Full wwPDB EM Validation Report ⓘ

Feb 25, 2024 – 10:33 AM EST

PDB ID	:	7JMF
EMDB ID	:	EMD-22392
Title	:	Functional Pathways of Biomolecules Retrieved from Single-particle Snapshots - Frame 42 - State 6 (S6)
Authors	:	Dashti, A.; des Georges, A.; Frank, J.; Ourmazd, A.
Deposited on	:	2020-07-31
Resolution	:	4.50 Å(reported)
Based on initial model	:	5TB4

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:

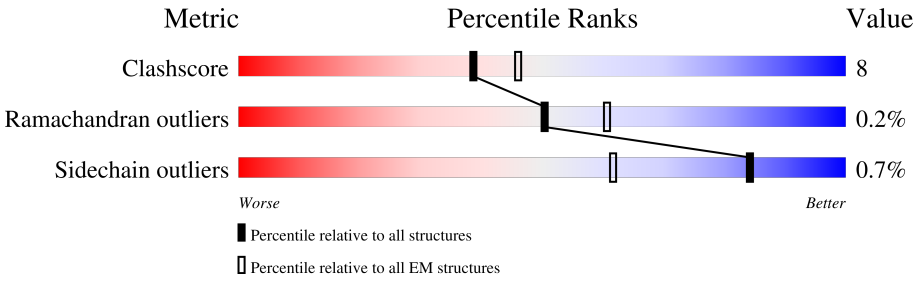
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.50 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	108	89% 69% 30%
1	F	108	84% 69% 30%
1	H	108	90% 69% 30%
1	J	108	87% 69% 30%
2	B	4687	63% 73% 15% 11%
2	E	4687	64% 73% 15% 11%
2	G	4687	69% 73% 16% 11%
2	I	4687	70% 73% 16% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120756 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	E	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	G	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	I	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	

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

Interest" by depositor).

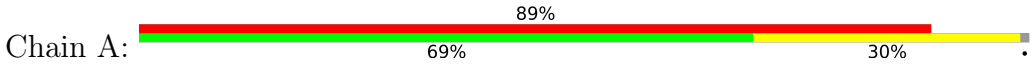
Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total Ca 1 1	0
4	E	1	Total Ca 1 1	0
4	G	1	Total Ca 1 1	0
4	I	1	Total Ca 1 1	0

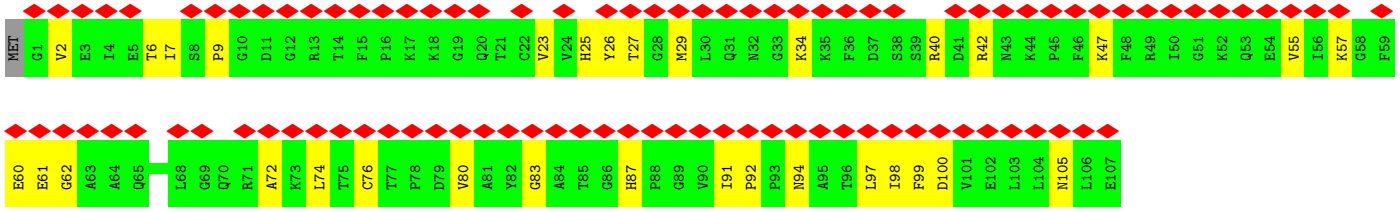
3 Residue-property plots (i)

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: Peptidyl-prolyl cis-trans isomerase FKBP1B

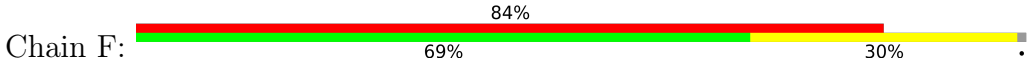
Chain A:

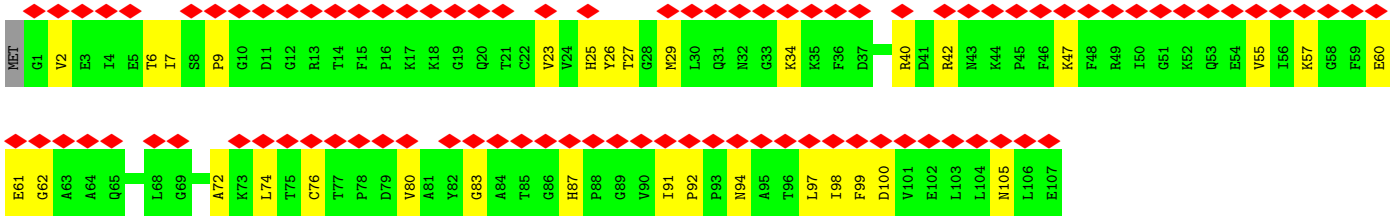




• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

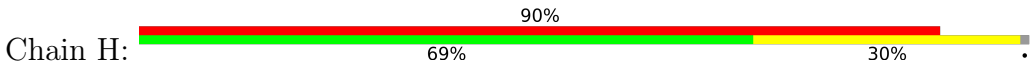
Chain F:





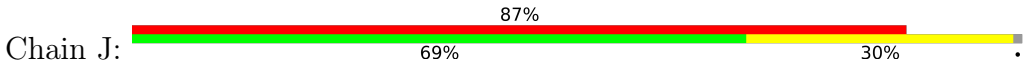
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

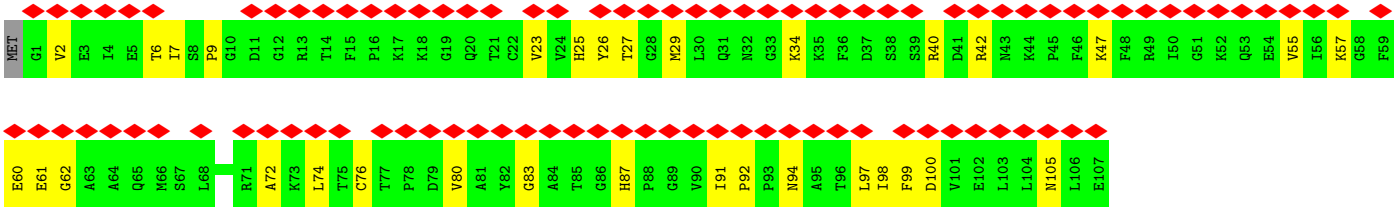
Chain H:



• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

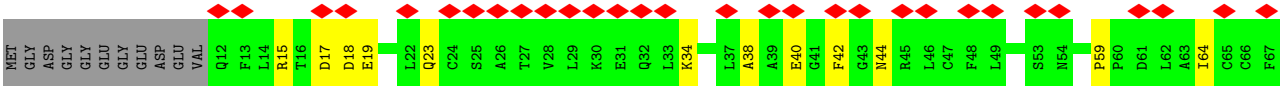
Chain J:

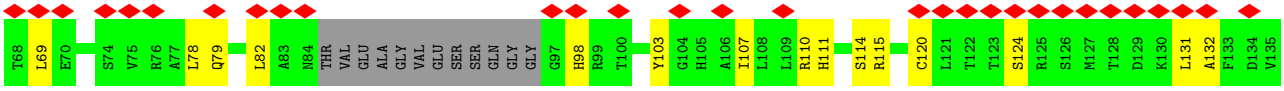


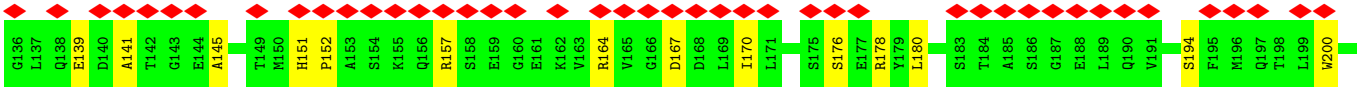


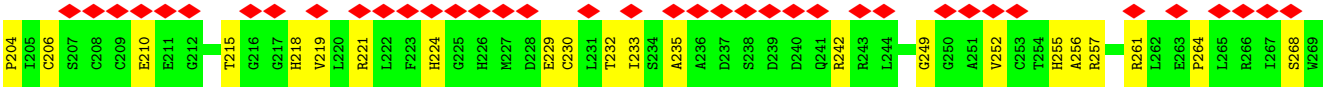
• Molecule 2: ryanodine receptor 1

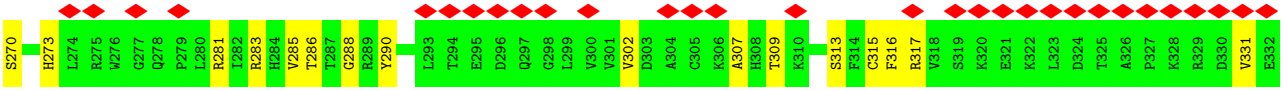
Chain B:

