	1:C:4486:GLN:HG3	2.22	0.40
1:D:244:CYS:SG	1:D:273:SER:HB2	2.61	0.40
1:D:398:HIS:HB3	1:D:400:ASP:OD1	2.22	0.40
1:D:1089:ARG:HB3	1:D:1204:VAL:HG23	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1111:GLY:HA3	1:D:1211:GLN:HE22	1.87	0.40
1:D:3868:ASN:HB3	1:D:3871:ILE:HB	2.03	0.40
1:A:1100:ARG:HG3	1:A:1167:ASP:CG	2.41	0.40
1:A:1642:ILE:HG23	1:A:1643:LEU:HD23	2.02	0.40
1:A:1783:PHE:HE2	1:A:1788:LEU:HB2	1.87	0.40
1:A:1843:ILE:O	1:A:1846:LEU:HG	2.21	0.40
1:A:3761:GLY:O	1:A:3764:ILE:HG22	2.21	0.40
1:A:4042:ILE:O	1:A:4076:THR:HA	2.22	0.40
1:A:4601:ARG:HD3	1:A:4707:TRP:HZ2	1.86	0.40
1:B:227:TYR:CE1	1:B:352:SER:HB3	2.57	0.40
1:B:314:LEU:HD11	1:B:393:MET:HG3	2.03	0.40
1:B:574:VAL:HA	1:B:577:CYS:HG	1.86	0.40
1:B:627:SER:O	1:B:631:LEU:HG	2.22	0.40
1:B:654:SER:H	1:B:841:LYS:HZ3	1.66	0.40
1:B:992:GLN:HA	1:B:995:MET:SD	2.61	0.40
1:B:1719:ARG:HD3	1:B:1832:MET:HA	2.04	0.40
1:B:2755:LEU:HD13	1:B:2764:GLU:OE2	2.21	0.40
1:B:4601:ARG:HD3	1:B:4707:TRP:HZ2	1.86	0.40
1:C:2071:GLU:O	1:C:3659:ARG:NH1	2.55	0.40
1:D:1686:LEU:HD11	1:D:1710:ILE:HD11	2.02	0.40
1:D:1719:ARG:HD3	1:D:1832:MET:HA	2.04	0.40
1:D:3878:LEU:HD22	1:D:3938:ARG:HE	1.86	0.40
1:D:4649:LYS:HA	1:D:4669:LEU:HD21	2.04	0.40
1:A:1111:GLY:HA3	1:A:1211:GLN:HE22	1.87	0.40
1:A:2230:SER:O	1:A:2230:SER:OG	2.39	0.40
1:A:2889:GLN:O	1:A:2893:LYS:HG3	2.22	0.40
1:A:3854:GLN:HB3	1:A:3930:ASN:HD21	1.87	0.40
1:A:3934:LEU:HD23	1:A:3939:LEU:HD22	2.04	0.40
1:B:34:LYS:HB3	1:B:34:LYS:HE3	1.92	0.40
1:B:191:TYR:HE2	1:C:2325:ARG:HD2	1.86	0.40
1:B:403:LEU:HD23	1:B:403:LEU:HA	1.90	0.40
1:B:548:CYS:HB2	1:B:582:SER:HB2	2.04	0.40
1:B:912:LYS:N	1:B:912:LYS:HD3	2.37	0.40
1:B:1609:VAL:HG12	1:B:1620:VAL:HG23	2.03	0.40
1:B:1783:PHE:HE2	1:B:1788:LEU:HB2	1.87	0.40
1:C:66:THR:HG23	1:C:124:SER:OG	2.21	0.40
1:C:709:GLY:N	1:C:721:ASP:OD2	2.55	0.40
1:C:712:GLU:OE1	1:C:838:ARG:HB3	2.21	0.40
1:C:2113:GLU:OE1	1:C:2113:GLU:N	2.37	0.40
1:D:66:THR:HG23	1:D:124:SER:OG	2.21	0.40
1:D:82:LEU:HD11	1:D:156:GLU:HB3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:TYR:CE1	1:D:352:SER:HB3	2.57	0.40
1:D:2084:PHE:CZ	1:D:3666:LEU:HB2	2.56	0.40
1:D:2157:HIS:O	1:D:2161:MET:HG2	2.22	0.40
1:D:4107:HIS:O	1:D:4109:PRO:HD3	2.22	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	3218/4966 (65%)	2999 (93%)	219 (7%)	0	100	100
1	B	3218/4966 (65%)	2997 (93%)	221 (7%)	0	100	100
1	C	3218/4966 (65%)	2994 (93%)	224 (7%)	0	100	100
1	D	3218/4966 (65%)	2997 (93%)	221 (7%)	0	100	100
2	G	105/176 (60%)	100 (95%)	5 (5%)	0	100	100
2	H	105/176 (60%)	100 (95%)	5 (5%)	0	100	100
2	I	105/176 (60%)	100 (95%)	5 (5%)	0	100	100
2	J	105/176 (60%)	100 (95%)	5 (5%)	0	100	100
All	All	13292/20568 (65%)	12387 (93%)	905 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	2827/3387 (84%)	2682 (95%)	145 (5%)	24	57
1	B	2827/3387 (84%)	2682 (95%)	145 (5%)	24	57
1	C	2827/3387 (84%)	2681 (95%)	146 (5%)	23	56
1	D	2827/3387 (84%)	2682 (95%)	145 (5%)	24	57
2	G	88/140 (63%)	84 (96%)	4 (4%)	27	61
2	H	88/140 (63%)	84 (96%)	4 (4%)	27	61
2	I	88/140 (63%)	84 (96%)	4 (4%)	27	61
2	J	88/140 (63%)	84 (96%)	4 (4%)	27	61
All	All	11660/14108 (83%)	11063 (95%)	597 (5%)	27	57