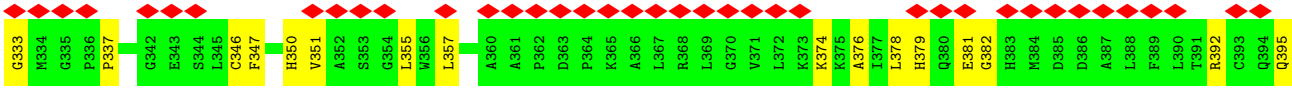


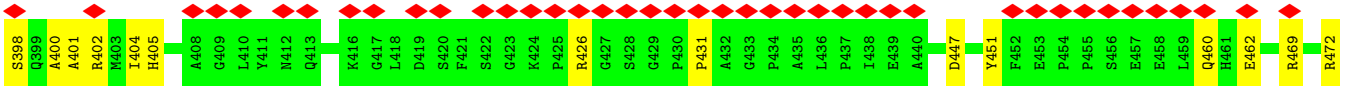


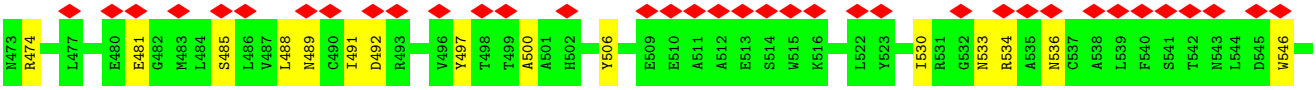


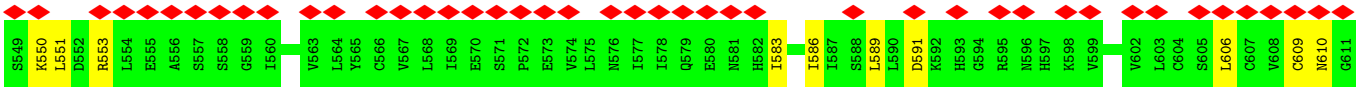


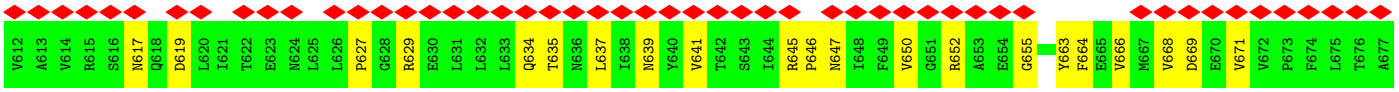


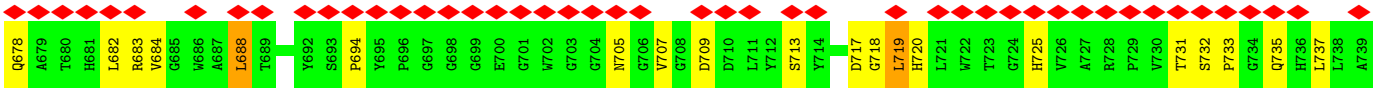


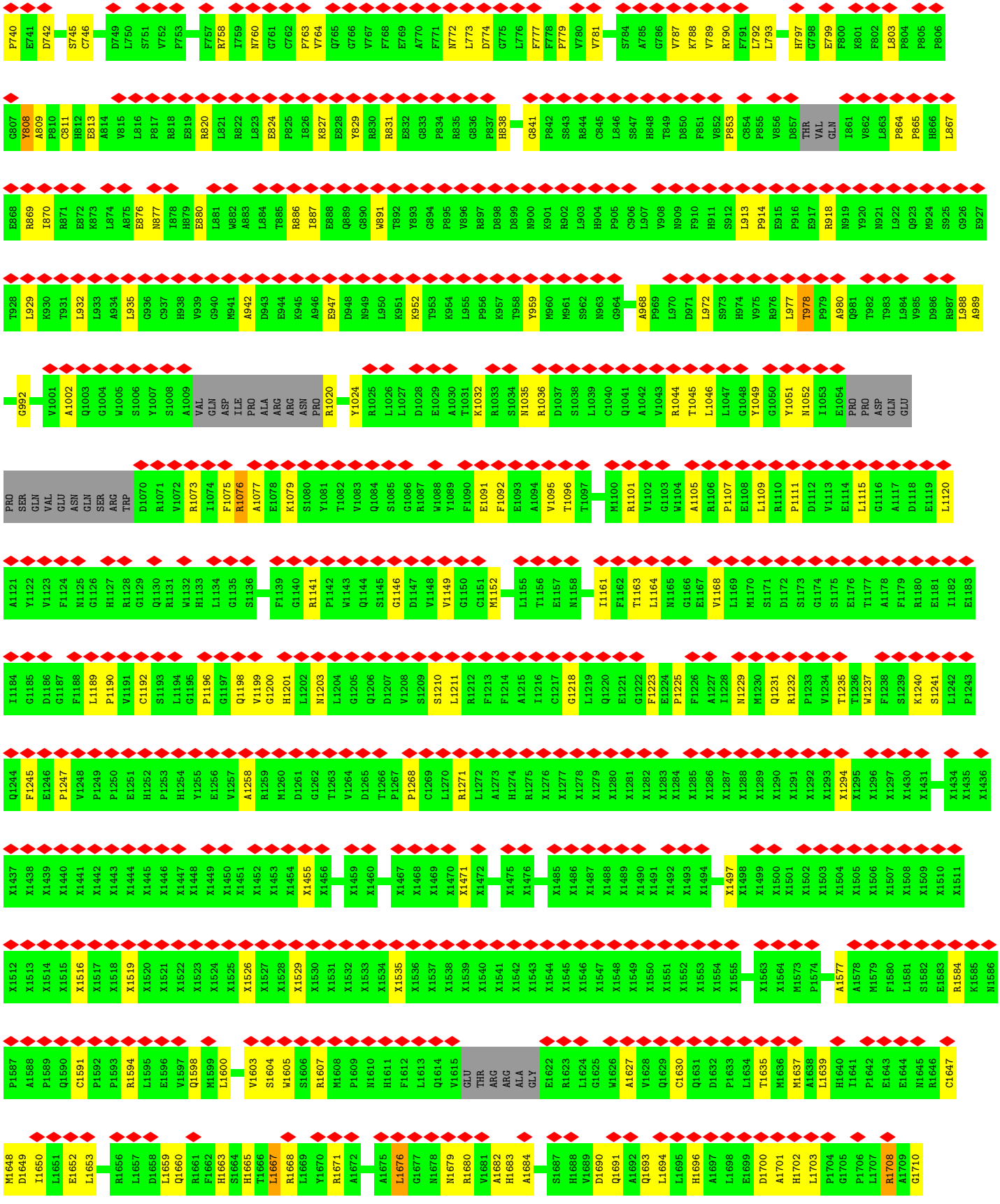








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G807 Y808 A809 P810 C811 H812 E813 A814 V815 L816 P817 R818 E819 R820 L821 R822 L823 E824 P825 I826 K827 E828 Y829 R830 R831 E832 G833 P834 R835 G836 P837 H838 G841 P842 S843 R844 C845 L846 S847 H848 T849 D850 F851 V852 P853 C854 P855 V856 D857 THR VAL GLN I861 V862 L863 P864 P865 H866 L867
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T928 L929 K930 T931 L932 L933 A934 L935 G936 C937 H938 V939 G940 M941 A942 D943 E944 K945 A946 E947 D948 N949 L950 K951 K952 T953 K954 L955 P956 K957 T958 Y959 M960 M961 S962 N963 G964 A968 P969 L970 D971 L972 S973 H974 V975 R976 L977 T978 P979 A980 Q981 T982 T983 L984 V985 D986 R987 L988 A989
G992 V1001 A1002 Q1003 G1004 W1005 S1006 Y1007 S1008 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 Y1024 R1025 L1026 L1027 D1028 E1029 A1030 T1031 K1032 R1033 S1034 N1035 R1036 D1037 S1038 L1039 C1040 Q1041 A1042 V1043 R1044 T1045 L1046 L1047 G1048 Y1049 G1050 Y1051 N1052 I1053 E1054 PRO PRO ASP GLN GLU
PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1071 V1072 R1073 I1074 F1075 R1076 A1077 E1078 K1079 S1080 Y1081 T1082 V1083 Q1084 S1085 G1086 R1087 W1088 Y1089 F1090 E1091 F1092 E1093 A1094 V1095 T1096 T1097 M1100 R1101 V1102 G1103 W1104 A1105 R1106 P1107 E1108 L1109 R1110 P1111 D1112 V1113 E1114 L1115 G1116 A1117 D1118 E1119 L1120
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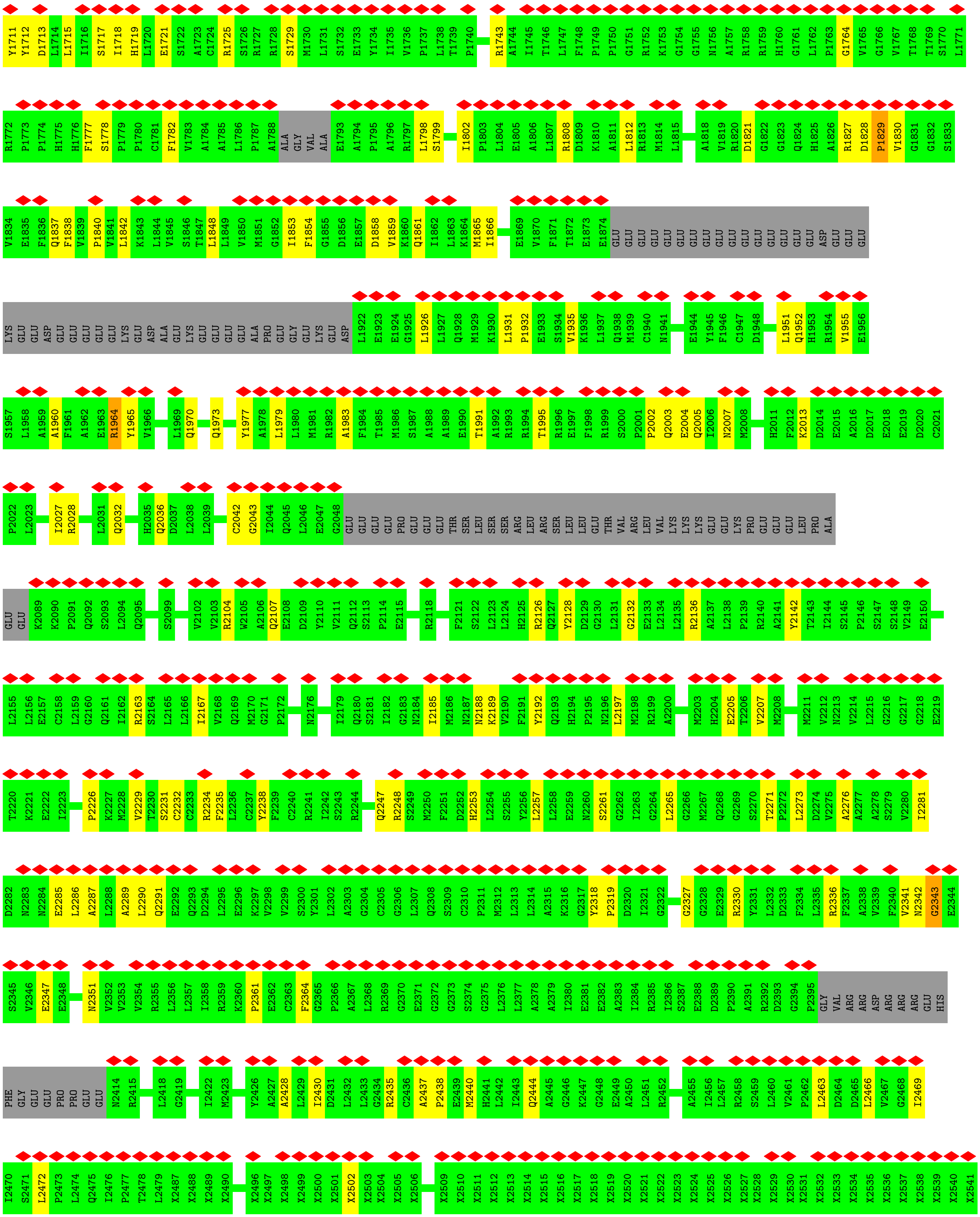