All (597) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	29	HIS
1	A	56	LYS
1	A	61	ASP
1	A	62	LEU
1	A	153	THR
1	A	166	SER
1	A	167	LYS
1	A	173	GLU
1	A	175	VAL
1	A	225	GLN
1	A	233	VAL
1	A	285	SER
1	A	297	LEU
1	A	302	THR
1	A	310	GLU
1	A	347	ASP
1	A	378	ASP
1	A	380	LYS
1	A	400	ASP
1	A	415	THR
1	A	439	LYS
1	A	446	ASP
1	A	450	GLU
1	A	473	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	501	CYS
1	A	516	ASP
1	A	524	GLU
1	A	528	SER
1	A	695	VAL
1	A	748	LEU
1	A	770	ILE
1	A	778	MET
1	A	830	GLU
1	A	867	VAL
1	A	887	GLU
1	A	893	TRP
1	A	894	VAL
1	A	904	TYR
1	A	912	LYS
1	A	914	GLN
1	A	919	VAL
1	A	920	GLU
1	A	922	CYS
1	A	926	GLU
1	A	935	MET
1	A	936	SER
1	A	944	LEU
1	A	946	LEU
1	A	952	ILE
1	A	971	GLN
1	A	972	LEU
1	A	976	TYR
1	A	982	ASP
1	A	986	ILE
1	A	987	LYS
1	A	999	LEU
1	A	1047	LYS
1	A	1057	LEU
1	A	1060	TYR
1	A	1161	VAL
1	A	1170	GLU
1	A	1186	SER
1	A	1261	VAL
1	A	1271	THR
1	A	1359	ILE
1	A	1373	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1598	SER
1	A	1691	GLU
1	A	1738	THR
1	A	1755	SER
1	A	1814	THR
1	A	1838	GLU
1	A	1896	LYS
1	A	1953	SER
1	A	1961	THR
1	A	1962	ARG
1	A	1997	ASP
1	A	2060	LEU
1	A	2245	SER
1	A	2246	VAL
1	A	2265	VAL
1	A	2351	LYS
1	A	2389	THR
1	A	2405	MET
1	A	2414	GLU
1	A	2436	SER
1	A	2441	MET
1	A	2464	LYS
1	A	2479	VAL
1	A	2489	VAL
1	A	2506	LEU
1	A	2715	LYS
1	A	2725	GLU
1	A	2727	SER
1	A	2729	ASP
1	A	2734	ASP
1	A	2736	LEU
1	A	2738	ASN
1	A	2741	ILE
1	A	2746	TYR
1	A	2768	GLU
1	A	2769	ILE
1	A	2774	ILE
1	A	2777	SER
1	A	2779	LYS
1	A	2835	ASP
1	A	2839	MET
1	A	2841	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2855	LYS
1	A	2858	GLU
1	A	2870	LEU
1	A	2880	GLU
1	A	2883	LYS
1	A	2884	ASP
1	A	2900	TYR
1	A	3620	LEU
1	A	3631	GLU
1	A	3692	ASP
1	A	3717	GLU
1	A	3800	SER
1	A	3824	SER
1	A	3885	SER
1	A	3899	GLU
1	A	3928	THR
1	A	3937	SER
1	A	3949	VAL
1	A	3962	SER
1	A	4017	ASP
1	A	4066	LEU
1	A	4072	ASP
1	A	4112	THR
1	A	4116	THR
1	A	4152	SER
1	A	4167	SER
1	A	4559	VAL
1	A	4612	ASP
1	A	4667	GLU
1	A	4697	LEU
1	A	4776	VAL
1	A	4797	ASP
1	A	4836	ASP
1	A	4842	ARG
1	A	4884	GLU
1	A	4955	ASP
2	G	22	THR
2	G	23	CYS
2	G	68	SER
2	G	69	LEU
1	B	22	LEU
1	B	29	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	56	LYS
1	B	61	ASP
1	B	62	LEU
1	B	153	THR
1	B	166	SER
1	B	167	LYS
1	B	173	GLU
1	B	175	VAL
1	B	225	GLN
1	B	233	VAL
1	B	285	SER
1	B	297	LEU
1	B	302	THR
1	B	310	GLU
1	B	347	ASP
1	B	378	ASP
1	B	380	LYS
1	B	400	ASP
1	B	415	THR
1	B	439	LYS
1	B	446	ASP
1	B	450	GLU
1	B	473	GLU
1	B	501	CYS
1	B	516	ASP
1	B	524	GLU
1	B	528	SER
1	B	695	VAL
1	B	748	LEU
1	B	770	ILE
1	B	778	MET
1	B	830	GLU
1	B	867	VAL
1	B	887	GLU
1	B	893	TRP
1	B	894	VAL
1	B	904	TYR
1	B	912	LYS
1	B	914	GLN
1	B	919	VAL
1	B	920	GLU
1	B	922	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	926	GLU
1	B	935	MET
1	B	936	SER
1	B	944	LEU
1	B	946	LEU
1	B	952	ILE
1	B	971	GLN
1	B	972	LEU
1	B	976	TYR
1	B	982	ASP
1	B	986	ILE
1	B	987	LYS
1	B	999	LEU
1	B	1047	LYS
1	B	1057	LEU
1	B	1060	TYR
1	B	1161	VAL
1	B	1170	GLU
1	B	1186	SER
1	B	1261	VAL
1	B	1271	THR
1	B	1359	ILE
1	B	1373	HIS
1	B	1598	SER
1	B	1691	GLU
1	B	1738	THR
1	B	1755	SER
1	B	1814	THR
1	B	1838	GLU
1	B	1896	LYS
1	B	1953	SER
1	B	1961	THR
1	B	1962	ARG
1	B	1997	ASP
1	B	2060	LEU
1	B	2245	SER
1	B	2246	VAL
1	B	2265	VAL
1	B	2351	LYS
1	B	2389	THR
1	B	2405	MET
1	B	2414	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2436	SER
1	B	2441	MET
1	B	2464	LYS
1	B	2479	VAL
1	B	2489	VAL
1	B	2506	LEU
1	B	2715	LYS
1	B	2725	GLU
1	B	2727	SER
1	B	2729	ASP
1	B	2734	ASP
1	B	2736	LEU
1	B	2738	ASN
1	B	2741	ILE
1	B	2746	TYR
1	B	2768	GLU
1	B	2769	ILE
1	B	2774	ILE
1	B	2777	SER
1	B	2779	LYS
1	B	2835	ASP
1	B	2839	MET
1	B	2841	GLU
1	B	2855	LYS
1	B	2858	GLU
1	B	2870	LEU
1	B	2880	GLU
1	B	2883	LYS
1	B	2884	ASP
1	B	2900	TYR
1	B	3620	LEU
1	B	3631	GLU
1	B	3692	ASP
1	B	3717	GLU
1	B	3800	SER
1	B	3824	SER
1	B	3885	SER
1	B	3899	GLU
1	B	3928	THR
1	B	3937	SER
1	B	3949	VAL
1	B	3962	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	4017	ASP
1	B	4066	LEU
1	B	4072	ASP
1	B	4112	THR
1	B	4116	THR
1	B	4152	SER
1	B	4167	SER
1	B	4559	VAL
1	B	4612	ASP
1	B	4667	GLU
1	B	4697	LEU
1	B	4776	VAL
1	B	4797	ASP
1	B	4836	ASP
1	B	4842	ARG
1	B	4884	GLU
1	B	4955	ASP
2	H	22	THR
2	H	23	CYS
2	H	68	SER
2	H	69	LEU
1	C	22	LEU
1	C	29	HIS
1	C	56	LYS
1	C	61	ASP
1	C	62	LEU
1	C	153	THR
1	C	166	SER
1	C	167	LYS
1	C	173	GLU
1	C	175	VAL
1	C	225	GLN
1	C	233	VAL
1	C	285	SER
1	C	297	LEU
1	C	302	THR
1	C	310	GLU
1	C	347	ASP
1	C	378	ASP
1	C	380	LYS
1	C	400	ASP
1	C	415	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	439	LYS
1	C	446	ASP
1	C	450	GLU
1	C	473	GLU
1	C	501	CYS
1	C	516	ASP
1	C	524	GLU
1	C	528	SER
1	C	695	VAL
1	C	748	LEU
1	C	770	ILE
1	C	778	MET
1	C	830	GLU
1	C	867	VAL
1	C	887	GLU
1	C	893	TRP
1	C	894	VAL
1	C	904	TYR
1	C	912	LYS
1	C	914	GLN
1	C	918	LEU
1	C	919	VAL
1	C	920	GLU
1	C	922	CYS
1	C	926	GLU
1	C	935	MET
1	C	936	SER
1	C	944	LEU
1	C	946	LEU
1	C	952	ILE
1	C	971	GLN
1	C	972	LEU
1	C	976	TYR
1	C	982	ASP
1	C	986	ILE
1	C	987	LYS
1	C	999	LEU
1	C	1047	LYS
1	C	1057	LEU
1	C	1060	TYR
1	C	1161	VAL
1	C	1170	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1186	SER
1	C	1261	VAL
1	C	1271	THR
1	C	1359	ILE
1	C	1373	HIS
1	C	1598	SER
1	C	1691	GLU
1	C	1738	THR
1	C	1755	SER
1	C	1814	THR
1	C	1838	GLU
1	C	1896	LYS
1	C	1953	SER
1	C	1961	THR
1	C	1962	ARG
1	C	1997	ASP
1	C	2060	LEU
1	C	2245	SER
1	C	2246	VAL
1	C	2265	VAL
1	C	2351	LYS
1	C	2389	THR
1	C	2405	MET
1	C	2414	GLU
1	C	2436	SER
1	C	2441	MET
1	C	2464	LYS
1	C	2479	VAL
1	C	2489	VAL
1	C	2506	LEU