M1648 D1649 I1650 L1651 E1652 L1653 R1656 L1657 D1658 L1659 Q1660 R1661 F1662 H1663 S1664 H1665 T1666 L1667 R1668 L1669 Y1670 R1671 A1672 A1675 L1676 G1677 N1678 N1679 R1680 V1681 A1682 H1683 A1684 S1687 H1688 V1689 D1690 Q1691 A1692 Q1693 L1694 L1695 H1696 A1697 L1698 E1699 D1700 A1701 H1702 L1703 P1704 G1705 P1706 L1707 R1708 A1709 G1710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LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 G1925 L1926 L1927 Q1928 M1929 K1930 L1931 P1932 E1933 S1934 V1935 K1936 L1937 Q1938 M1939 C1940 N1941 E1944 Y1945 F1946 C1947 D1948 L1951 Q1952 H1953 R1954 V1955 E1956
S1957 L1958 A1959 A1960 F1961 A1962 E1963 R1964 Y1965 V1966 L1969 Q1970 Q1973 Y1977 A1978 L1979 L1980 M1981 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 R1996 E1997 F1998 R1999 S2000 P2001 P2002 Q2003 E2004 Q2005 I2006 N2007 M2008 H2011 F2012 K2013 D2014 E2015 A2016 D2017 E2018 E2019 D2020 C2021
P2022 L2023 I2027 R2028 L2031 Q2032 H2035 Q2036 D2037 L2038 L2039 C2042 G2043 I2044 Q2045 L2046 E2047 G2048 GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA
GLU GLU K2089 K2090 P2091 Q2092 S2093 L2094 Q2095 S2099 V2102 V2103 R2104 W2105 A2106 Q2107 E2108 D2109 Y2110 V2111 Q2112 S2113 P2114 E2115 R2118 F2121 S2122 L2123 L2124 H2125 R2126 Q2127 Y2128 D2129 G2130 L2131 G2132 E2133 L2134 L2135 R2136 A2137 L2138 P2139 R2140 A2141 Y2142 T2143 I2144 S2145 P2146 S2147 S2148 V2149 E2150
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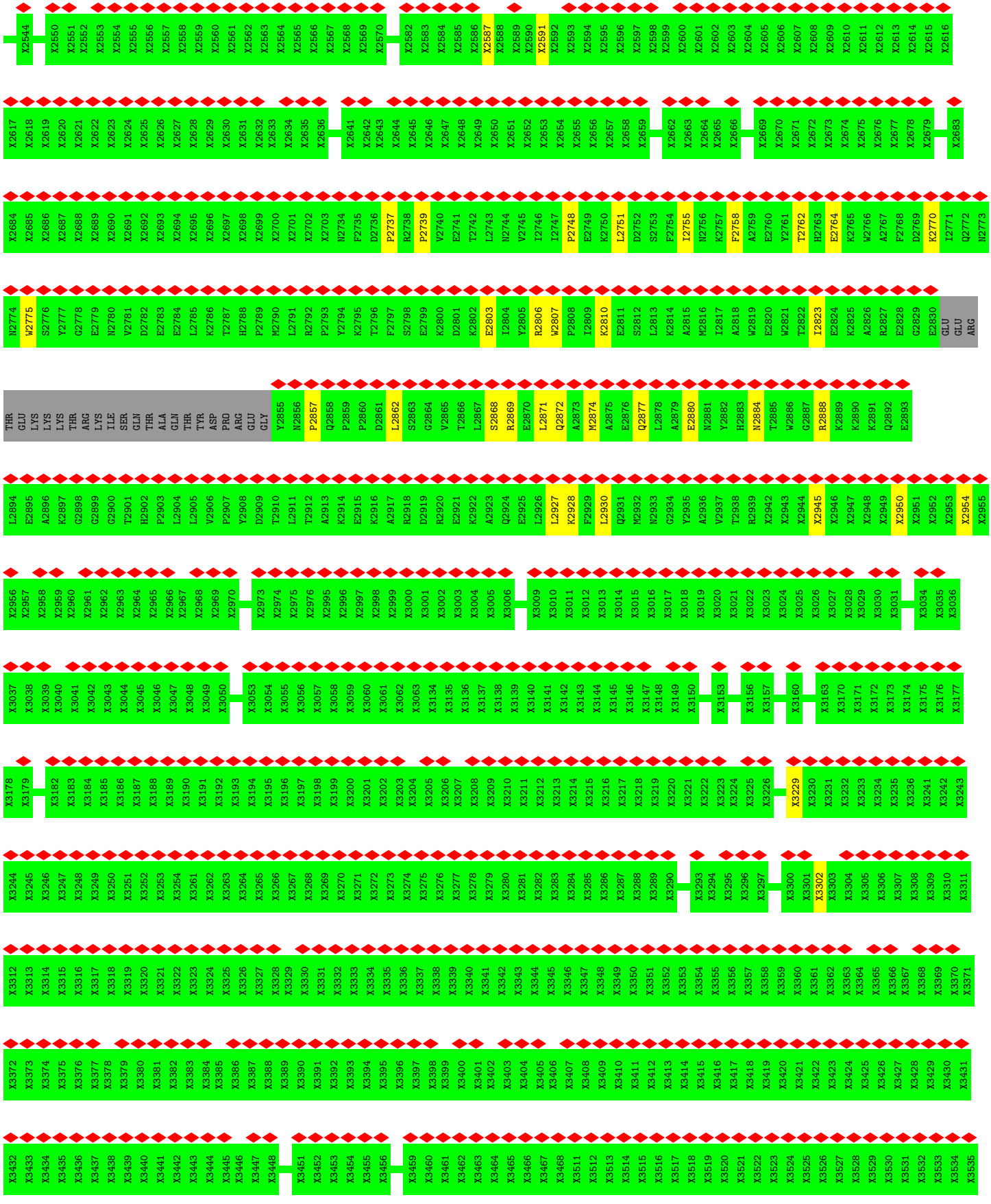
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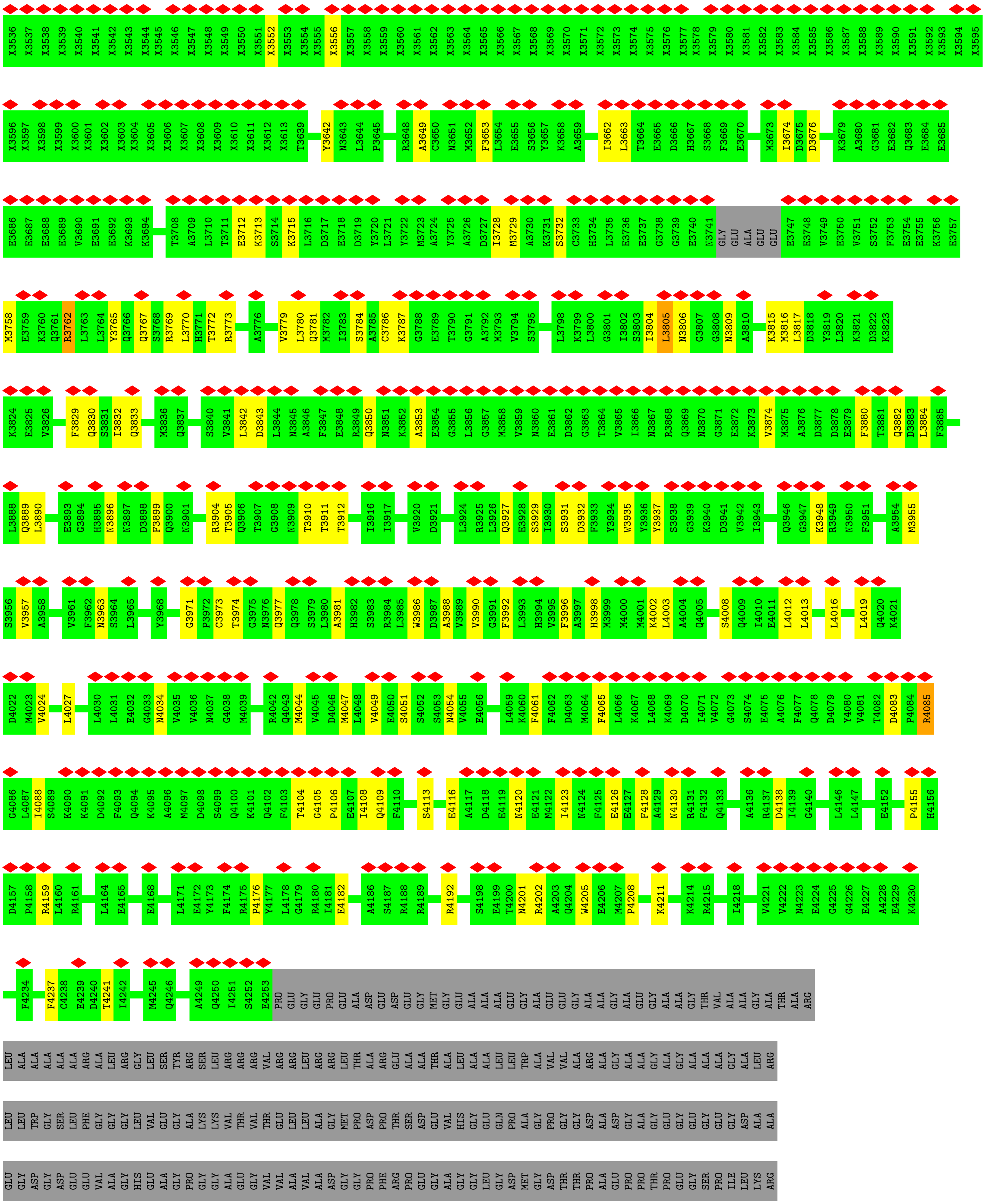
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LEU ALA ALA ALA ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG LEU ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA ALA ALA LEU LEU TRP ALA VAL VAL ALA ARG ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA LEU ARG
LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA
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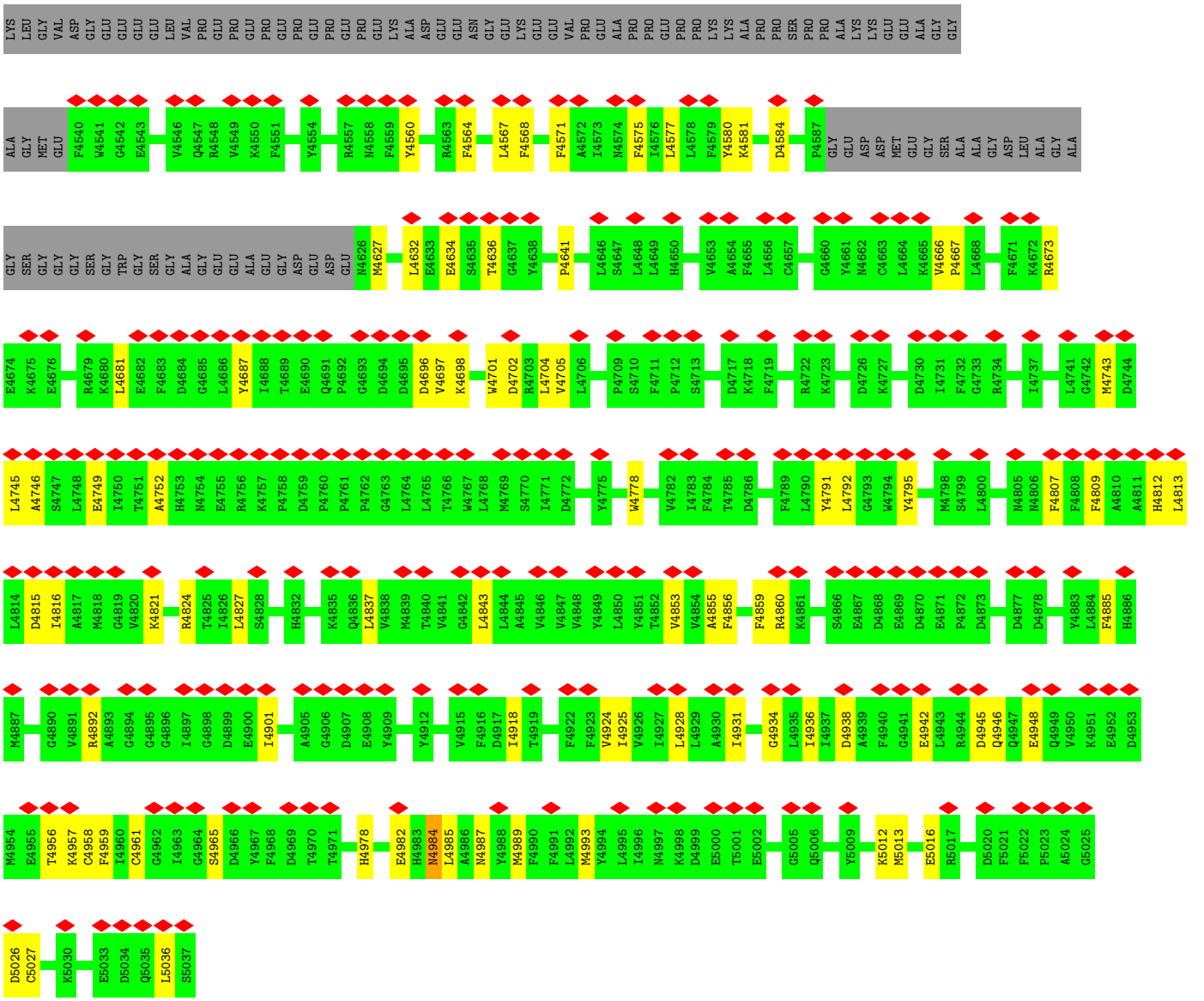
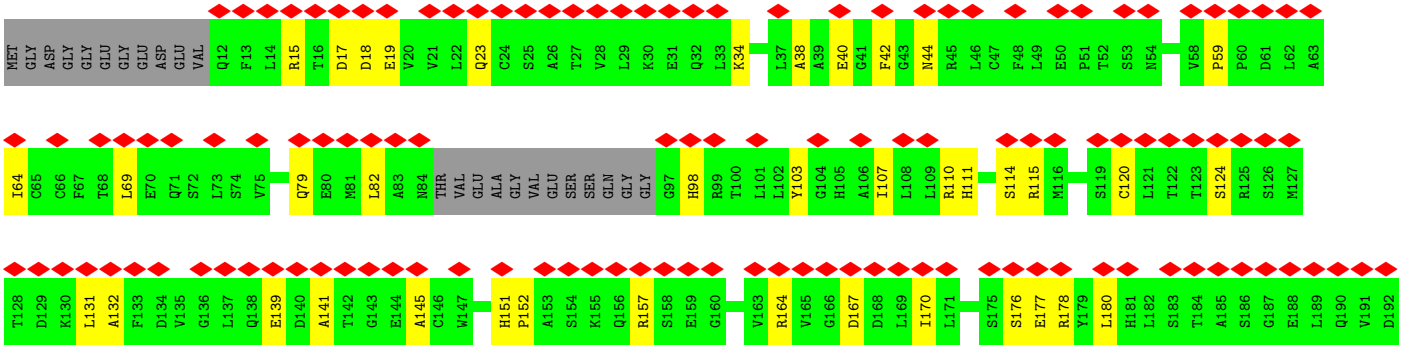
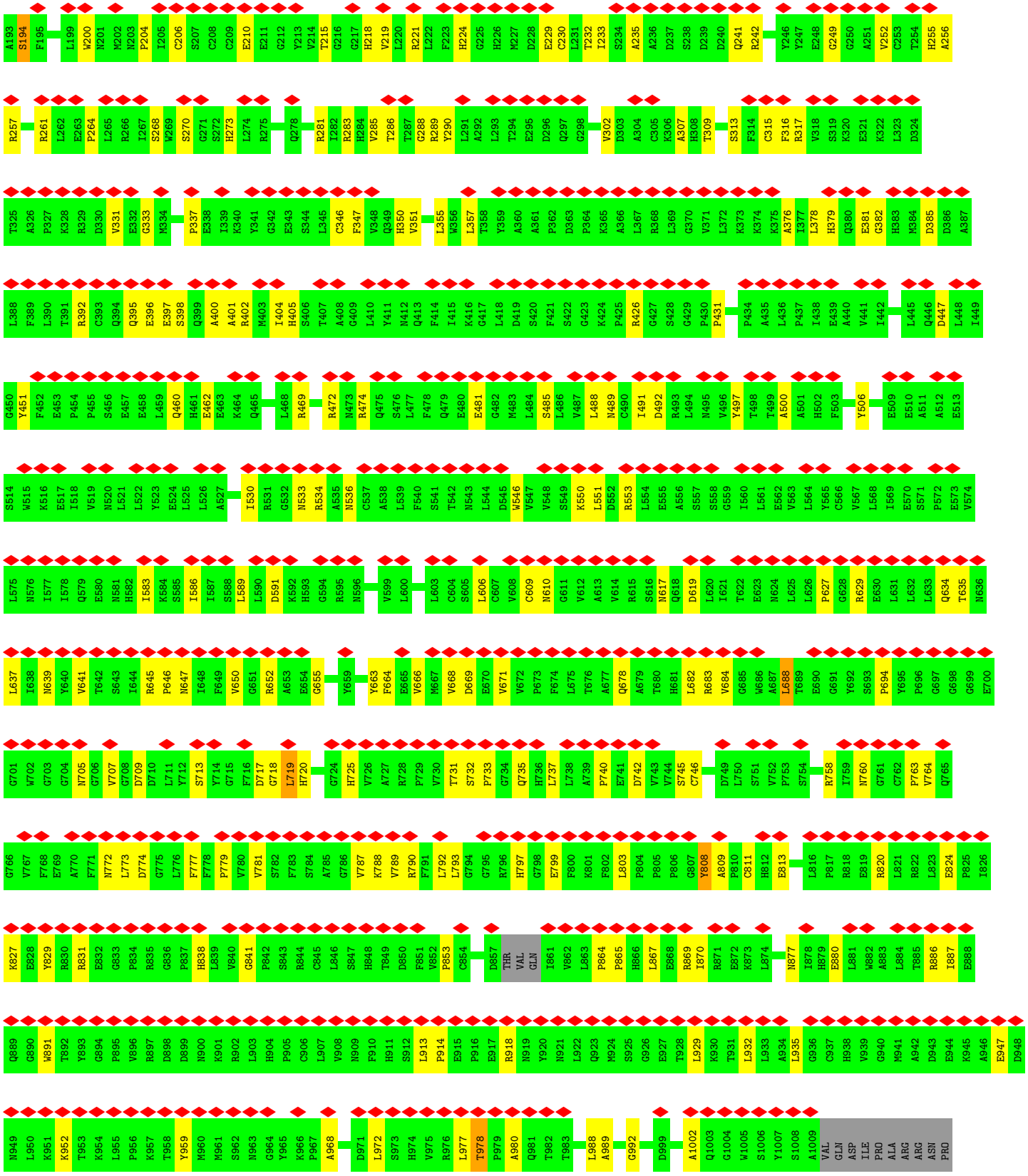