1	C	2715	LYS
1	C	2725	GLU
1	C	2727	SER
1	C	2729	ASP
1	C	2734	ASP
1	C	2736	LEU
1	C	2738	ASN
1	C	2741	ILE
1	C	2746	TYR
1	C	2768	GLU
1	C	2769	ILE
1	C	2774	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	2777	SER
1	C	2779	LYS
1	C	2835	ASP
1	C	2839	MET
1	C	2841	GLU
1	C	2855	LYS
1	C	2858	GLU
1	C	2870	LEU
1	C	2880	GLU
1	C	2883	LYS
1	C	2884	ASP
1	C	2900	TYR
1	C	3620	LEU
1	C	3631	GLU
1	C	3692	ASP
1	C	3717	GLU
1	C	3800	SER
1	C	3824	SER
1	C	3885	SER
1	C	3899	GLU
1	C	3928	THR
1	C	3937	SER
1	C	3949	VAL
1	C	3962	SER
1	C	4017	ASP
1	C	4066	LEU
1	C	4072	ASP
1	C	4112	THR
1	C	4116	THR
1	C	4152	SER
1	C	4167	SER
1	C	4559	VAL
1	C	4612	ASP
1	C	4667	GLU
1	C	4697	LEU
1	C	4776	VAL
1	C	4797	ASP
1	C	4836	ASP
1	C	4842	ARG
1	C	4884	GLU
1	C	4955	ASP
2	I	22	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	23	CYS
2	I	68	SER
2	I	69	LEU
1	D	22	LEU
1	D	29	HIS
1	D	56	LYS
1	D	61	ASP
1	D	62	LEU
1	D	153	THR
1	D	166	SER
1	D	167	LYS
1	D	173	GLU
1	D	175	VAL
1	D	225	GLN
1	D	233	VAL
1	D	285	SER
1	D	297	LEU
1	D	302	THR
1	D	310	GLU
1	D	347	ASP
1	D	378	ASP
1	D	380	LYS
1	D	400	ASP
1	D	415	THR
1	D	439	LYS
1	D	446	ASP
1	D	450	GLU
1	D	473	GLU
1	D	501	CYS
1	D	516	ASP
1	D	524	GLU
1	D	528	SER
1	D	695	VAL
1	D	748	LEU
1	D	770	ILE
1	D	778	MET
1	D	830	GLU
1	D	867	VAL
1	D	887	GLU
1	D	893	TRP
1	D	894	VAL
1	D	904	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	912	LYS
1	D	914	GLN
1	D	919	VAL
1	D	920	GLU
1	D	922	CYS
1	D	926	GLU
1	D	935	MET
1	D	936	SER
1	D	944	LEU
1	D	946	LEU
1	D	952	ILE
1	D	971	GLN
1	D	972	LEU
1	D	976	TYR
1	D	982	ASP
1	D	986	ILE
1	D	987	LYS
1	D	999	LEU
1	D	1047	LYS
1	D	1057	LEU
1	D	1060	TYR
1	D	1161	VAL
1	D	1170	GLU
1	D	1186	SER
1	D	1261	VAL
1	D	1271	THR
1	D	1359	ILE
1	D	1373	HIS
1	D	1598	SER
1	D	1691	GLU
1	D	1738	THR
1	D	1755	SER
1	D	1814	THR
1	D	1838	GLU
1	D	1896	LYS
1	D	1953	SER
1	D	1961	THR
1	D	1962	ARG
1	D	1997	ASP
1	D	2060	LEU
1	D	2245	SER
1	D	2246	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	2265	VAL
1	D	2351	LYS
1	D	2389	THR
1	D	2405	MET
1	D	2414	GLU
1	D	2436	SER
1	D	2441	MET
1	D	2464	LYS
1	D	2479	VAL
1	D	2489	VAL
1	D	2506	LEU
1	D	2715	LYS
1	D	2725	GLU
1	D	2727	SER
1	D	2729	ASP
1	D	2734	ASP
1	D	2736	LEU
1	D	2738	ASN
1	D	2741	ILE
1	D	2746	TYR
1	D	2768	GLU
1	D	2769	ILE
1	D	2774	ILE
1	D	2777	SER
1	D	2779	LYS
1	D	2835	ASP
1	D	2839	MET
1	D	2841	GLU
1	D	2855	LYS
1	D	2858	GLU
1	D	2870	LEU
1	D	2880	GLU
1	D	2883	LYS
1	D	2884	ASP
1	D	2900	TYR
1	D	3620	LEU
1	D	3631	GLU
1	D	3692	ASP
1	D	3717	GLU
1	D	3800	SER
1	D	3824	SER
1	D	3885	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	3899	GLU
1	D	3928	THR
1	D	3937	SER
1	D	3949	VAL
1	D	3962	SER
1	D	4017	ASP
1	D	4066	LEU
1	D	4072	ASP
1	D	4112	THR
1	D	4116	THR
1	D	4152	SER
1	D	4167	SER
1	D	4559	VAL
1	D	4612	ASP
1	D	4667	GLU
1	D	4697	LEU
1	D	4776	VAL
1	D	4797	ASP
1	D	4836	ASP
1	D	4842	ARG
1	D	4884	GLU
1	D	4955	ASP
2	J	22	THR
2	J	23	CYS
2	J	68	SER
2	J	69	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (178) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	54	ASN
1	A	79	GLN
1	A	123	HIS
1	A	240	HIS
1	A	299	HIS
1	A	394	HIS
1	A	410	HIS
1	A	476	GLN
1	A	487	ASN
1	A	496	ASN
1	A	593	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	629	GLN
1	A	651	HIS
1	A	669	GLN
1	A	1002	ASN
1	A	1265	HIS
1	A	1353	HIS
1	A	1590	GLN
1	A	1627	GLN
1	A	1653	GLN
1	A	1685	GLN
1	A	1711	HIS
1	A	1836	HIS
1	A	1837	ASN
1	A	1944	ASN
1	A	1999	HIS
1	A	2159	ASN
1	A	2317	ASN
1	A	3633	HIS
1	A	3721	GLN
1	A	3860	GLN
1	A	3932	GLN
1	A	3959	GLN
1	A	3974	GLN
1	A	4096	ASN
1	A	4158	GLN
1	A	4170	GLN
1	A	4491	ASN
1	A	4496	ASN
1	A	4628	GLN
1	A	4637	GLN
1	A	4716	ASN
1	A	4862	GLN
1	A	4960	GLN
2	G	32	GLN
1	B	12	GLN
1	B	54	ASN
1	B	79	GLN
1	B	123	HIS
1	B	299	HIS
1	B	394	HIS
1	B	410	HIS
1	B	476	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	487	ASN
1	B	496	ASN
1	B	593	HIS
1	B	629	GLN
1	B	651	HIS
1	B	669	GLN
1	B	731	HIS
1	B	1002	ASN
1	B	1265	HIS
1	B	1353	HIS
1	B	1590	GLN
1	B	1627	GLN
1	B	1653	GLN
1	B	1685	GLN
1	B	1711	HIS
1	B	1836	HIS
1	B	1837	ASN
1	B	1944	ASN
1	B	1999	HIS
1	B	2159	ASN
1	B	2317	ASN
1	B	3633	HIS
1	B	3721	GLN
1	B	3860	GLN
1	B	3932	GLN
1	B	3959	GLN
1	B	3974	GLN
1	B	4096	ASN
1	B	4158	GLN
1	B	4170	GLN
1	B	4491	ASN
1	B	4496	ASN
1	B	4637	GLN
1	B	4716	ASN
1	B	4960	GLN
2	H	32	GLN
1	C	12	GLN
1	C	54	ASN
1	C	79	GLN
1	C	123	HIS
1	C	299	HIS
1	C	394	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	410	HIS
1	C	476	GLN
1	C	487	ASN
1	C	496	ASN
1	C	593	HIS
1	C	629	GLN
1	C	651	HIS
1	C	669	GLN
1	C	1002	ASN
1	C	1265	HIS
1	C	1353	HIS
1	C	1590	GLN
1	C	1627	GLN
1	C	1653	GLN
1	C	1685	GLN
1	C	1711	HIS
1	C	1836	HIS
1	C	1837	ASN
1	C	1944	ASN
1	C	1999	HIS
1	C	2159	ASN
1	C	2317	ASN
1	C	3633	HIS
1	C	3721	GLN
1	C	3860	GLN
1	C	3932	GLN
1	C	3959	GLN
1	C	3974	GLN
1	C	4096	ASN
1	C	4158	GLN
1	C	4170	GLN
1	C	4491	ASN
1	C	4496	ASN
1	C	4637	GLN
1	C	4716	ASN
1	C	4960	GLN
2	I	32	GLN
1	D	12	GLN
1	D	54	ASN
1	D	79	GLN
1	D	123	HIS
1	D	168	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	299	HIS
1	D	394	HIS
1	D	410	HIS
1	D	476	GLN
1	D	487	ASN
1	D	496	ASN
1	D	593	HIS
1	D	629	GLN
1	D	651	HIS
1	D	669	GLN
1	D	731	HIS
1	D	1002	ASN
1	D	1265	HIS
1	D	1353	HIS
1	D	1590	GLN
1	D	1627	GLN
1	D	1653	GLN
1	D	1685	GLN
1	D	1711	HIS
1	D	1836	HIS
1	D	1837	ASN
1	D	1944	ASN
1	D	1999	HIS
1	D	2159	ASN
1	D	2317	ASN
1	D	3633	HIS
1	D	3721	GLN
1	D	3860	GLN
1	D	3932	GLN
1	D	3959	GLN
1	D	3974	GLN
1	D	4096	ASN
1	D	4158	GLN
1	D	4170	GLN
1	D	4491	ASN
1	D	4496	ASN
1	D	4637	GLN
1	D	4716	ASN
1	D	4960	GLN
2	J	32	GLN

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

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

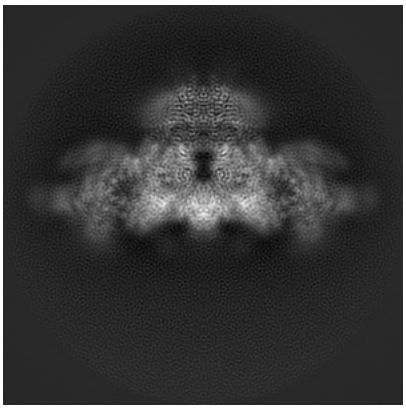
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33939. These allow visual inspection of the internal detail of the map and identification of artifacts.

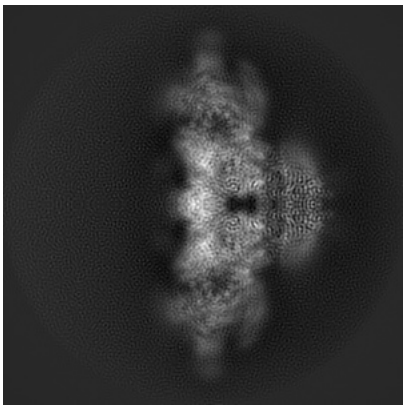
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

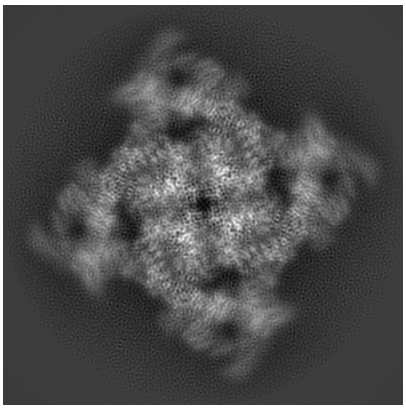
6.1.1 Primary map



X

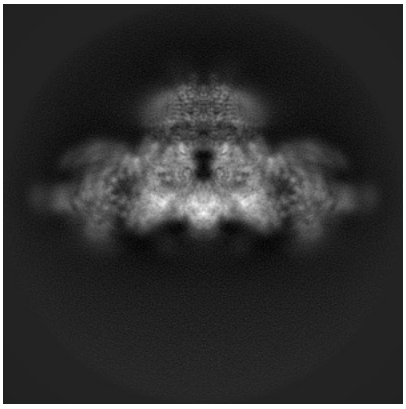


Y

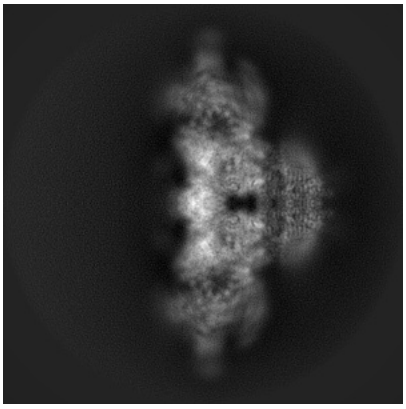


Z

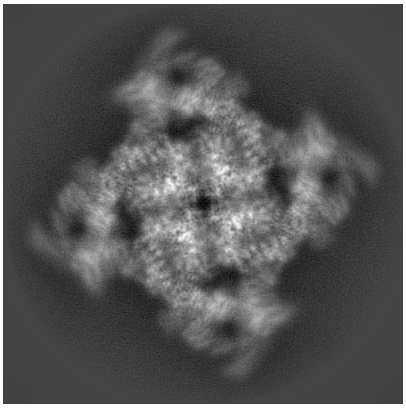
6.1.2 Raw map



X



Y

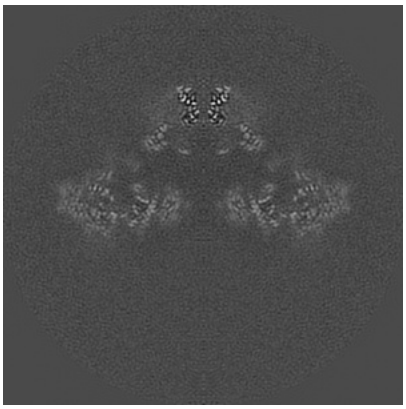


Z

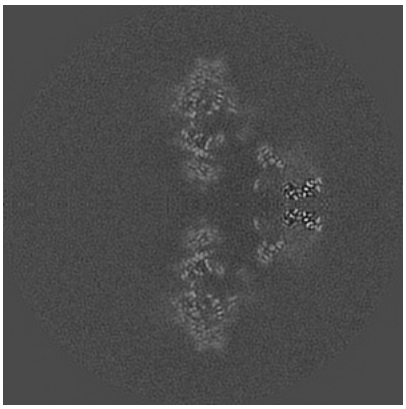
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