• Molecule 2: ryanodine receptor 1

Chain E:

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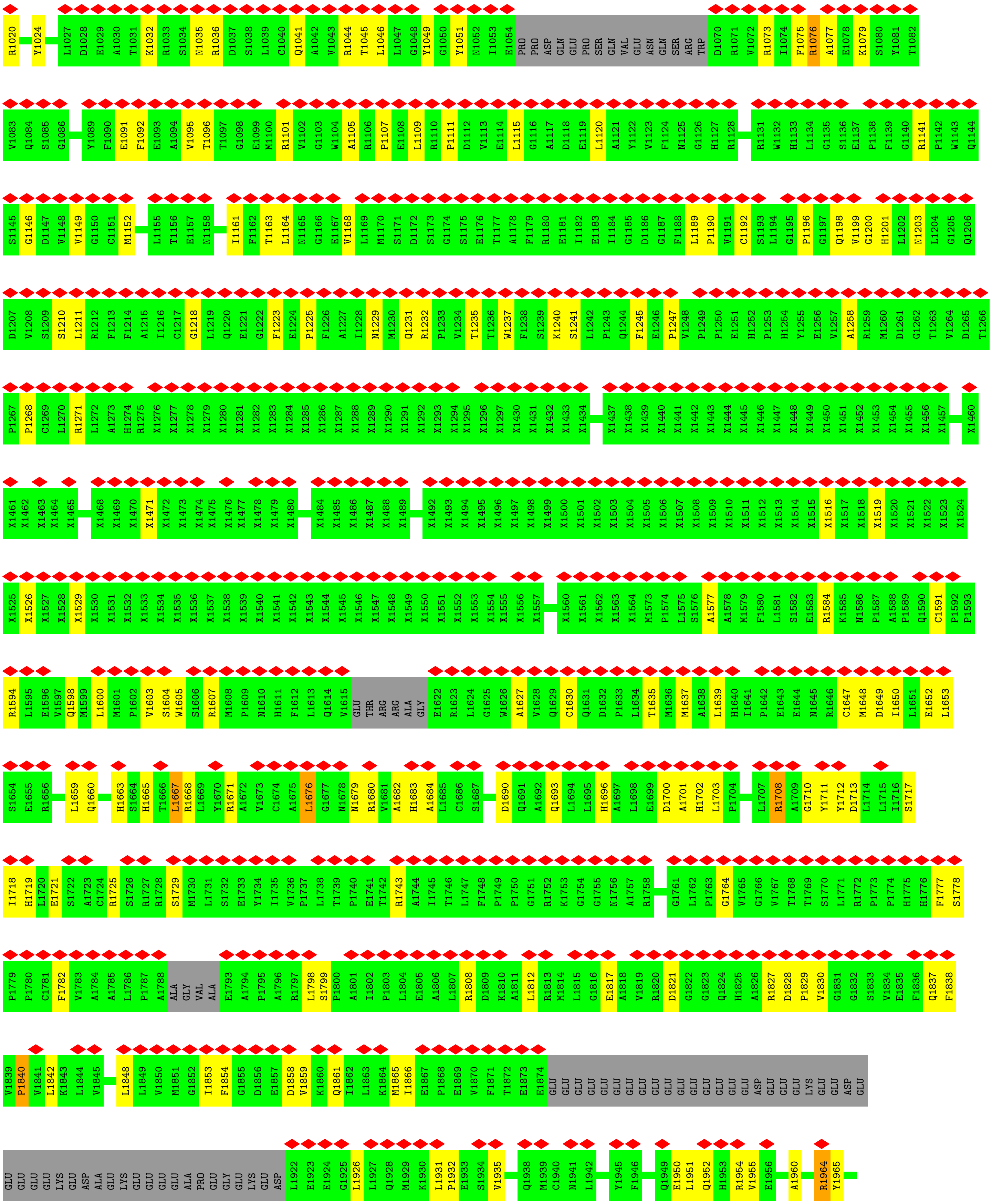
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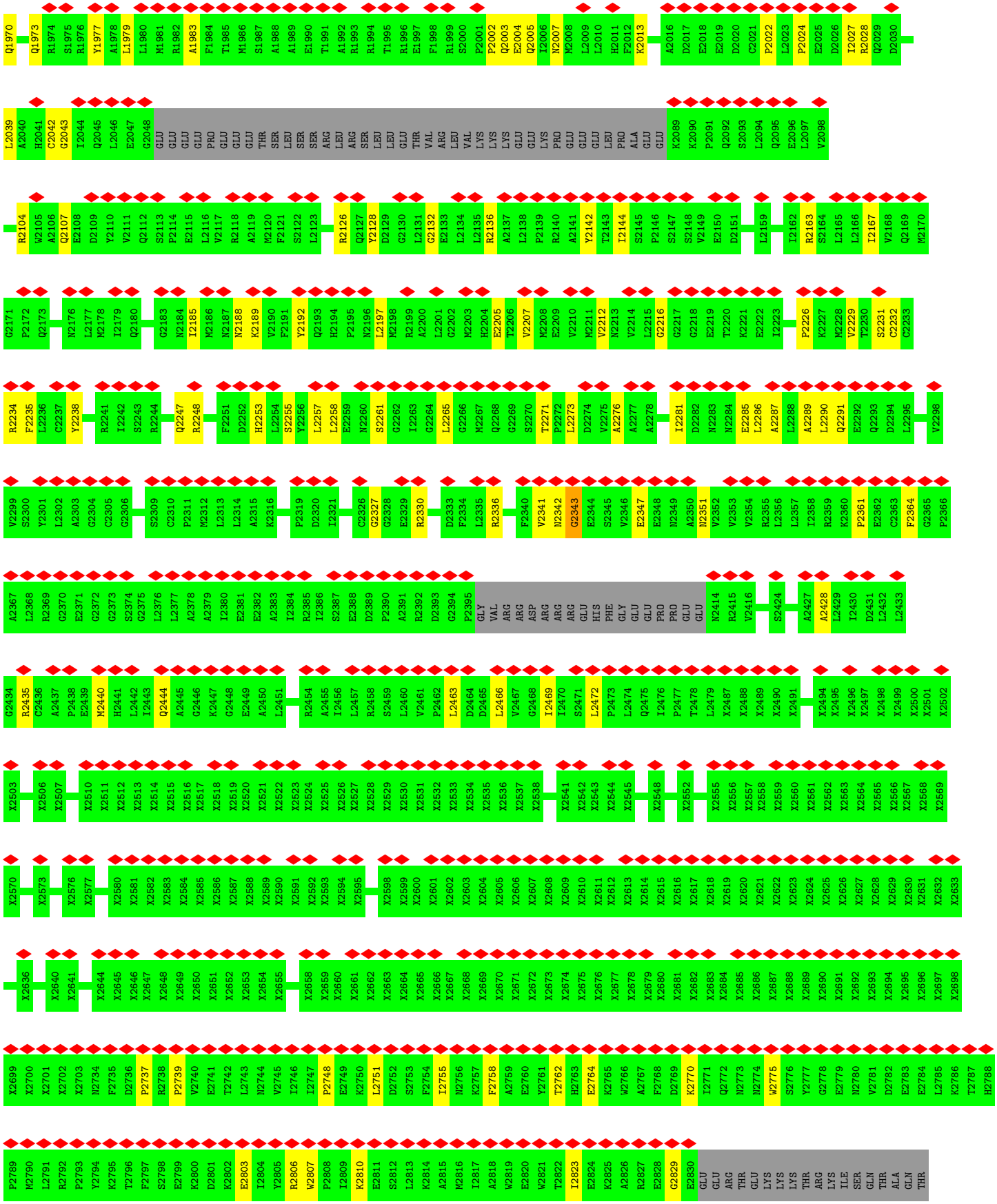
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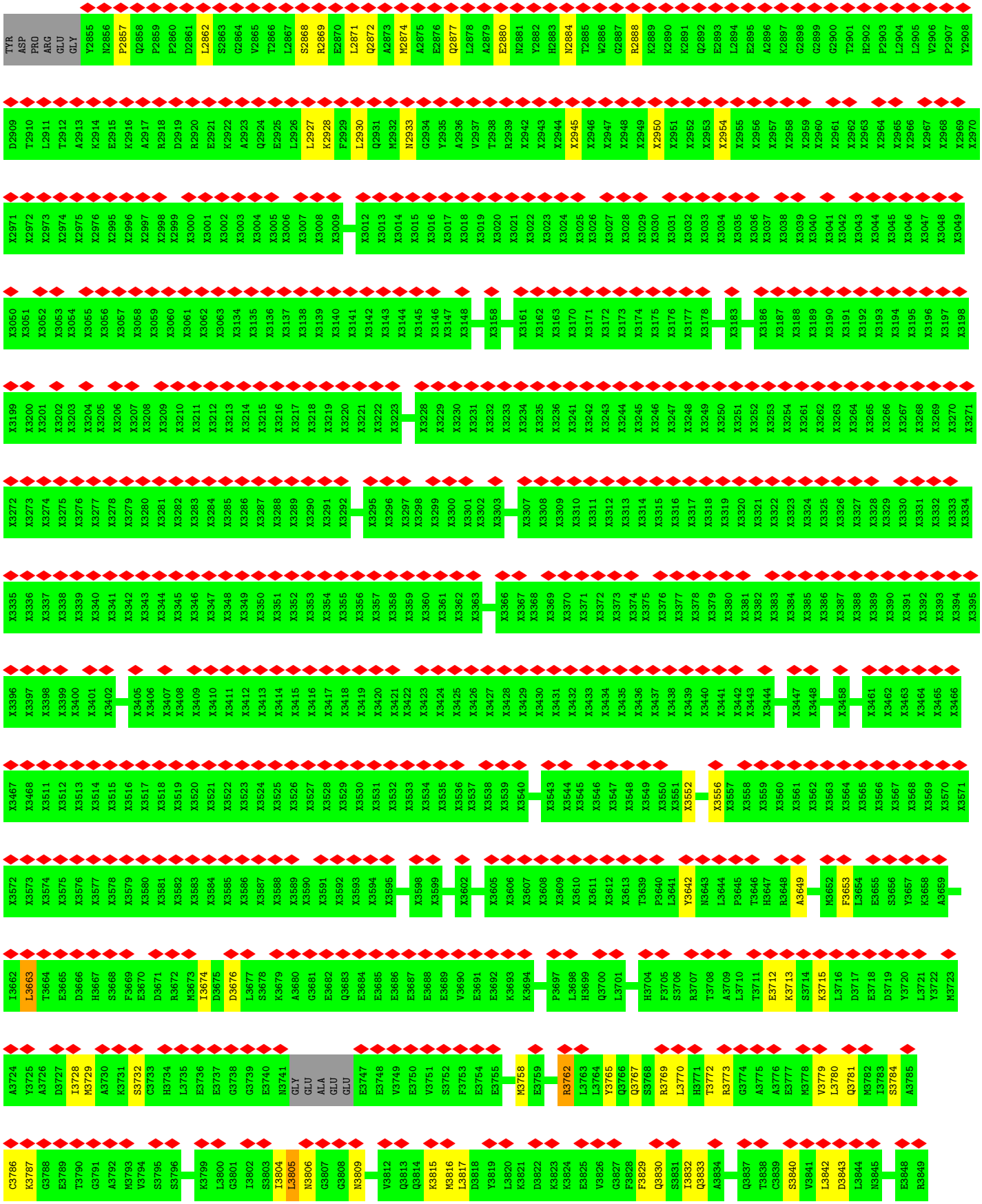
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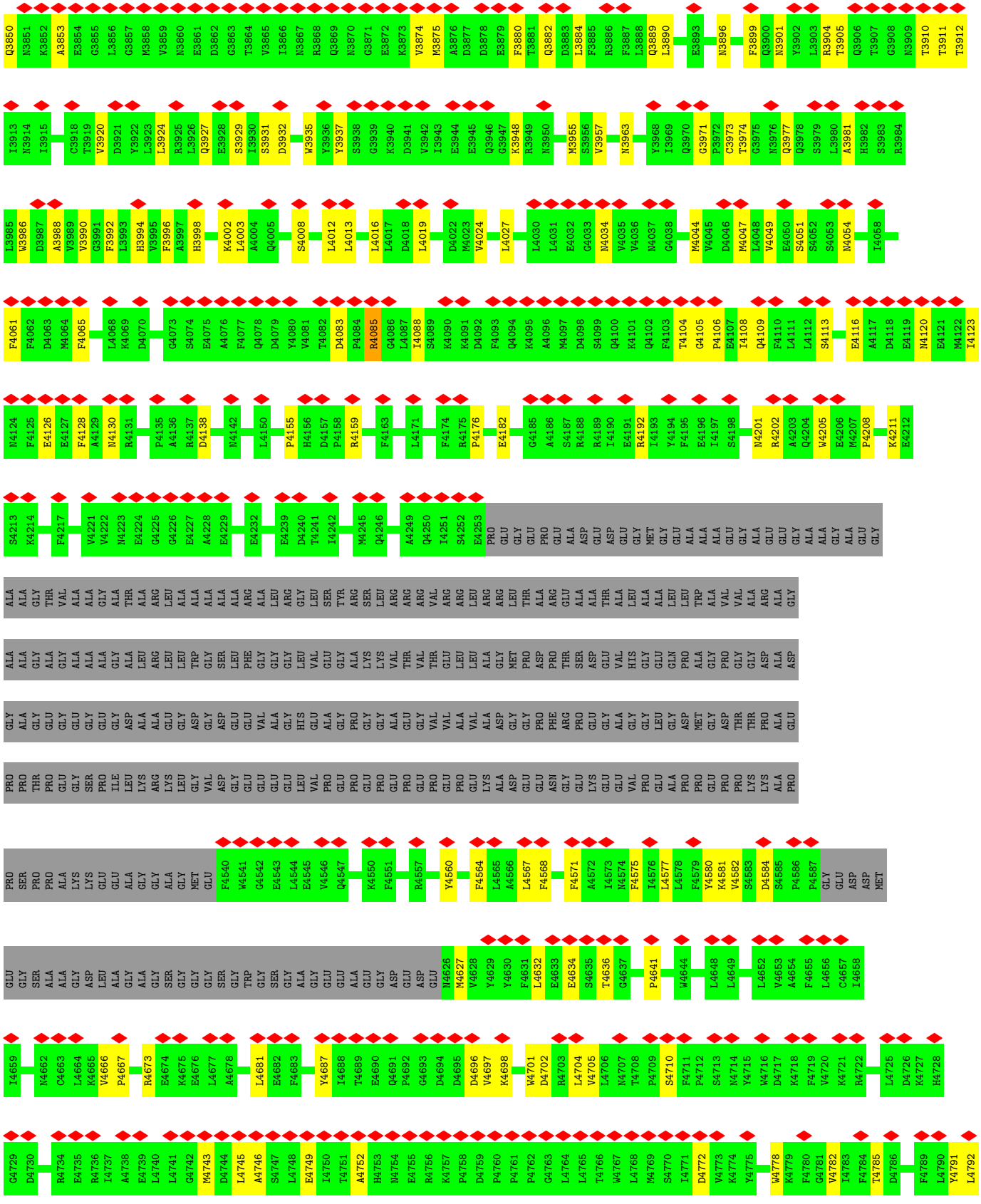
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GLY ALA GLY GLU GLY GLY GLU GLY GLU GLY ASP ALA ALA GLU GLY ASP GLY ASP GLU GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA VAL ALA ASP ALA GLY GLY PRO PHE ARG PRO GLU GLY ALA GLY GLY LEU GLY ASP MET GLY ASP THR THR PRO ALA GLU
PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU LYS ALA ASP GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO GLU PRO PRO LYS LYS ALA PRO
PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU F4540 W4541 G4542 E4543 L4544 E4545 V4546 Q4547 K4550 F4551 R4557 Y4560 F4564 L4565 A4566 L4567 F4568 F4571 A4572 I4573 N4574 F4575 I4576 L4577 L4578 F4579 Y4580 K4581 V4582 S4583 D4584 S4585 P4586 P4587 GLY GLU ASP ASP MET
GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY GLY SER GLY TRP GLY GLY SER GLY GLY ALA GLY GLU GLU ALA GLU GLY GLY ASP GLU GLU N4626 M4627 V4628 Y4629 Y4630 F4631 L4632 E4633 E4634 S4635 T4636 G4637 P4641 W4644 L4648 L4649 L4652 V4653 A4654 F4655 L4656 C4657 I4658
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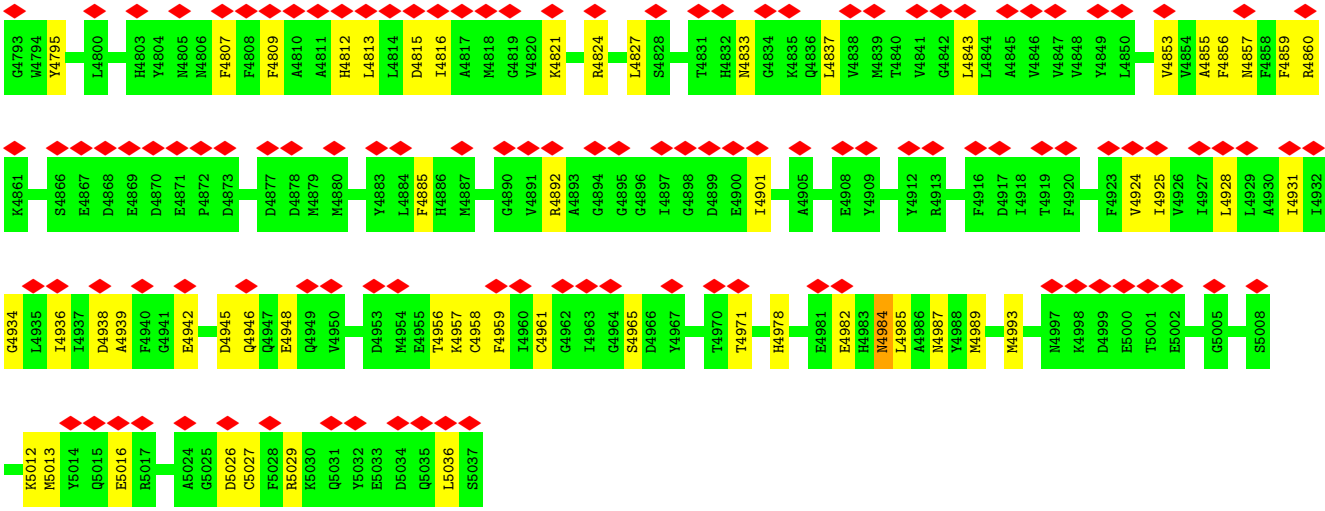
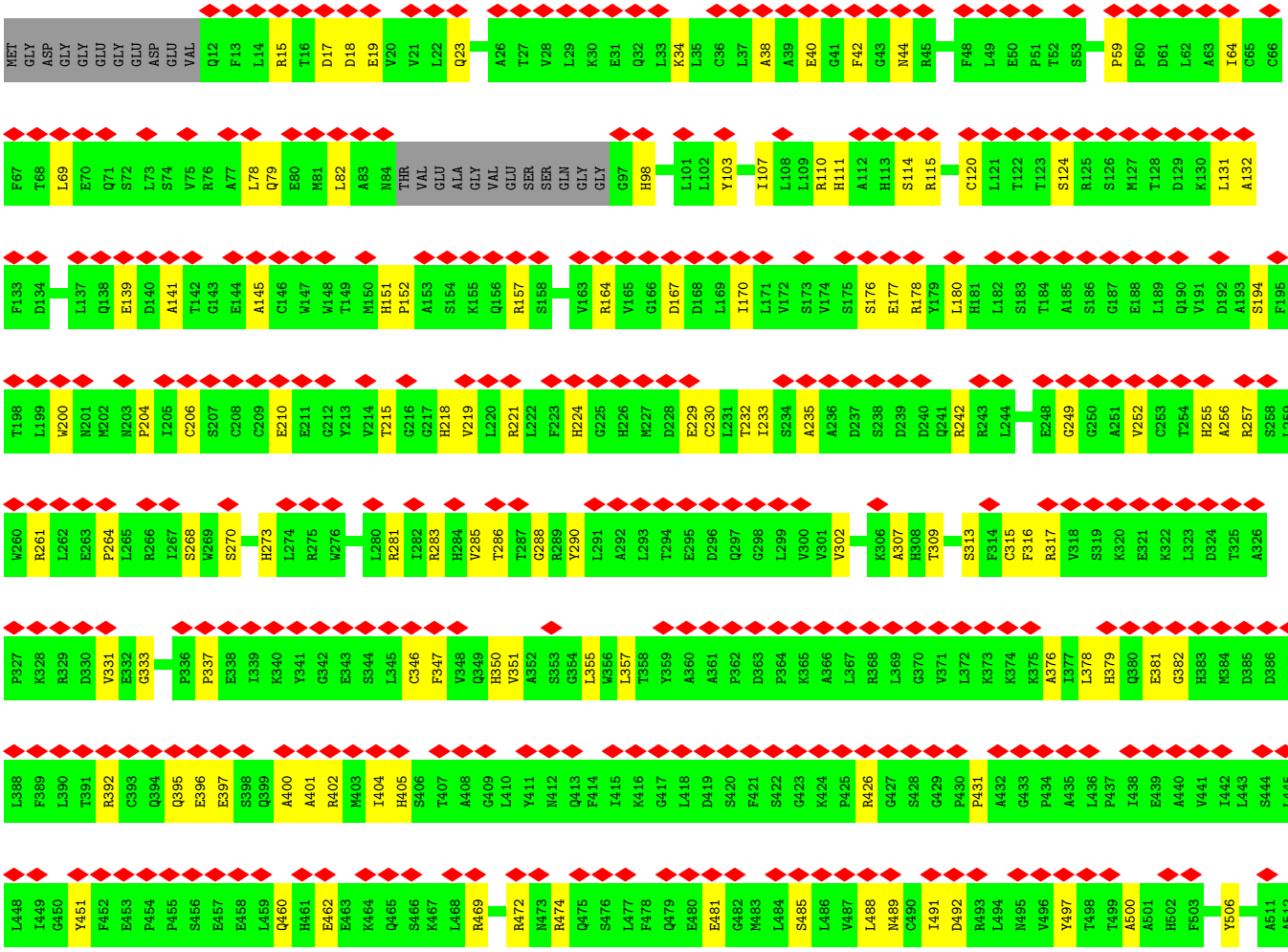
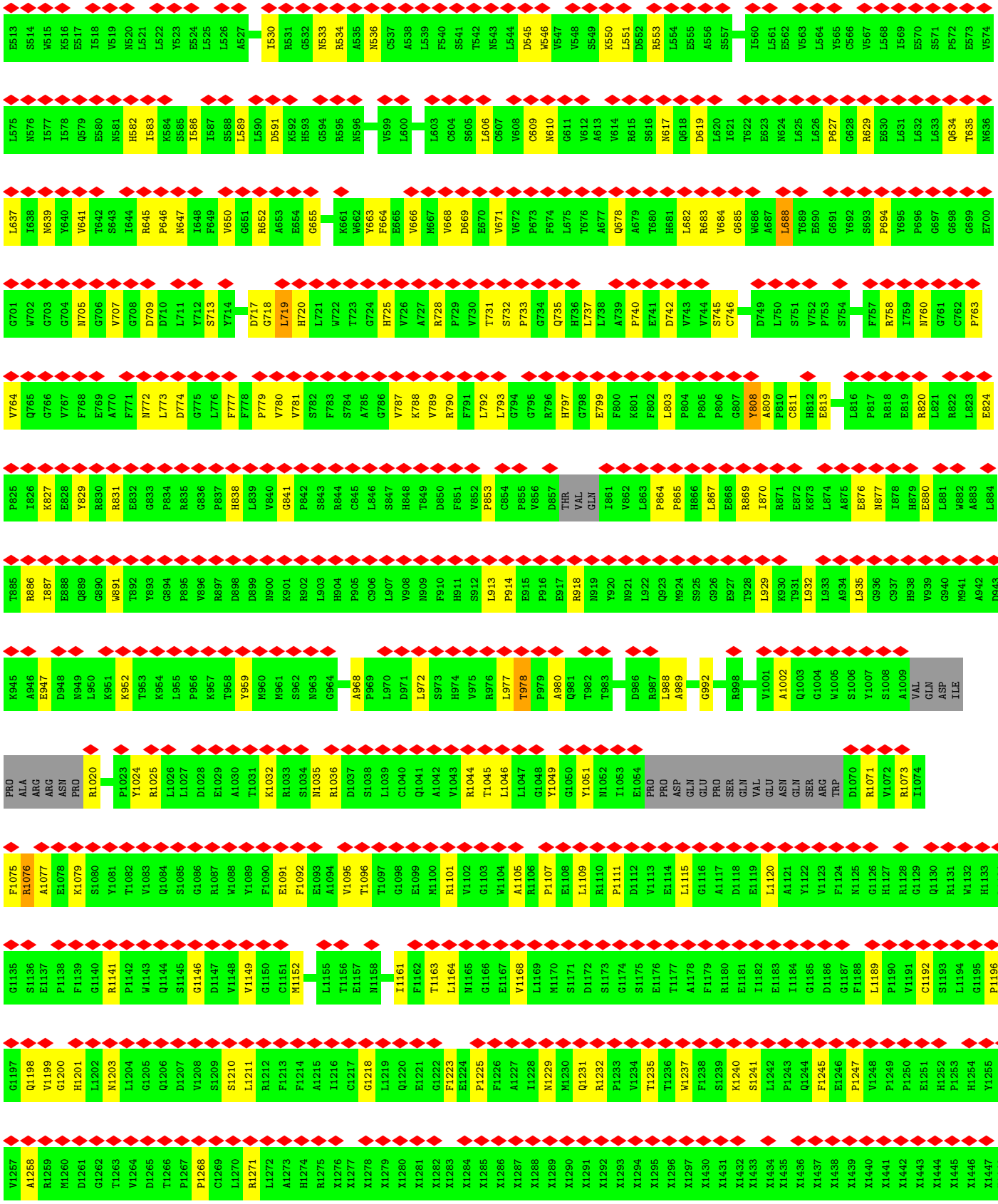


• Molecule 2: ryanodine receptor 1

Chain G:

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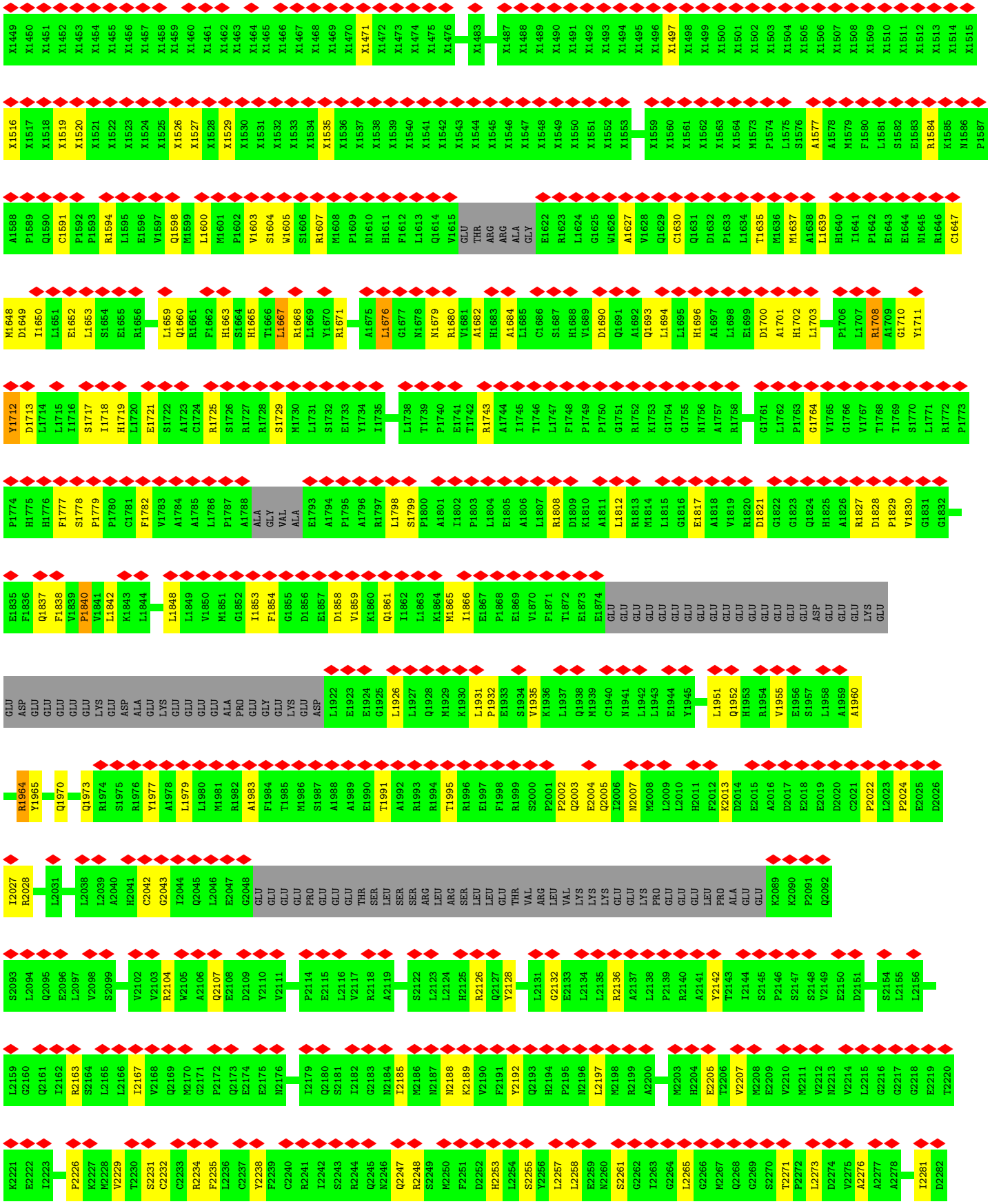