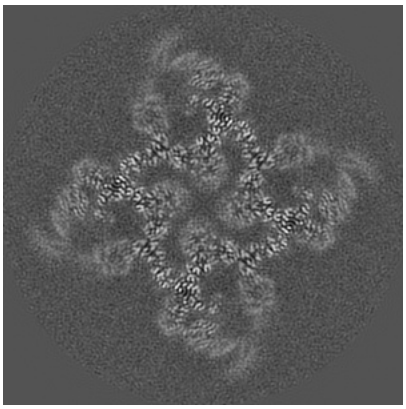
6.2.1 Primary map



X Index: 170

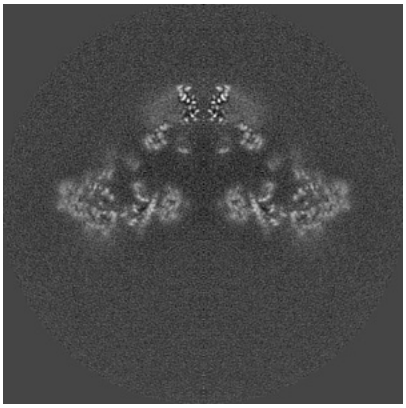


Y Index: 170

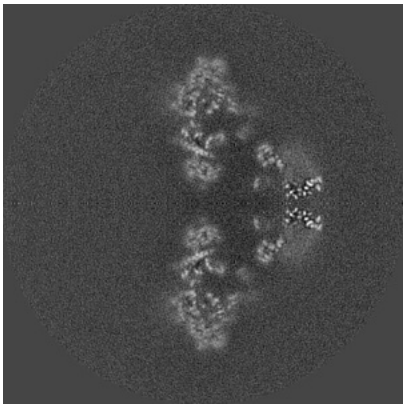


Z Index: 170

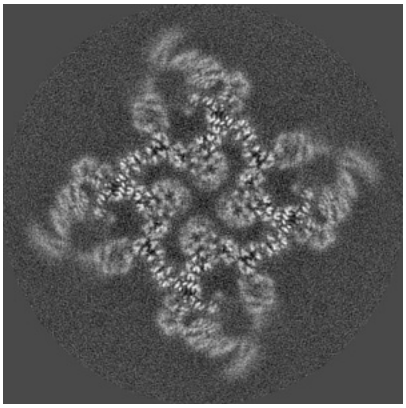
6.2.2 Raw map



X Index: 170



Y Index: 170

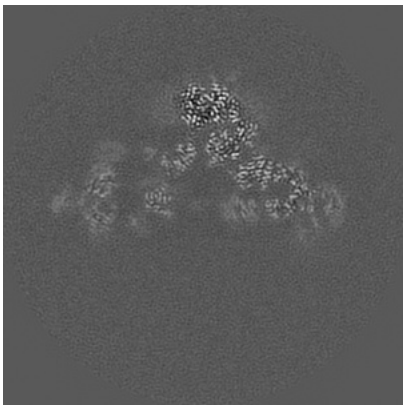


Z Index: 170

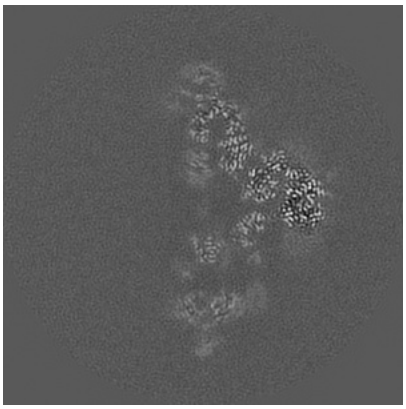
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

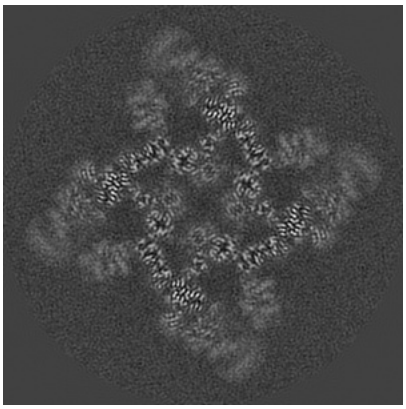
6.3.1 Primary map



X Index: 182

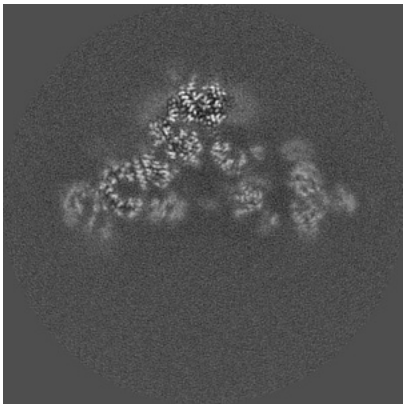


Y Index: 158

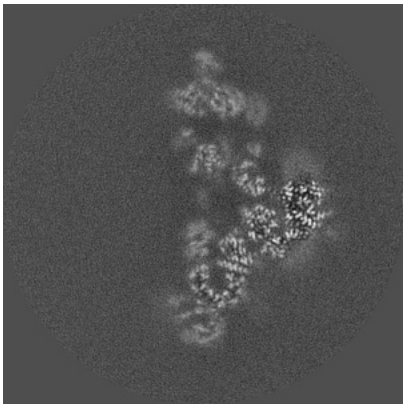


Z Index: 174

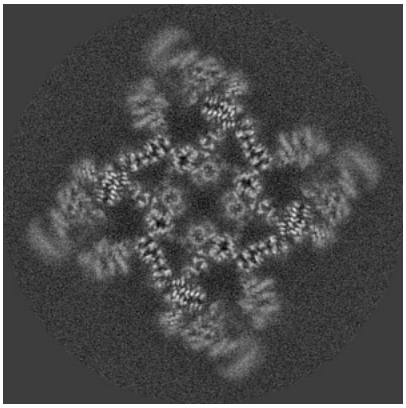
6.3.2 Raw map



X Index: 158



Y Index: 182

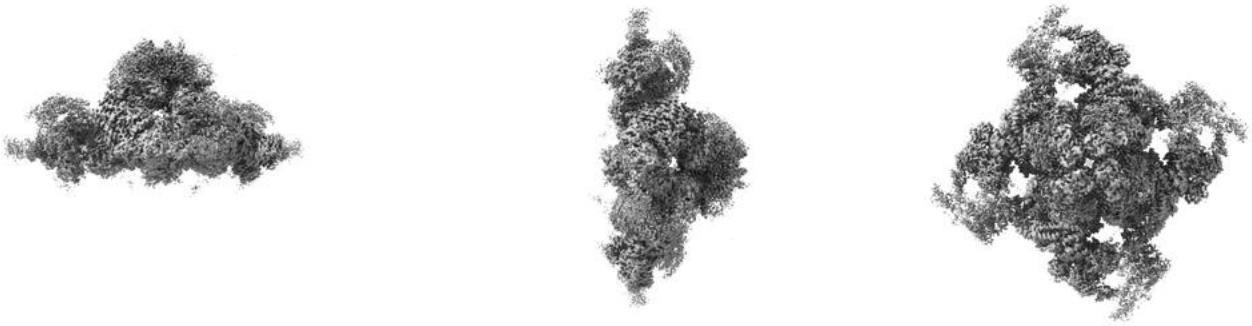


Z Index: 174

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

6.4 Orthogonal surface views (i)

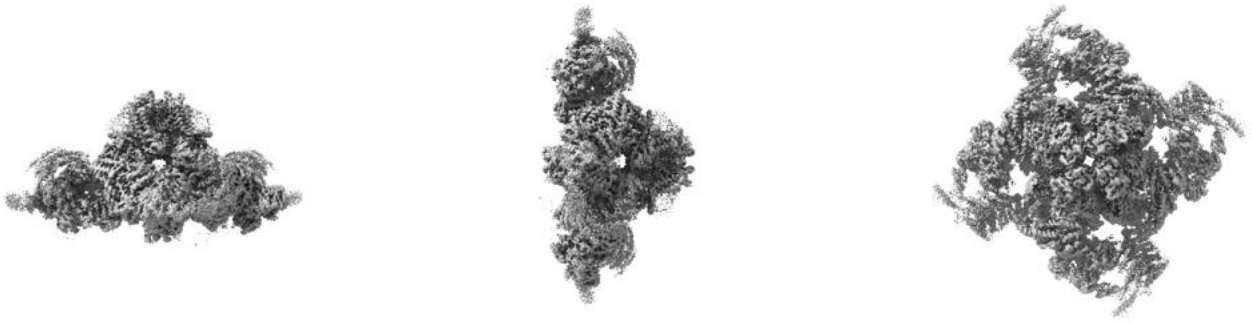
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.021. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

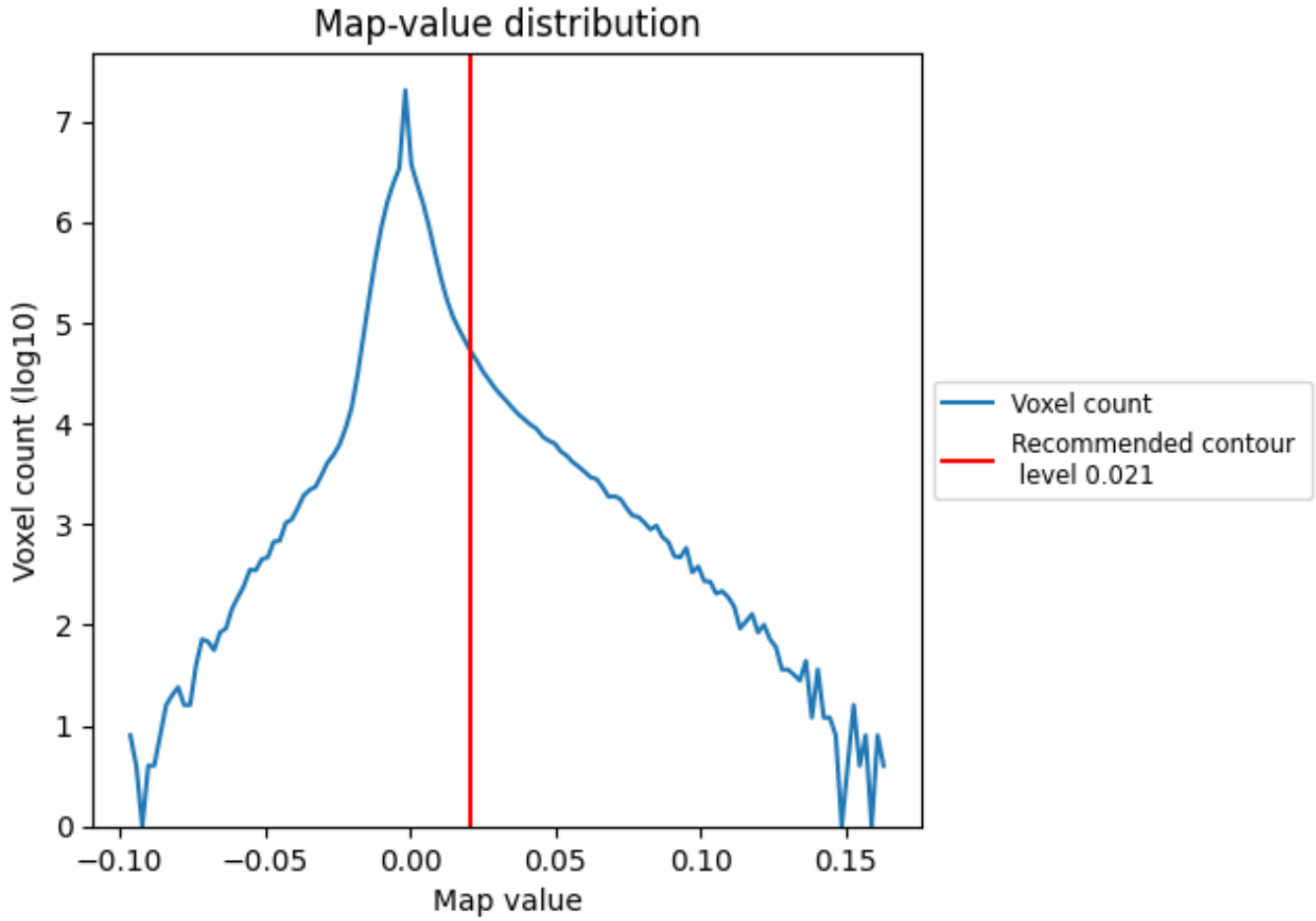
6.5 Mask visualisation (i)

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

7 Map analysis

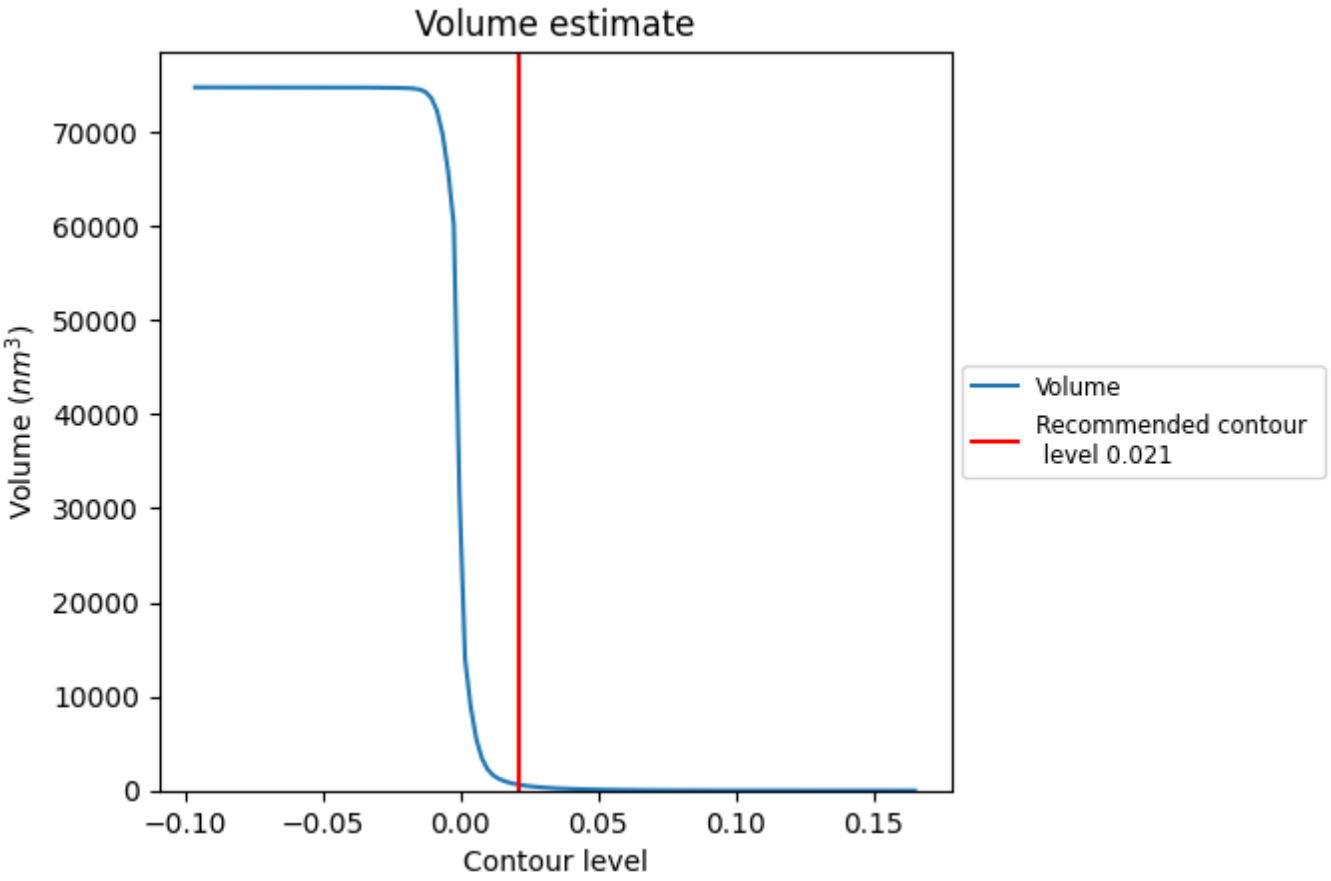
This section contains the results of statistical analysis of the map.

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.