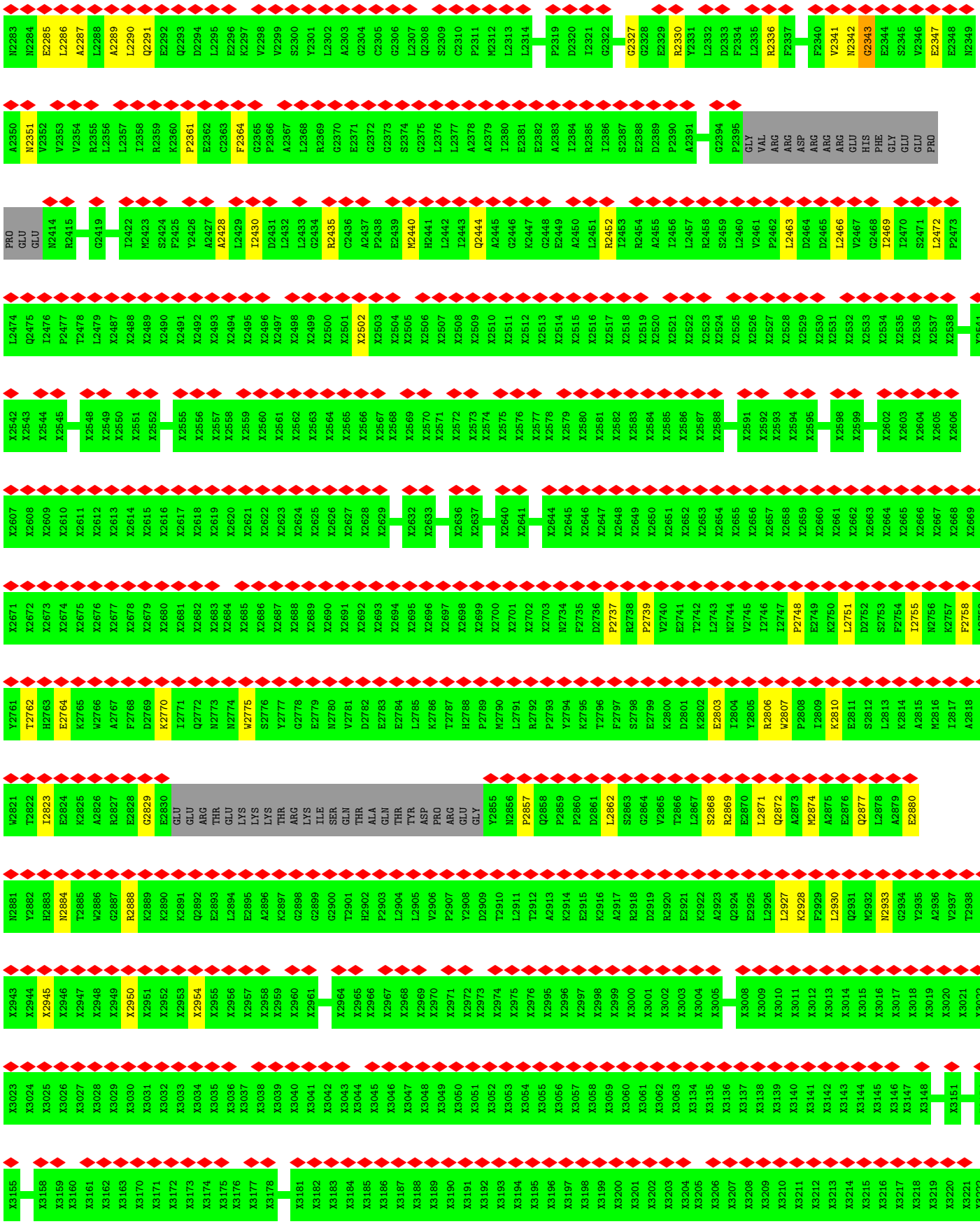
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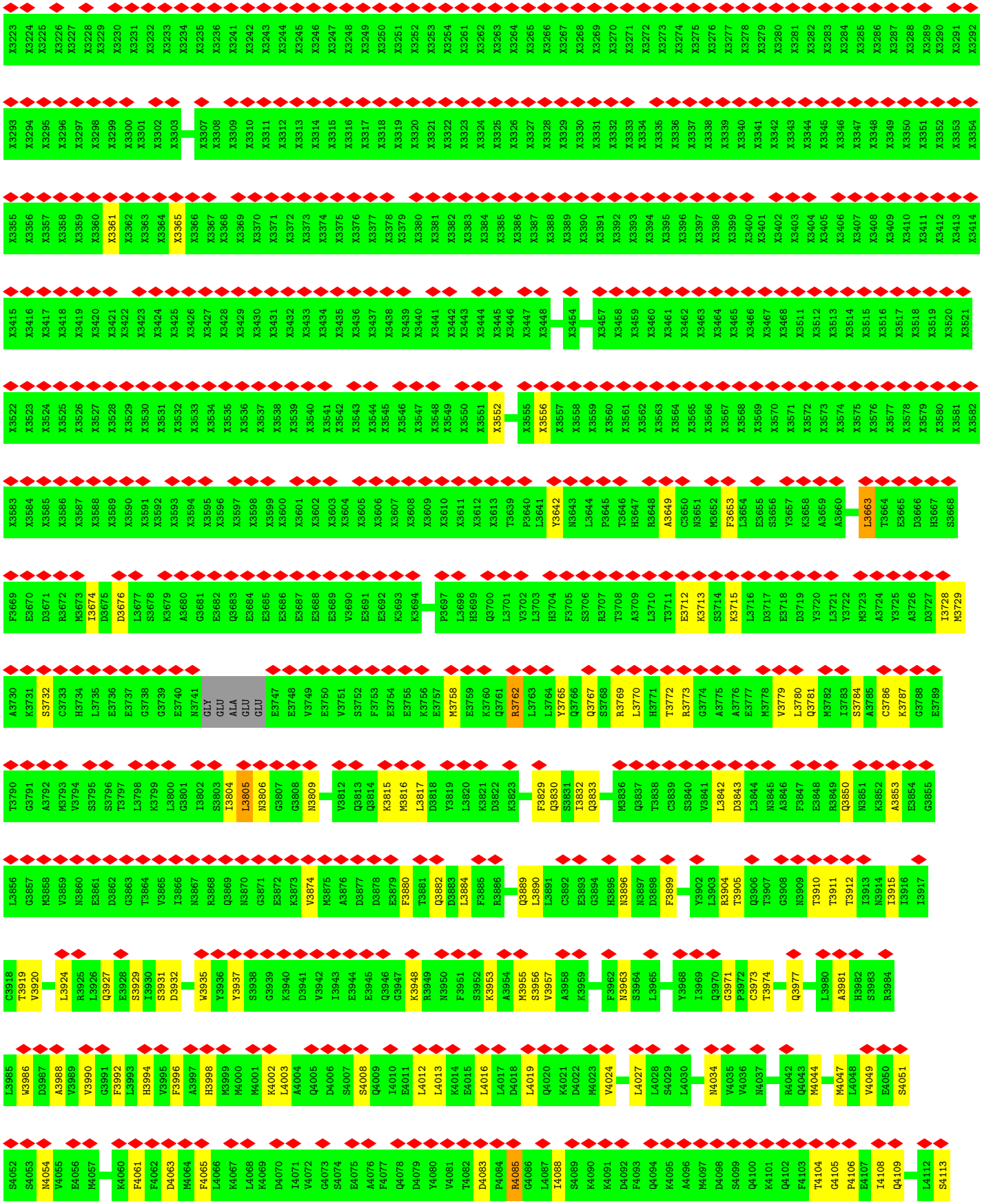
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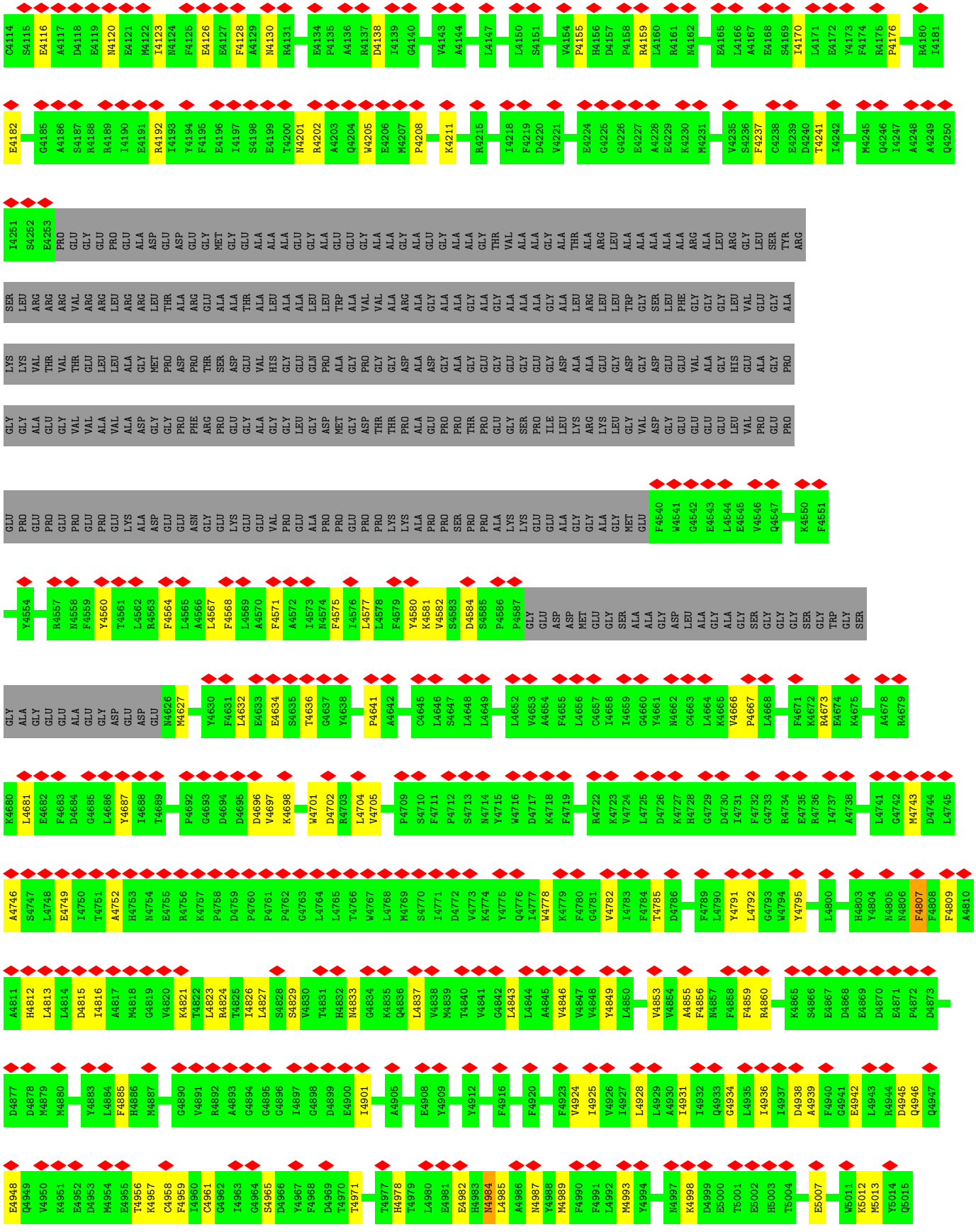
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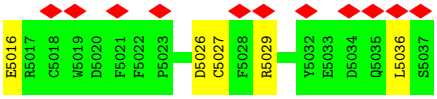
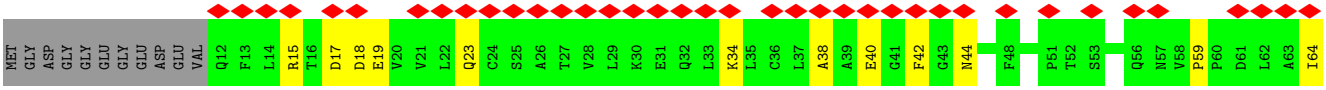
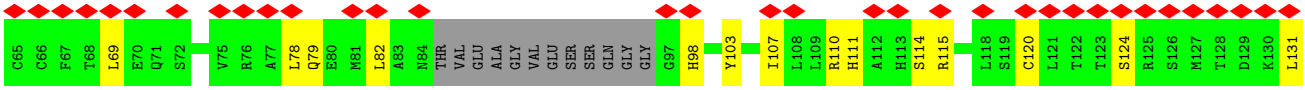
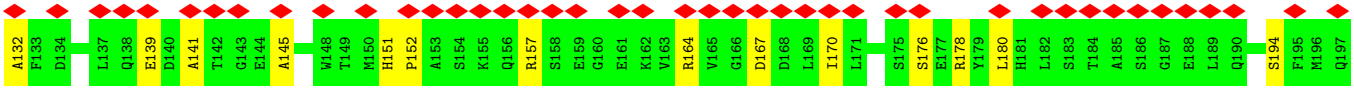
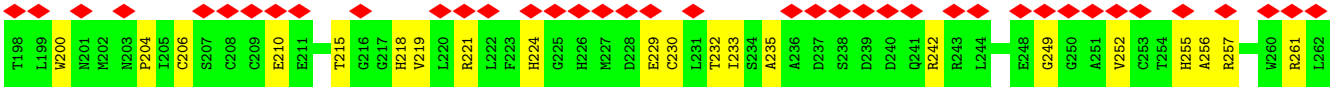