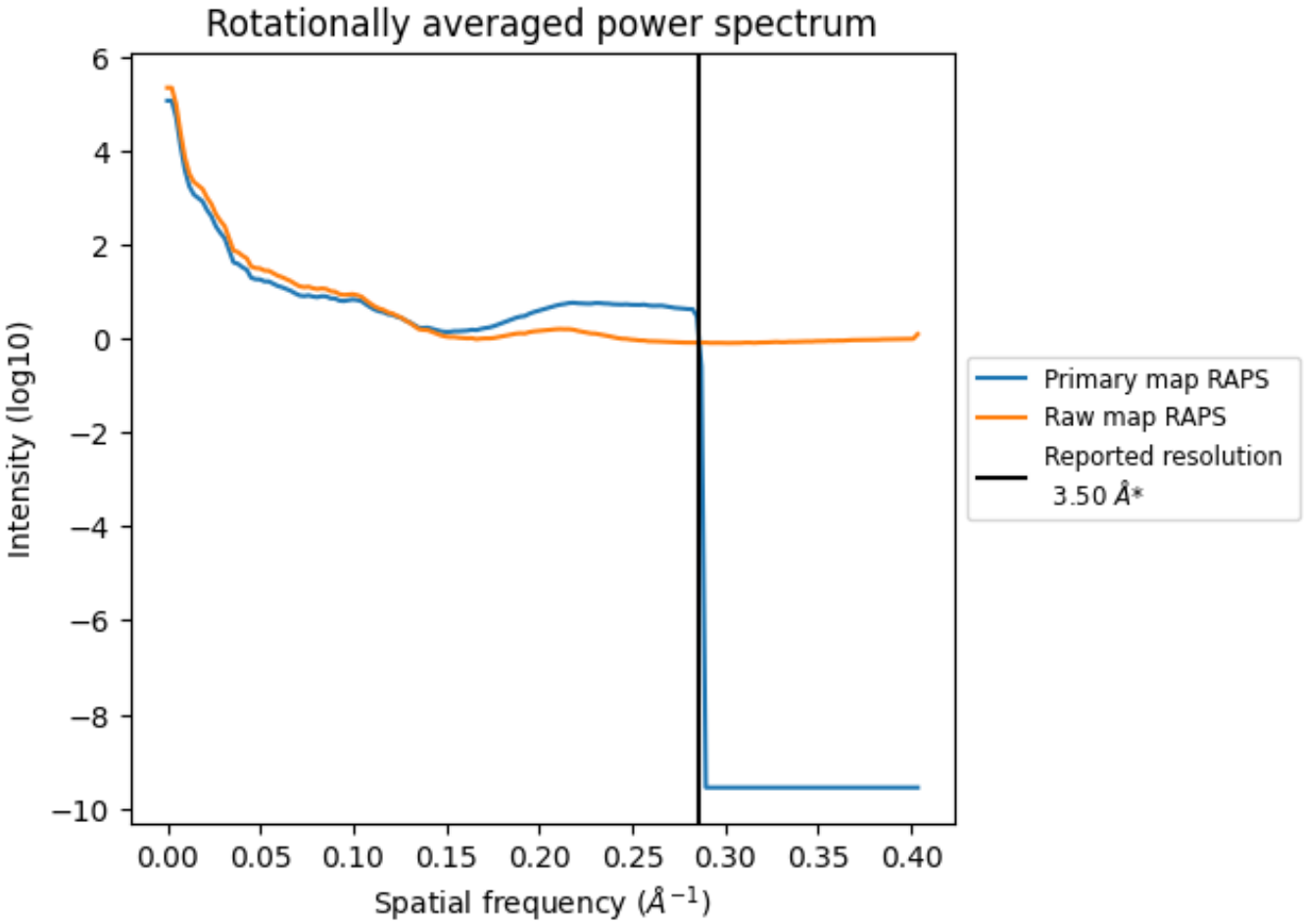
7.2 Volume estimate



The volume at the recommended contour level is 638 nm^3; this corresponds to an approximate mass of 576 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)

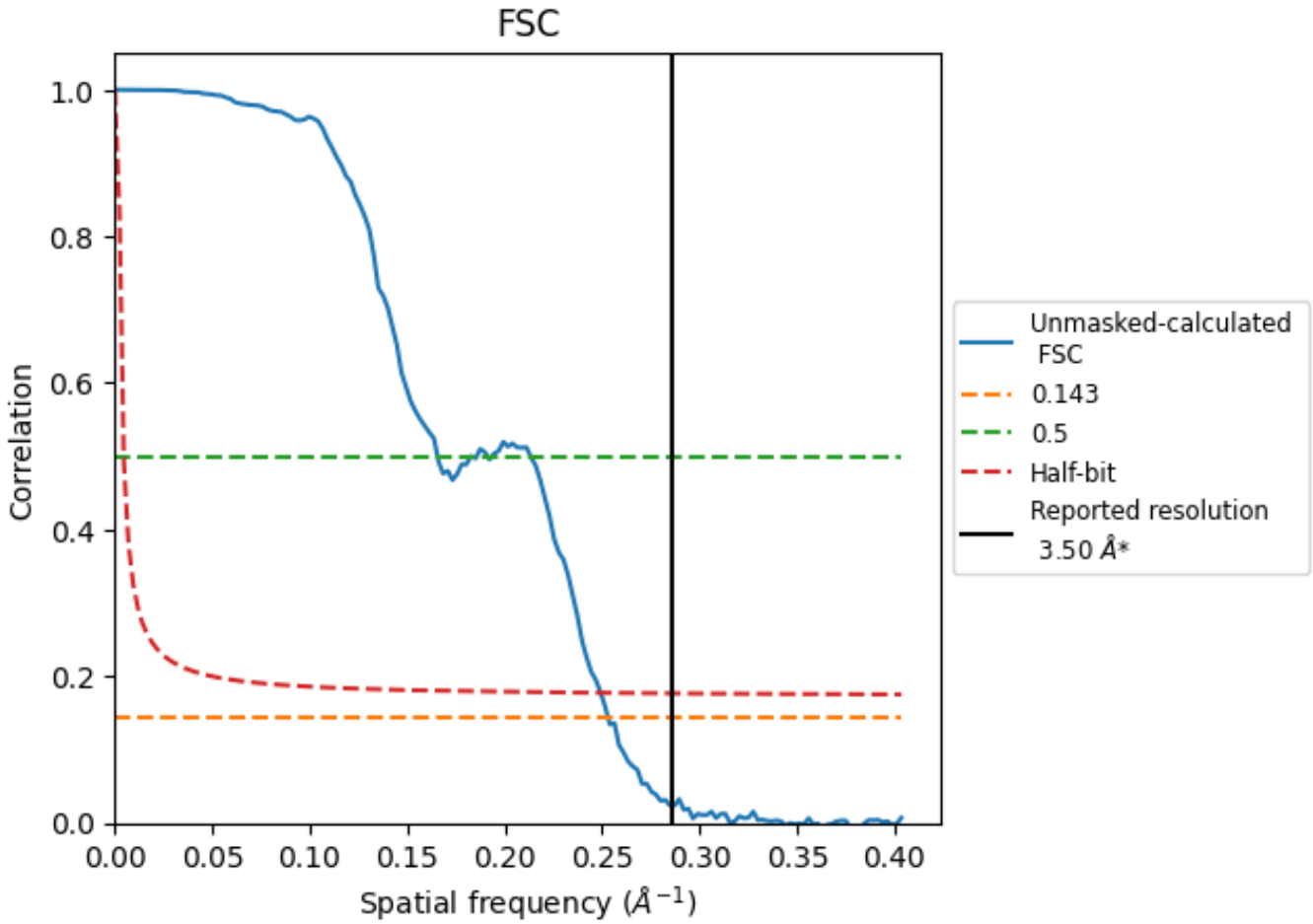


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

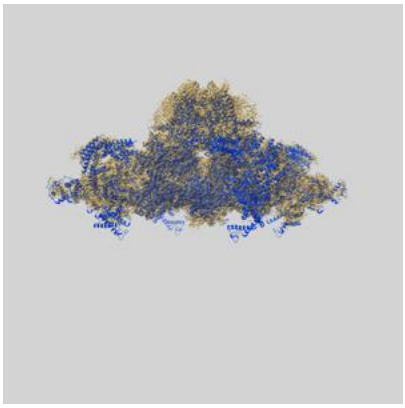
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.95	6.04	4.01

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.95 differs from the reported value 3.5 by more than 10 %

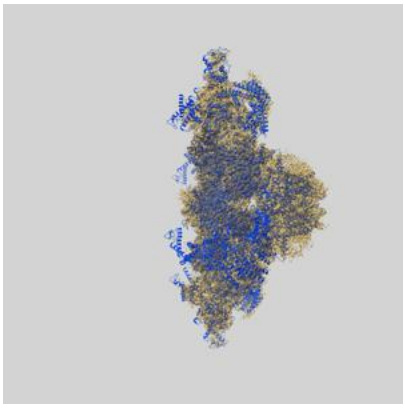
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33939 and PDB model 7VMP. Per-residue inclusion information can be found in section 3 on page 11.