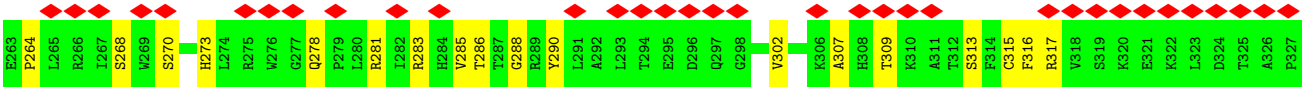
• Molecule 2: ryanodine receptor 1

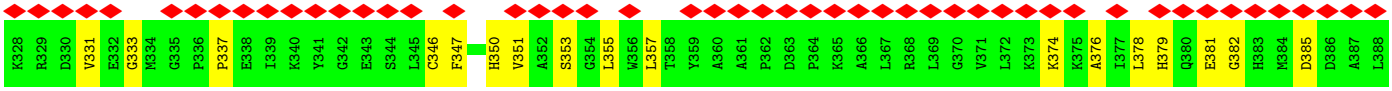


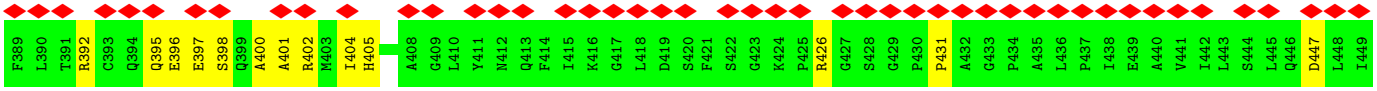


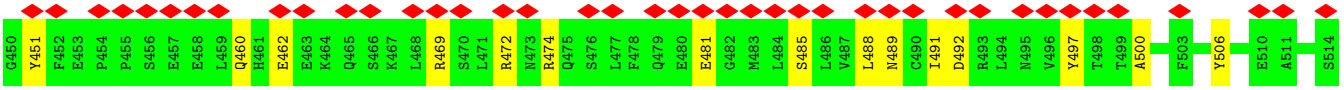


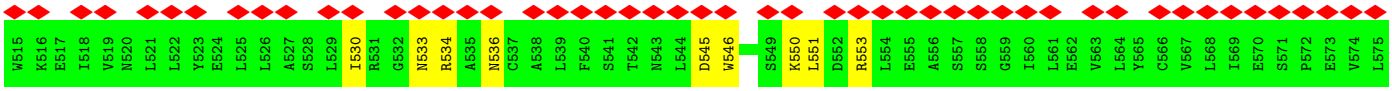


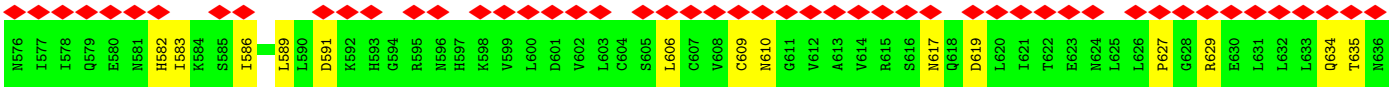


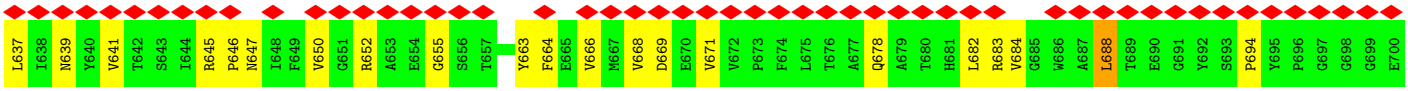


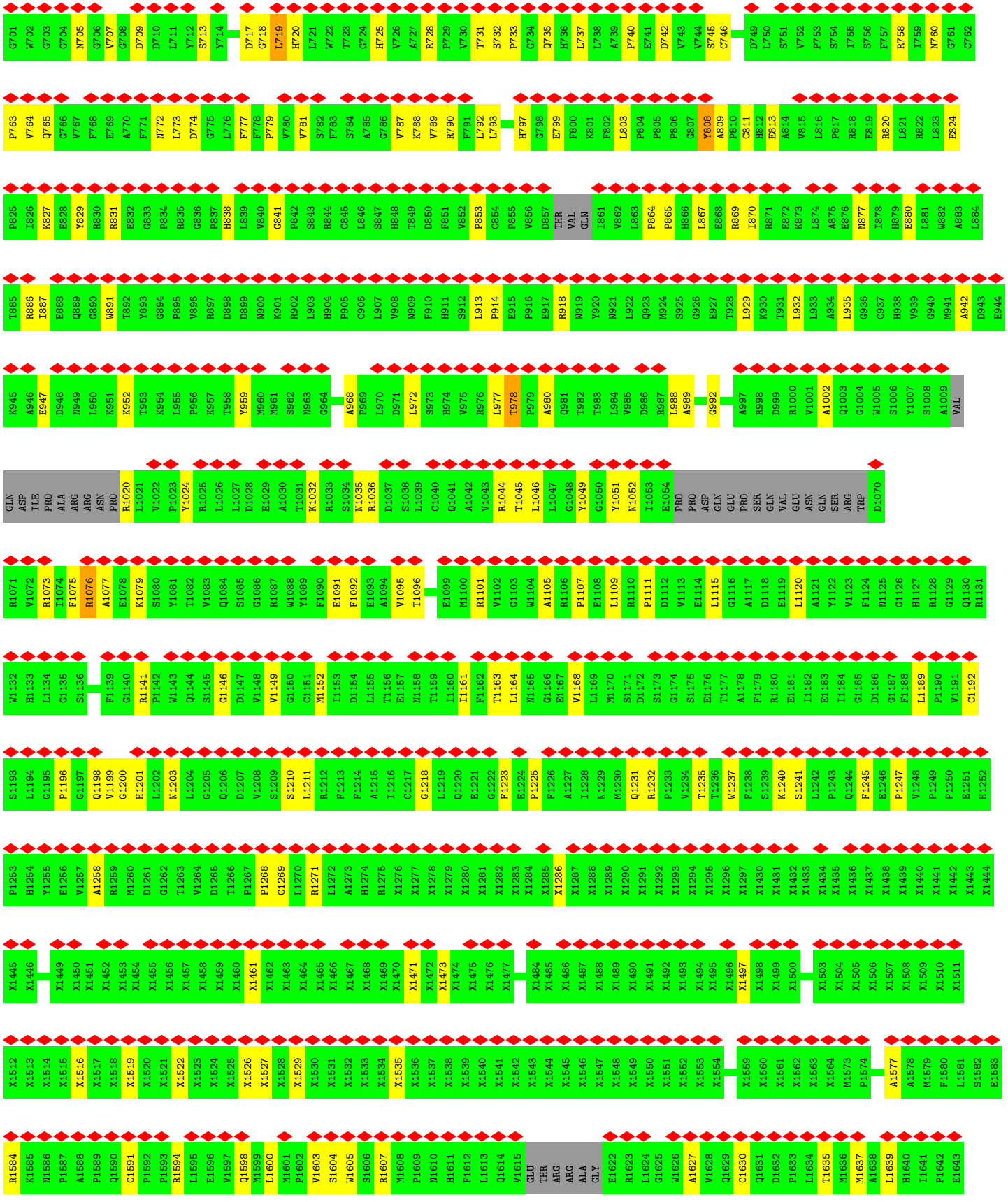








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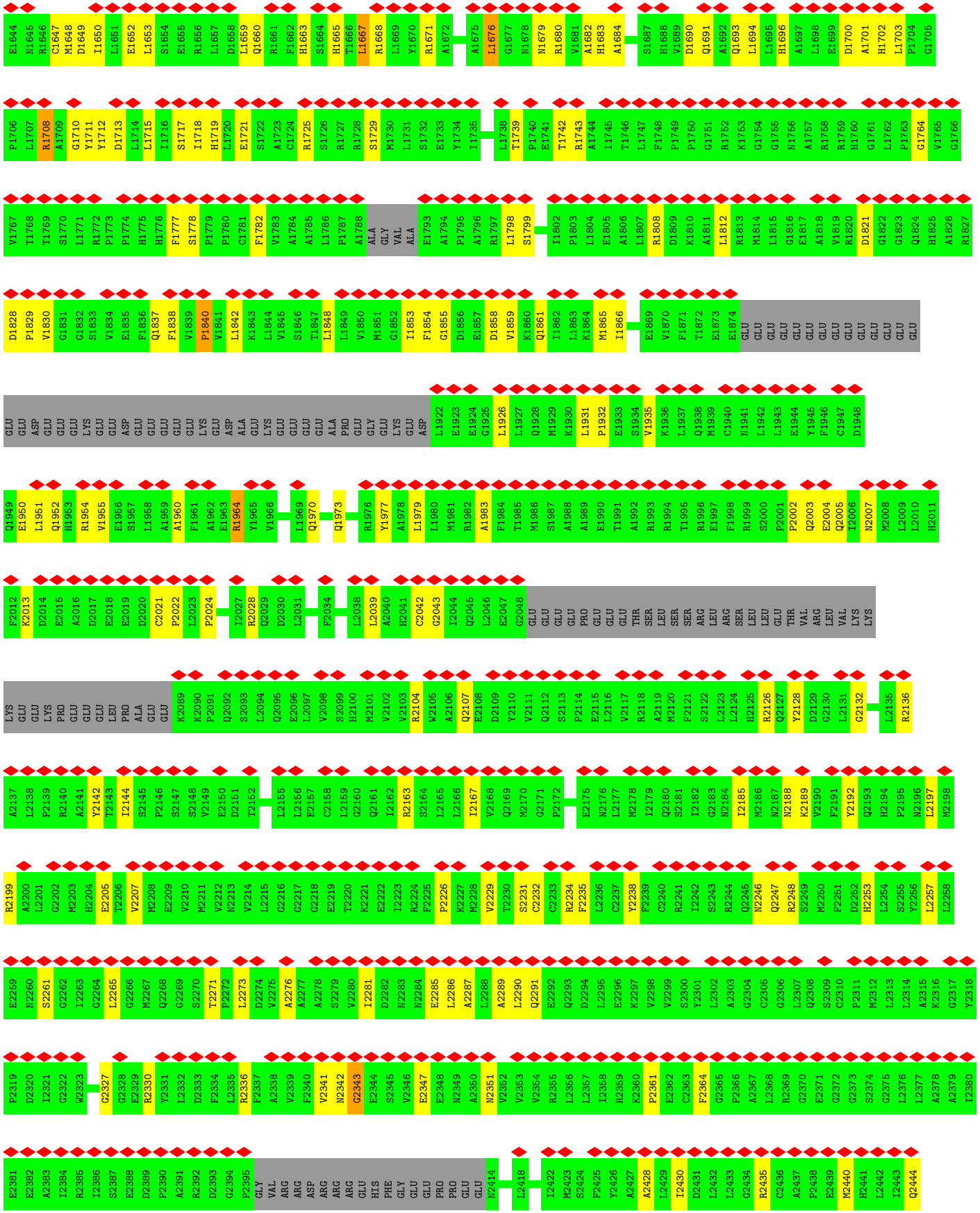
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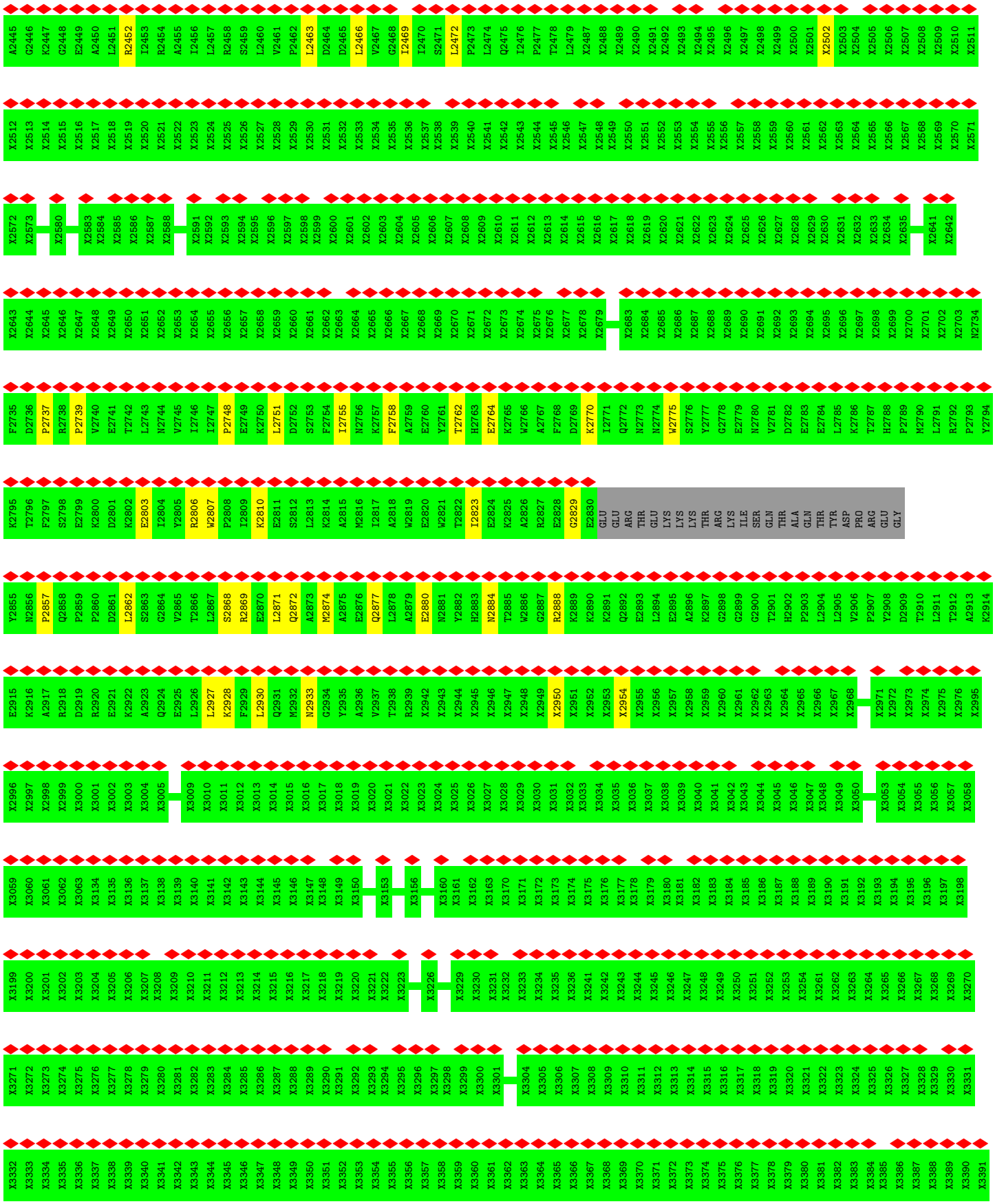
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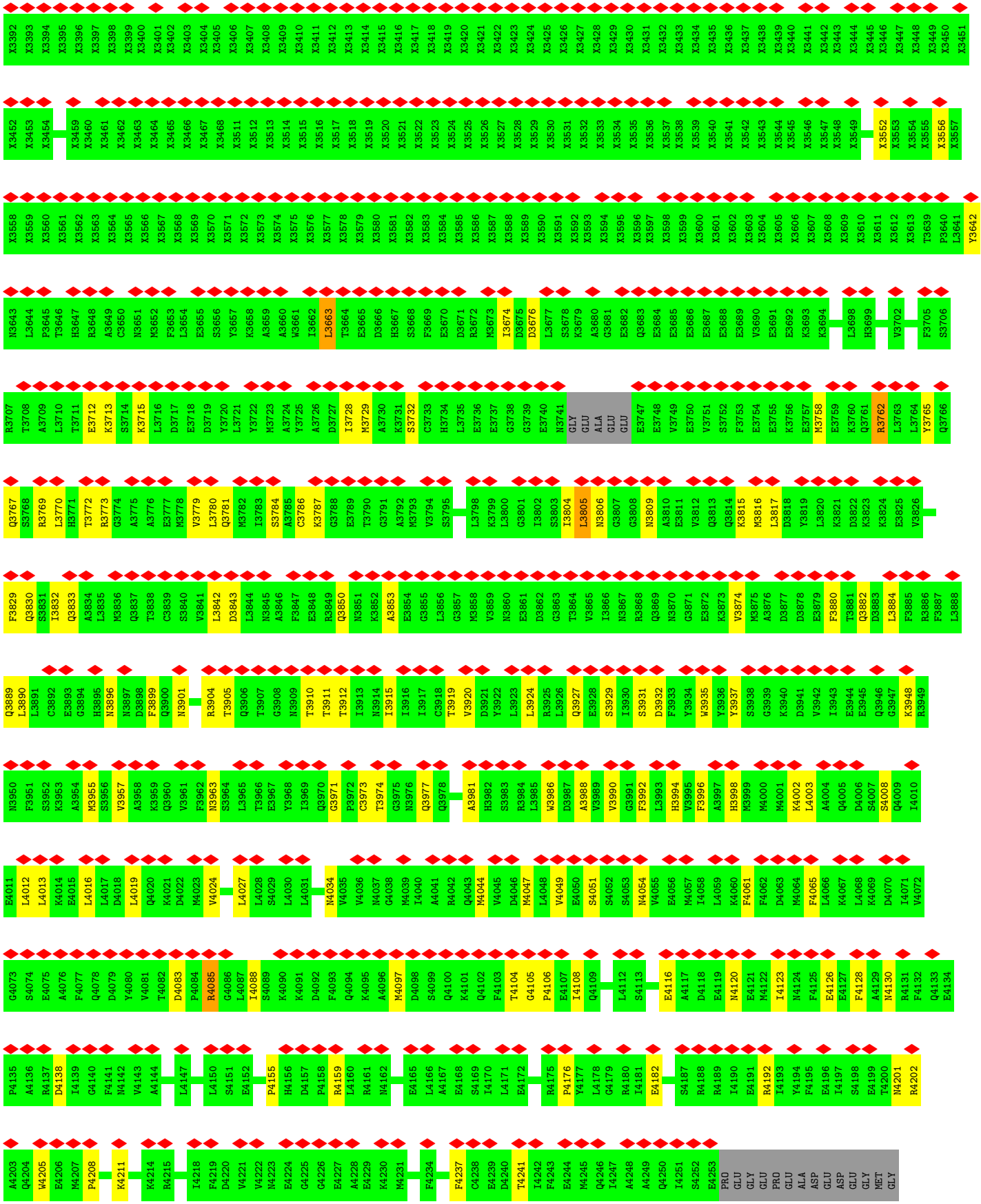
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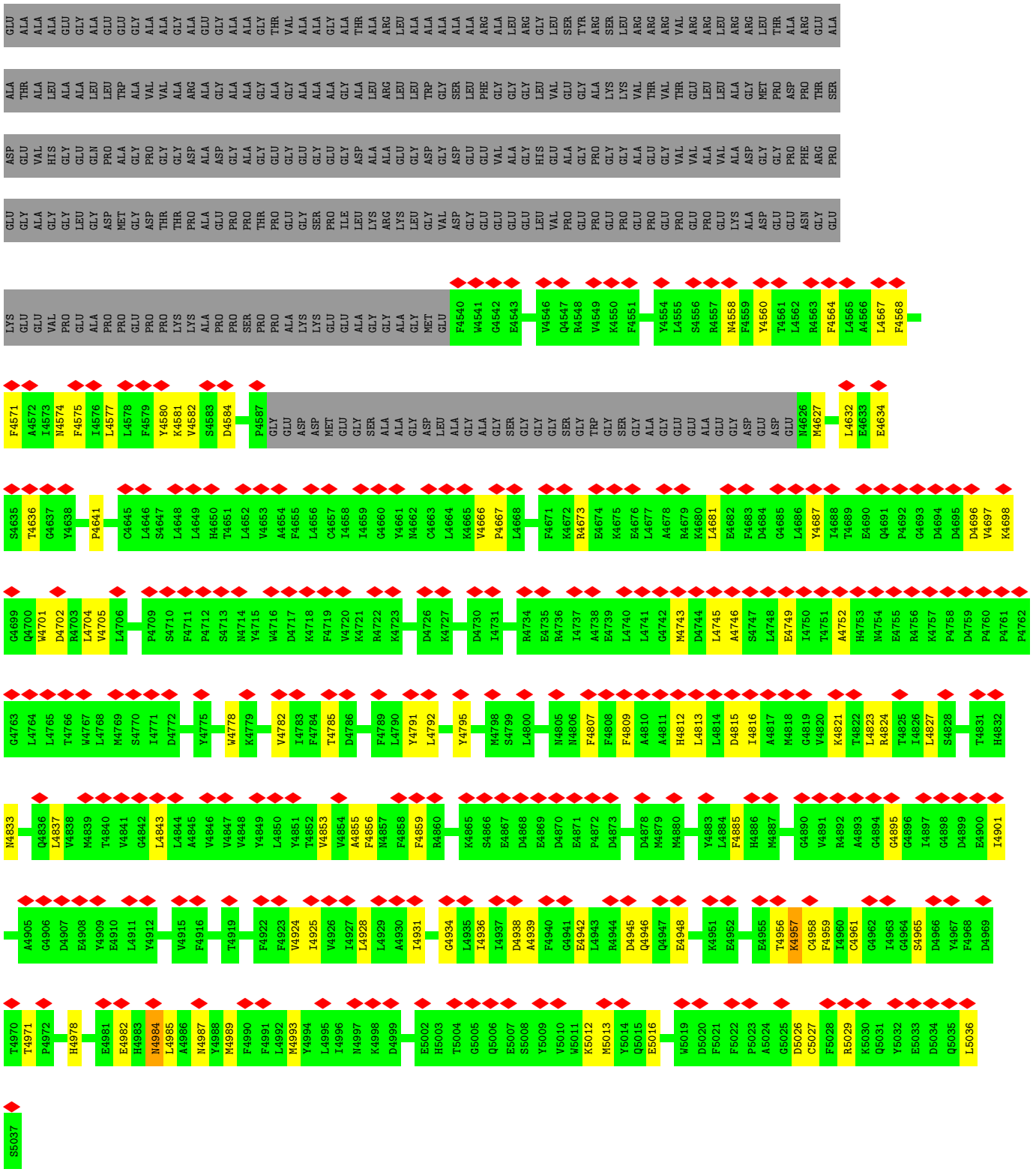

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	791956	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.404	Depositor
Minimum map value	-0.232	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

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	0.32	0/834	0.58	0/1123
1	F	0.32	0/834	0.57	0/1123
1	H	0.32	0/834	0.58	0/1123
1	J	0.32	0/834	0.57	0/1123
2	B	0.32	0/25428	0.57	5/34534 (0.0%)
2	E	0.33	0/25428	0.57	5/34534 (0.0%)
2	G	0.33	0/25428	0.57	5/34534 (0.0%)
2	I	0.33	0/25428	0.57	5/34534 (0.0%)
All	All	0.33	0/105048	0.57	20/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	17
2	E	0	18
2	G	0	17
2	I	0	17
All	All	0	69

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	719	LEU	CA-CB-CG	6.48	130.21	115.30
2	E	719	LEU	CA-CB-CG	6.45	130.14	115.30
2	G	719	LEU	CA-CB-CG	6.45	130.13	115.30
2	B	719	LEU	CA-CB-CG	6.44	130.11	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	977	LEU	CA-CB-CG	6.06	129.24	115.30
2	I	977	LEU	CA-CB-CG	6.06	129.24	115.30
2	G	977	LEU	CA-CB-CG	6.04	129.19	115.30
2	E	977	LEU	CA-CB-CG	6.03	129.17	115.30
2	B	1667	LEU	CA-CB-CG	5.27	127.41	115.30
2	I	1667	LEU	CA-CB-CG	5.26	127.40	115.30
2	G	1667	LEU	CA-CB-CG	5.25	127.37	115.30
2	E	1667	LEU	CA-CB-CG	5.24	127.36	115.30
2	B	4985	LEU	CA-CB-CG	5.13	127.10	115.30
2	E	4985	LEU	CA-CB-CG	5.12	127.07	115.30
2	I	4985	LEU	CA-CB-CG	5.10	127.04	115.30
2	G	4985	LEU	CA-CB-CG	5.10	127.02	115.30
2	I	2463	LEU	CA-CB-CG	5.09	127.01	115.30
2	E	2463	LEU	CA-CB-CG	5.07	126.97	115.30
2	G	2463	LEU	CA-CB-CG	5.06	126.93	115.30
2	B	2463	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

All (69) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1712	TYR	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2342	ASN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3786	CYS	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	4696	ASP	Peptide
2	B	4807	PHE	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1712	TYR	Peptide
2	E	1828	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	E	1840	PRO	Peptide
2	E	194	SER	Peptide
2	E	2291	GLN	Peptide
2	E	2342	ASN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3786	CYS	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	4696	ASP	Peptide
2	E	4807	PHE	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1712	TYR	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2342	ASN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3786	CYS	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	4696	ASP	Peptide
2	G	4807	PHE	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide
2	I	1712	TYR	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	2291	GLN	Peptide
2	I	2342	ASN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3786	CYS	Peptide

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Mol	Chain	Res	Type	Group
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	4696	ASP	Peptide
2	I	4807	PHE	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	19	0
1	F	818	0	824	19	0
1	H	818	0	824	19	0
1	J	818	0	824	21	0
2	B	29369	0	24710	415	0
2	E	29369	0	24708	425	0
2	G	29369	0	24708	429	0
2	I	29369	0	24711	430	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	120756	0	102133	1756	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 8.