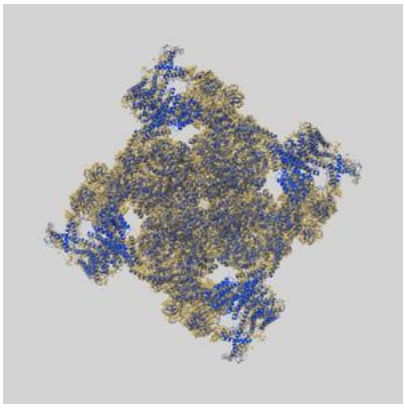
9.1 Map-model overlay



X



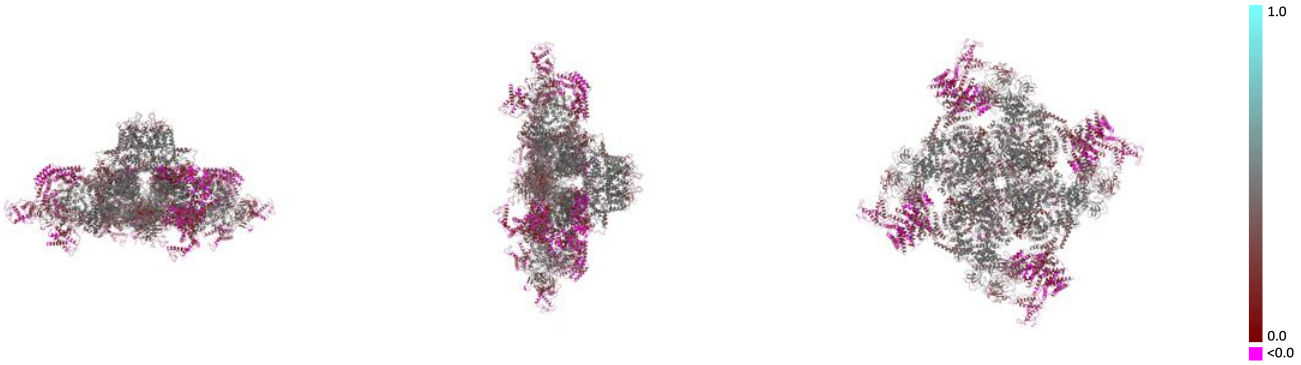
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.021 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.

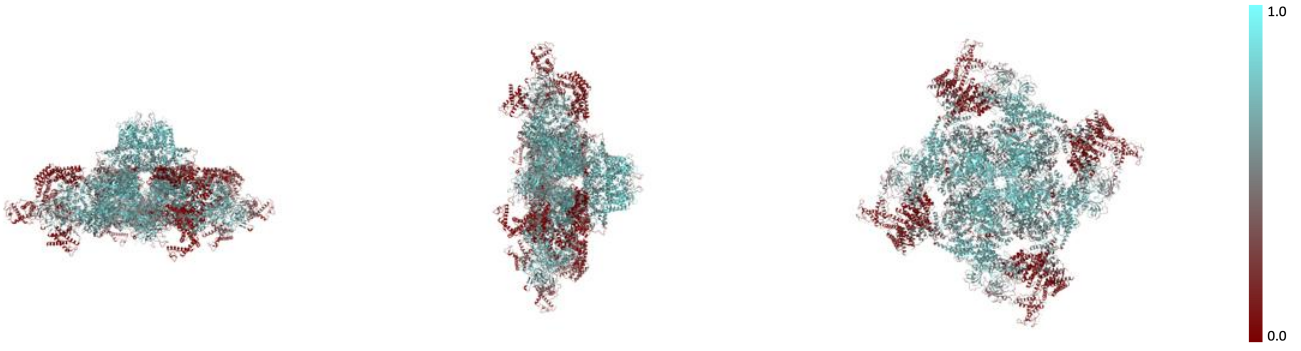
9.2 Q-score mapped to coordinate model



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.

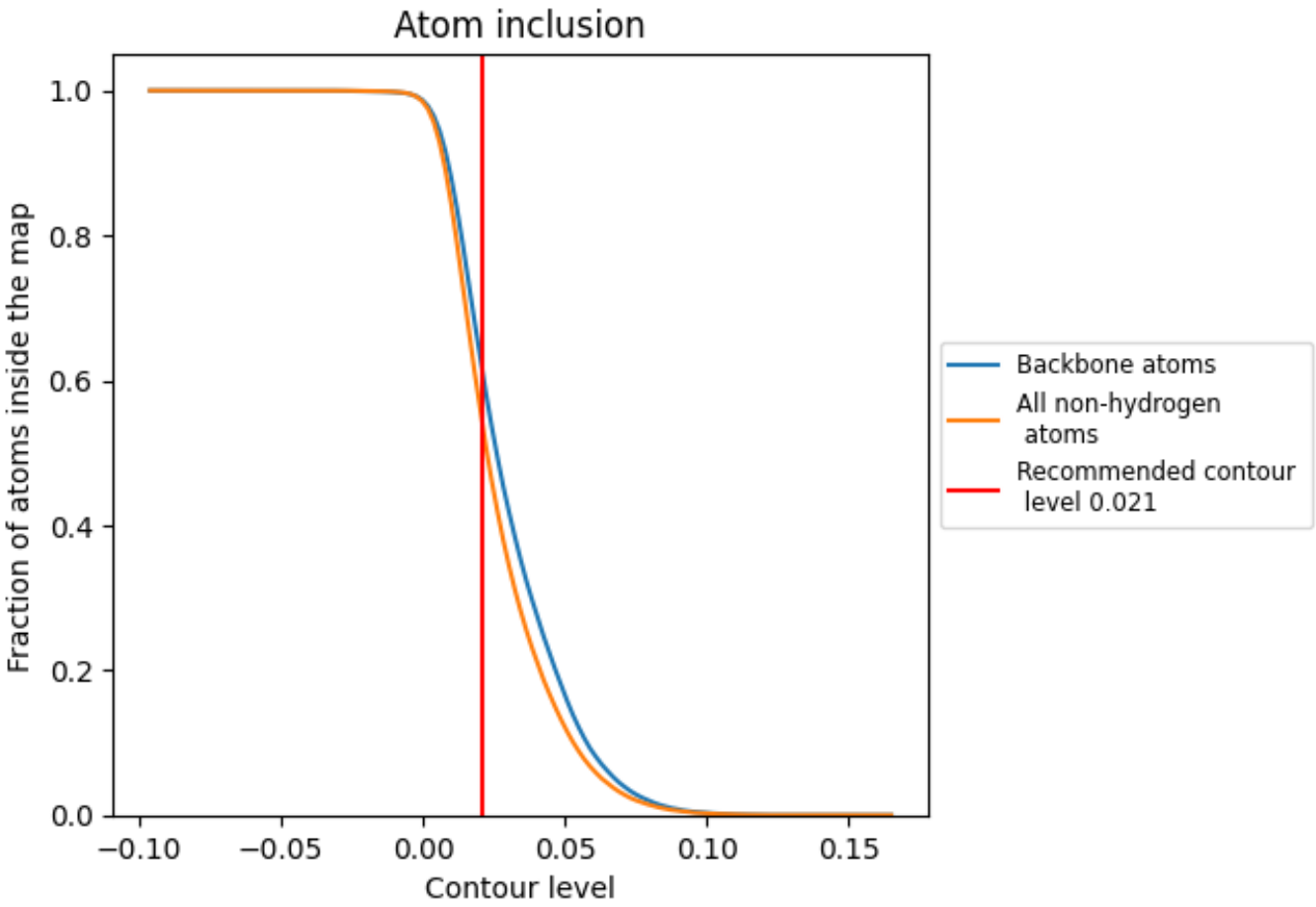
9.3 Atom inclusion mapped to coordinate model



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 (0.021).

9.4 Atom inclusion (i)



At the recommended contour level, 61% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5373	0.3360
A	0.5361	0.3340
B	0.5368	0.3380
C	0.5335	0.3330
D	0.5348	0.3310
G	0.6072	0.4090
H	0.6097	0.4110
I	0.6047	0.4090
J	0.6134	0.4090