All (1756) 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)
2:G:4860:ARG:HD2	2:I:4582:VAL:HG11	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:177:GLU:HG3	2:I:2452:ARG:HH12	1.54	0.70
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.72	0.70
2:G:111:HIS:HD2	2:G:114:SER:H	1.38	0.70
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.72	0.70
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.72	0.70
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.57	0.70
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.57	0.70
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.72	0.70
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.57	0.70
2:B:111:HIS:HD2	2:B:114:SER:H	1.38	0.69
2:E:111:HIS:HD2	2:E:114:SER:H	1.38	0.69
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.57	0.69
2:I:111:HIS:HD2	2:I:114:SER:H	1.38	0.69
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.27	0.68
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.27	0.68
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.27	0.68
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.75	0.68
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.75	0.68
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.27	0.67
2:E:4855:ALA:HA	2:E:4859:PHE:HB2	1.76	0.67
2:I:4855:ALA:HA	2:I:4859:PHE:HB2	1.76	0.67
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.75	0.67
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.60	0.67
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.75	0.67
2:G:4855:ALA:HA	2:G:4859:PHE:HB2	1.76	0.67
2:B:4855:ALA:HA	2:B:4859:PHE:HB2	1.76	0.66
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.60	0.66
2:I:224:HIS:H	2:I:230:CYS:HA	1.61	0.66
2:G:224:HIS:H	2:G:230:CYS:HA	1.61	0.66
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.78	0.65
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.60	0.65
2:E:224:HIS:H	2:E:230:CYS:HA	1.61	0.65
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.78	0.65
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.78	0.65
2:B:224:HIS:H	2:B:230:CYS:HA	1.61	0.65
2:E:2764:GLU:HG3	2:E:2857:PRO:HB2	1.79	0.65
2:B:2764:GLU:HG3	2:B:2857:PRO:HB2	1.79	0.64
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.78	0.64
2:G:2764:GLU:HG3	2:G:2857:PRO:HB2	1.79	0.64
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.79	0.64
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.30	0.64
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.60	0.64
2:B:3767:GLN:HB3	2:B:3772:THR:HG22	1.80	0.64
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.30	0.64
2:G:1247:PRO:HA	2:G:1598:GLN:HA	1.80	0.64
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.80	0.64
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.78	0.64
2:I:4821:LYS:HA	2:I:4824:ARG:HE	1.64	0.64
2:B:4821:LYS:HA	2:B:4824:ARG:HE	1.63	0.63
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.78	0.63
2:I:2764:GLU:HG3	2:I:2857:PRO:HB2	1.79	0.63
2:I:3767:GLN:HB3	2:I:3772:THR:HG22	1.80	0.63
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.81	0.63
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.32	0.63
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.32	0.63
2:I:1247:PRO:HA	2:I:1598:GLN:HA	1.80	0.63
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.32	0.63
2:B:742:ASP:HA	2:B:760:ASN:HD21	1.63	0.63
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.32	0.63
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.80	0.63
2:E:742:ASP:HA	2:E:760:ASN:HD21	1.63	0.63
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.30	0.63
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.80	0.63
2:G:4821:LYS:HA	2:G:4824:ARG:HE	1.63	0.63
2:G:3767:GLN:HB3	2:G:3772:THR:HG22	1.80	0.63
2:B:606:LEU:O	2:B:617:ASN:ND2	2.32	0.63
2:E:4821:LYS:HA	2:E:4824:ARG:HE	1.63	0.63
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.30	0.63
2:E:3767:GLN:HB3	2:E:3772:THR:HG22	1.80	0.62
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.80	0.62
2:G:742:ASP:HA	2:G:760:ASN:HD21	1.63	0.62
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.82	0.62
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.81	0.62
2:I:742:ASP:HA	2:I:760:ASN:HD21	1.64	0.62
2:E:1247:PRO:HA	2:E:1598:GLN:HA	1.80	0.62
2:G:606:LEU:O	2:G:617:ASN:ND2	2.32	0.62
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.82	0.62
2:B:1830:VAL:HB	2:B:1837:GLN:HA	1.82	0.62
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.33	0.62
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.33	0.62
2:E:606:LEU:O	2:E:617:ASN:ND2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.81	0.62
2:I:606:LEU:O	2:I:617:ASN:ND2	2.32	0.62
2:B:1247:PRO:HA	2:B:1598:GLN:HA	1.81	0.61
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.33	0.61
2:G:853:PRO:HB3	2:G:1024:TYR:H	1.65	0.61
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.82	0.61
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.33	0.61
2:E:1830:VAL:HB	2:E:1837:GLN:HA	1.82	0.61
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.82	0.61
2:I:853:PRO:HB3	2:I:1024:TYR:H	1.66	0.61
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.33	0.61
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.33	0.61
2:I:728:ARG:NH2	2:I:1527:UNK:O	2.33	0.61
2:I:1830:VAL:HB	2:I:1837:GLN:HA	1.82	0.61
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.82	0.61
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.33	0.61
2:G:1830:VAL:HB	2:G:1837:GLN:HA	1.81	0.61
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.81	0.61
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.33	0.61
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.81	0.61
2:E:4978:HIS:HA	2:E:4982:GLU:HB2	1.83	0.60
2:I:1091:GLU:HB3	2:I:1203:ASN:HB3	1.83	0.60
2:I:4978:HIS:HA	2:I:4982:GLU:HB2	1.83	0.60
2:B:4978:HIS:HA	2:B:4982:GLU:HB2	1.83	0.60
2:E:395:GLN:HG3	2:E:397:GLU:H	1.67	0.60
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.83	0.60
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.83	0.60
2:G:1101:ARG:HE	2:G:1115:LEU:HB3	1.67	0.60
2:B:853:PRO:HB3	2:B:1024:TYR:H	1.66	0.60
2:I:1101:ARG:HE	2:I:1115:LEU:HB3	1.67	0.60
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.84	0.60
2:E:853:PRO:HB3	2:E:1024:TYR:H	1.66	0.60
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.83	0.60
2:G:221:ARG:NH2	2:G:255:HIS:O	2.34	0.60
2:E:4083:ASP:HA	2:E:4085:ARG:HH11	1.66	0.60
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.83	0.60
2:G:4978:HIS:HA	2:G:4982:GLU:HB2	1.83	0.60
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.84	0.60
2:E:4809:PHE:HA	2:E:4812:HIS:HD1	1.67	0.60
1:J:27:THR:HB	1:J:100:ASP:HB3	1.84	0.60
2:B:395:GLN:HG3	2:B:397:GLU:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4809:PHE:HA	2:B:4812:HIS:HD1	1.67	0.59
2:E:1241:SER:HA	2:E:1603:VAL:HA	1.84	0.59
2:G:1241:SER:HA	2:G:1603:VAL:HA	1.84	0.59
2:I:1241:SER:HA	2:I:1603:VAL:HA	1.84	0.59
2:B:1241:SER:HA	2:B:1603:VAL:HA	1.84	0.59
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.84	0.59
2:E:1091:GLU:HB3	2:E:1203:ASN:HB3	1.83	0.59
1:F:27:THR:HB	1:F:100:ASP:HB3	1.84	0.59
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.84	0.59
1:H:27:THR:HB	1:H:100:ASP:HB3	1.84	0.59
2:I:395:GLN:HG3	2:I:397:GLU:H	1.67	0.59
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.34	0.59
2:G:1973:GLN:O	2:G:1977:TYR:N	2.36	0.59
2:G:2281:ILE:HG23	2:G:2341:VAL:HG11	1.85	0.59
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.34	0.59
2:B:1091:GLU:HB3	2:B:1203:ASN:HB3	1.83	0.59
2:B:221:ARG:NH2	2:B:255:HIS:O	2.34	0.59
2:B:1218:GLY:HA2	2:B:1223:PHE:HB2	1.84	0.59
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.84	0.59
2:G:395:GLN:HG3	2:G:397:GLU:H	1.67	0.59
1:A:6:THR:HA	1:A:72:ALA:HA	1.85	0.59
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.84	0.59
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.34	0.59
2:G:4809:PHE:HA	2:G:4812:HIS:HD1	1.67	0.59
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.83	0.59
2:B:4083:ASP:HA	2:B:4085:ARG:HH11	1.66	0.59
2:E:18:ASP:HB2	2:E:69:LEU:HD12	1.84	0.59
2:E:1973:GLN:O	2:E:1977:TYR:N	2.36	0.59
2:G:242:ARG:NH1	2:G:481:GLU:OE1	2.36	0.59
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.84	0.59
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.84	0.59
1:A:27:THR:HB	1:A:100:ASP:HB3	1.84	0.59
2:G:1091:GLU:HB3	2:G:1203:ASN:HB3	1.83	0.59
2:G:1096:THR:HG23	2:G:1199:VAL:HG22	1.84	0.59
2:I:2281:ILE:HG23	2:I:2341:VAL:HG11	1.84	0.59
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.34	0.59
2:E:242:ARG:NH1	2:E:481:GLU:OE1	2.36	0.59
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.36	0.59
2:I:1973:GLN:O	2:I:1977:TYR:N	2.36	0.59
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.84	0.59
2:E:1101:ARG:HE	2:E:1115:LEU:HB3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.36	0.59
2:I:4083:ASP:HA	2:I:4085:ARG:HH11	1.67	0.59
2:I:4809:PHE:HA	2:I:4812:HIS:HD1	1.67	0.59
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.85	0.58
2:B:1101:ARG:HE	2:B:1115:LEU:HB3	1.66	0.58
2:E:1218:GLY:HA2	2:E:1223:PHE:HB2	1.84	0.58
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.68	0.58
2:G:4061:PHE:HA	2:G:4065:PHE:HB3	1.85	0.58
2:I:242:ARG:NH1	2:I:481:GLU:OE1	2.36	0.58
2:B:18:ASP:HB2	2:B:69:LEU:HD12	1.85	0.58
2:B:4892:ARG:NH2	2:I:4895:GLY:O	2.33	0.58
2:E:2281:ILE:HG23	2:E:2341:VAL:HG11	1.85	0.58
2:E:4061:PHE:HA	2:E:4065:PHE:HB3	1.85	0.58
2:G:18:ASP:HB2	2:G:69:LEU:HD12	1.84	0.58
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.84	0.58
2:G:1218:GLY:HA2	2:G:1223:PHE:HB2	1.84	0.58
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.84	0.58
2:E:591:ASP:O	2:E:1594:ARG:NH2	2.36	0.58
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.86	0.58
2:G:4083:ASP:HA	2:G:4085:ARG:HH11	1.66	0.58
2:B:650:VAL:HB	2:B:777:PHE:HB2	1.86	0.58
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.86	0.58
2:G:591:ASP:O	2:G:1594:ARG:NH2	2.36	0.58
2:I:18:ASP:HB2	2:I:69:LEU:HD12	1.84	0.58
2:B:242:ARG:NH1	2:B:481:GLU:OE1	2.36	0.58
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.84	0.58
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.37	0.58
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.36	0.58
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.85	0.58
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.36	0.58
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.76	0.58
1:F:6:THR:HA	1:F:72:ALA:HA	1.85	0.58
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.37	0.58
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.84	0.58
2:E:650:VAL:HB	2:E:777:PHE:HB2	1.86	0.58
2:E:1096:THR:HG23	2:E:1199:VAL:HG22	1.84	0.58
2:G:1271:ARG:HA	2:G:1471:UNK:HA	1.85	0.58
2:I:379:HIS:HD2	2:I:382:GLY:H	1.52	0.58
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.86	0.58
2:I:1096:THR:HG23	2:I:1199:VAL:HG22	1.84	0.58
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:591:ASP:O	2:B:1594:ARG:NH2	2.36	0.58
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.86	0.58
2:B:2281:ILE:HG23	2:B:2341:VAL:HG11	1.84	0.58
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.37	0.58
2:B:1096:THR:HG23	2:B:1199:VAL:HG22	1.84	0.58
2:B:1973:GLN:O	2:B:1977:TYR:N	2.36	0.58
2:E:221:ARG:NH2	2:E:255:HIS:O	2.34	0.58
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.76	0.58
2:I:650:VAL:HB	2:I:777:PHE:HB2	1.86	0.58
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.69	0.58
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.36	0.58
2:B:2440:MET:O	2:B:2444:GLN:N	2.37	0.58
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.68	0.58
2:E:827:LYS:O	2:E:1073:ARG:NH2	2.37	0.58
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.36	0.58
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.68	0.58
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.84	0.57
2:B:827:LYS:O	2:B:1073:ARG:NH2	2.37	0.57
2:E:177:GLU:HG3	2:G:2452:ARG:HH12	1.69	0.57
2:I:1218:GLY:HA2	2:I:1223:PHE:HB2	1.84	0.57
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.69	0.57
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.70	0.57
2:G:650:VAL:HB	2:G:777:PHE:HB2	1.86	0.57
2:I:827:LYS:O	2:I:1073:ARG:NH2	2.37	0.57
2:B:379:HIS:HD2	2:B:382:GLY:H	1.51	0.57
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.84	0.57
2:I:609:CYS:SG	2:I:610:ASN:N	2.78	0.57
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.84	0.57
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.86	0.57
2:B:4061:PHE:HA	2:B:4065:PHE:HB3	1.85	0.57
2:E:1271:ARG:HA	2:E:1471:UNK:HA	1.85	0.57
2:I:1232:ARG:HH21	2:I:1701:ALA:HB1	1.70	0.57
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.76	0.57
2:I:4061:PHE:HA	2:I:4065:PHE:HB3	1.85	0.57
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.69	0.57
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.86	0.57
2:G:2440:MET:O	2:G:2444:GLN:N	2.37	0.57
2:I:591:ASP:O	2:I:1594:ARG:NH2	2.36	0.57
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.85	0.57
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.87	0.57
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:639:ASN:H	2:G:678:GLN:HE22	1.53	0.57
2:G:2205:GLU:HG2	2:G:2253:HIS:HE1	1.70	0.57
1:H:6:THR:HA	1:H:72:ALA:HA	1.85	0.57
2:I:2205:GLU:HG2	2:I:2253:HIS:HE1	1.70	0.57
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.87	0.57
1:J:6:THR:HA	1:J:72:ALA:HA	1.85	0.57
2:E:2440:MET:O	2:E:2444:GLN:N	2.37	0.57
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.70	0.57
2:G:827:LYS:O	2:G:1073:ARG:NH2	2.37	0.57
2:G:3904:ARG:NH2	2:G:3973:CYS:SG	2.78	0.57
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.86	0.57
2:I:3904:ARG:NH2	2:I:3973:CYS:SG	2.78	0.57
2:E:609:CYS:SG	2:E:610:ASN:N	2.78	0.57
2:E:639:ASN:H	2:E:678:GLN:HE22	1.53	0.57
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.86	0.57
2:G:379:HIS:HD2	2:G:382:GLY:H	1.51	0.57
2:G:1232:ARG:HH21	2:G:1701:ALA:HB1	1.69	0.57
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.69	0.57
2:B:609:CYS:SG	2:B:610:ASN:N	2.78	0.57
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.70	0.57
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.68	0.56
2:B:451:TYR:O	2:B:474:ARG:NH1	2.38	0.56
2:B:813:GLU:OE2	2:B:1020:ARG:N	2.38	0.56
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.87	0.56
2:G:4584:ASP:HA	2:G:4627:MET:HA	1.87	0.56
2:I:221:ARG:NH2	2:I:255:HIS:O	2.34	0.56
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.70	0.56
2:B:256:ALA:HB1	2:B:286:THR:HG21	1.87	0.56
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	1.88	0.56
2:E:4584:ASP:HA	2:E:4627:MET:HA	1.87	0.56
2:G:609:CYS:SG	2:G:610:ASN:N	2.78	0.56
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.85	0.56
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.86	0.56
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.37	0.56
2:B:1232:ARG:HH21	2:B:1701:ALA:HB1	1.70	0.56
2:E:813:GLU:OE2	2:E:1020:ARG:N	2.38	0.56
2:G:813:GLU:OE2	2:G:1020:ARG:N	2.38	0.56
2:I:256:ALA:HB1	2:I:286:THR:HG21	1.87	0.56
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.37	0.56
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.85	0.56
2:I:4581:LYS:HB2	2:I:4632:LEU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:639:ASN:H	2:B:678:GLN:HE22	1.53	0.56
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.87	0.56
2:E:3904:ARG:NH2	2:E:3973:CYS:SG	2.78	0.56
2:E:4581:LYS:HB2	2:E:4632:LEU:HB2	1.87	0.56
2:G:256:ALA:HB1	2:G:286:THR:HG21	1.87	0.56
2:I:2440:MET:O	2:I:2444:GLN:N	2.37	0.56
2:B:3904:ARG:NH2	2:B:3973:CYS:SG	2.78	0.56
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	1.88	0.56
2:B:2205:GLU:HG2	2:B:2253:HIS:HE1	1.70	0.56
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.86	0.56
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.69	0.56
2:E:256:ALA:HB1	2:E:286:THR:HG21	1.87	0.56
2:E:2205:GLU:HG2	2:E:2253:HIS:HE1	1.70	0.56
2:E:4843:LEU:HD12	2:G:4823:LEU:HD21	1.86	0.56
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.39	0.56
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.69	0.56
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.39	0.56
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.39	0.56
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.88	0.56
2:E:157:ARG:NH2	2:E:167:ASP:OD1	2.38	0.56
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.88	0.56
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.69	0.56
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.38	0.56
2:G:4581:LYS:HB2	2:G:4632:LEU:HB2	1.87	0.56
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	1.88	0.56
2:I:813:GLU:OE2	2:I:1020:ARG:N	2.38	0.56
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.38	0.56
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.88	0.56
2:B:4918:ILE:HG23	2:E:4892:ARG:HD3	1.88	0.56
2:E:379:HIS:HD2	2:E:382:GLY:H	1.52	0.56
2:I:639:ASN:H	2:I:678:GLN:HE22	1.53	0.56
2:I:1271:ARG:HA	2:I:1471:UNK:HA	1.87	0.56
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.86	0.56
2:B:157:ARG:NH2	2:B:167:ASP:OD1	2.38	0.56
2:B:1211:LEU:HD11	2:B:1225:PRO:HB3	1.88	0.56
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.70	0.56
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.39	0.56
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.38	0.56
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.88	0.56
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	1.88	0.56
2:E:1232:ARG:HH21	2:E:1701:ALA:HB1	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.39	0.56
2:E:4984:ASN:OD1	2:E:4987:ASN:ND2	2.39	0.55
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.88	0.55
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.39	0.55
2:I:1808:ARG:NH1	2:I:1853:ILE:O	2.39	0.55
2:B:1838:PHE:HB3	2:B:1842:LEU:HD11	1.89	0.55
2:G:1838:PHE:HB3	2:G:1842:LEU:HD11	1.89	0.55
2:I:4584:ASP:HA	2:I:4627:MET:HA	1.87	0.55
2:B:331:VAL:HG12	2:B:333:GLY:H	1.71	0.55
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.87	0.55
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.88	0.55
2:B:4584:ASP:HA	2:B:4627:MET:HA	1.87	0.55
2:E:1211:LEU:HD11	2:E:1225:PRO:HB3	1.88	0.55
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.88	0.55
2:G:451:TYR:O	2:G:474:ARG:NH1	2.38	0.55
2:I:331:VAL:HG12	2:I:333:GLY:H	1.71	0.55
2:I:451:TYR:O	2:I:474:ARG:NH1	2.38	0.55
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.88	0.55
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.88	0.55
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.88	0.55
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.88	0.55
2:E:1808:ARG:NH1	2:E:1853:ILE:O	2.39	0.55
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.88	0.55
2:B:4984:ASN:OD1	2:B:4987:ASN:ND2	2.40	0.55
2:G:132:ALA:HA	2:G:194:SER:HB2	1.89	0.55
2:I:132:ALA:HA	2:I:194:SER:HB2	1.89	0.55
2:B:283:ARG:HH21	2:B:402:ARG:HH12	1.54	0.55
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.39	0.55
2:E:627:PRO:HB2	1:F:92:PRO:HD3	1.89	0.55
2:E:1838:PHE:HB3	2:E:1842:LEU:HD11	1.89	0.55
2:B:4581:LYS:HB2	2:B:4632:LEU:HB2	1.87	0.55
2:E:451:TYR:O	2:E:474:ARG:NH1	2.38	0.55
2:G:1211:LEU:HD11	2:G:1225:PRO:HB3	1.88	0.55
2:I:864:PRO:HD2	2:I:867:LEU:HD12	1.89	0.55
2:I:1211:LEU:HD11	2:I:1225:PRO:HB3	1.88	0.55
2:I:1838:PHE:HB3	2:I:1842:LEU:HD11	1.89	0.55
2:I:4984:ASN:OD1	2:I:4987:ASN:ND2	2.39	0.55
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.89	0.55
2:B:3767:GLN:NE2	2:B:3804:ILE:O	2.40	0.55
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.76	0.54
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.88	0.54
2:G:23:GLN:HE21	2:G:34:LYS:HB3	1.73	0.54
2:G:3767:GLN:NE2	2:G:3804:ILE:O	2.40	0.54
2:G:4984:ASN:OD1	2:G:4987:ASN:ND2	2.40	0.54
2:I:283:ARG:HH21	2:I:402:ARG:HH12	1.54	0.54
2:I:3767:GLN:NE2	2:I:3804:ILE:O	2.40	0.54
2:B:23:GLN:HE21	2:B:34:LYS:HB3	1.73	0.54
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.89	0.54
2:B:864:PRO:HD2	2:B:867:LEU:HD12	1.89	0.54
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.90	0.54
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.89	0.54
2:E:331:VAL:HG12	2:E:333:GLY:H	1.71	0.54
2:E:647:ASN:ND2	2:E:820:ARG:O	2.39	0.54
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.90	0.54
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.90	0.54
2:I:157:ARG:NH2	2:I:167:ASP:OD1	2.38	0.54
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.88	0.54
2:I:683:ARG:NH1	2:I:707:VAL:O	2.40	0.54
1:A:25:HIS:HB3	1:A:40:ARG:HD3	1.90	0.54
2:E:3767:GLN:NE2	2:E:3804:ILE:O	2.40	0.54
2:G:157:ARG:NH2	2:G:167:ASP:OD1	2.38	0.54
2:G:1667:LEU:O	2:G:1671:ARG:NH1	2.41	0.54
2:B:1667:LEU:O	2:B:1671:ARG:NH1	2.41	0.54
2:E:3843:ASP:H	2:E:3874:VAL:HG13	1.73	0.54
2:G:283:ARG:HH21	2:G:402:ARG:HH12	1.54	0.54
2:B:669:ASP:OD2	2:B:790:ARG:NH2	2.41	0.54
2:B:2248:ARG:NH2	2:B:2285:GLU:OE1	2.41	0.54
2:G:331:VAL:HG12	2:G:333:GLY:H	1.71	0.54
2:B:132:ALA:HA	2:B:194:SER:HB2	1.89	0.54
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.88	0.54
2:E:283:ARG:HH21	2:E:402:ARG:HH12	1.54	0.54
2:I:2248:ARG:NH2	2:I:2285:GLU:OE1	2.41	0.54
1:A:26:TYR:OH	1:A:42:ARG:NH2	2.36	0.54
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.90	0.54
2:E:132:ALA:HA	2:E:194:SER:HB2	1.89	0.54
2:G:864:PRO:HD2	2:G:867:LEU:HD12	1.89	0.54
2:I:669:ASP:OD2	2:I:790:ARG:NH2	2.41	0.54
2:B:396:GLU:O	2:B:400:ALA:N	2.40	0.53
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.88	0.53
2:I:655:GLY:HA2	2:I:1002:ALA:HB2	1.90	0.53
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:25:HIS:HB3	1:J:40:ARG:HD3	1.90	0.53
2:B:1808:ARG:NH1	2:B:1853:ILE:O	2.39	0.53
2:E:1667:LEU:O	2:E:1671:ARG:NH1	2.41	0.53
2:I:1667:LEU:O	2:I:1671:ARG:NH1	2.41	0.53
2:E:655:GLY:HA2	2:E:1002:ALA:HB2	1.90	0.53
2:E:683:ARG:NH1	2:E:707:VAL:O	2.40	0.53
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.89	0.53
1:F:25:HIS:HB3	1:F:40:ARG:HD3	1.90	0.53
2:G:669:ASP:OD2	2:G:790:ARG:NH2	2.41	0.53
2:I:23:GLN:HE21	2:I:34:LYS:HB3	1.73	0.53
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.90	0.53
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.38	0.53
2:E:2248:ARG:NH2	2:E:2285:GLU:OE1	2.41	0.53
2:G:17:ASP:HB2	2:G:98:HIS:HE1	1.73	0.53
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.41	0.53
2:B:3843:ASP:H	2:B:3874:VAL:HG13	1.73	0.53
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.91	0.53
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.91	0.53
2:G:551:LEU:HD11	2:G:589:LEU:HD13	1.90	0.53
2:G:2248:ARG:NH2	2:G:2285:GLU:OE1	2.41	0.53
2:G:3843:ASP:H	2:G:3874:VAL:HG13	1.73	0.53
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.91	0.53
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.41	0.53
2:E:23:GLN:HE21	2:E:34:LYS:HB3	1.73	0.53
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.89	0.53
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.91	0.53
1:H:25:HIS:HB3	1:H:40:ARG:HD3	1.90	0.53
2:I:17:ASP:HB2	2:I:98:HIS:HE1	1.73	0.53
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.91	0.53
2:B:683:ARG:NH1	2:B:707:VAL:O	2.40	0.53
2:E:3992:PHE:O	2:E:3996:PHE:N	2.37	0.53
2:G:261:ARG:HB3	2:G:283:ARG:HB3	1.91	0.53
2:G:647:ASN:ND2	2:G:820:ARG:O	2.40	0.53
1:H:26:TYR:OH	1:H:42:ARG:NH2	2.36	0.53
2:I:551:LEU:HD11	2:I:589:LEU:HD13	1.90	0.53
2:I:4958:CYS:SG	2:I:4959:PHE:N	2.82	0.53
2:B:647:ASN:ND2	2:B:820:ARG:O	2.40	0.53
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.91	0.53
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.90	0.53
2:G:3992:PHE:O	2:G:3996:PHE:N	2.38	0.53
2:G:4924:VAL:HG23	2:G:4925:ILE:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:ASP:HB2	2:B:98:HIS:HE1	1.73	0.53
2:B:551:LEU:HD11	2:B:589:LEU:HD13	1.90	0.53
2:E:645:ARG:N	2:E:824:GLU:O	2.39	0.53
2:E:4924:VAL:HG23	2:E:4925:ILE:HG12	1.90	0.53
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.91	0.53
2:G:4843:LEU:HD12	2:I:4823:LEU:HD21	1.91	0.53
2:B:655:GLY:HA2	2:B:1002:ALA:HB2	1.90	0.52
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.90	0.52
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.91	0.52
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.90	0.52
2:G:655:GLY:HA2	2:G:1002:ALA:HB2	1.90	0.52
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.90	0.52
2:B:1679:ASN:HA	2:B:1682:ALA:HB3	1.92	0.52
2:E:669:ASP:OD2	2:E:790:ARG:NH2	2.41	0.52
2:G:4958:CYS:SG	2:G:4959:PHE:N	2.82	0.52
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.91	0.52
2:E:1196:PRO:O	2:E:1198:GLN:NE2	2.41	0.52
2:E:4958:CYS:SG	2:E:4959:PHE:N	2.82	0.52
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.41	0.52
2:I:914:PRO:O	2:I:918:ARG:N	2.42	0.52
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.43	0.52
2:I:3843:ASP:H	2:I:3874:VAL:HG13	1.73	0.52
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.43	0.52
2:E:261:ARG:HB3	2:E:283:ARG:HB3	1.91	0.52
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.41	0.52
2:I:627:PRO:HB2	1:J:92:PRO:HD3	1.92	0.52
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.38	0.52
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	1.91	0.52
1:J:26:TYR:OH	1:J:42:ARG:NH2	2.36	0.52
2:B:4958:CYS:SG	2:B:4959:PHE:N	2.82	0.52
2:E:17:ASP:HB2	2:E:98:HIS:HE1	1.73	0.52
2:E:4012:LEU:O	2:E:4016:LEU:N	2.43	0.52
2:G:1808:ARG:NH1	2:G:1853:ILE:O	2.39	0.52
2:I:2128:TYR:OH	2:I:3676:ASP:OD2	2.28	0.52
2:I:4924:VAL:HG23	2:I:4925:ILE:HG12	1.90	0.52
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.91	0.52
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.43	0.52
2:I:261:ARG:HB3	2:I:283:ARG:HB3	1.91	0.52
2:I:488:LEU:O	2:I:492:ASP:N	2.41	0.52
2:E:396:GLU:O	2:E:400:ALA:N	2.40	0.52
2:E:551:LEU:HD11	2:E:589:LEU:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4704:LEU:HD22	2:E:4778:TRP:HB2	1.92	0.52
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	1.92	0.52
2:G:4704:LEU:HD22	2:G:4778:TRP:HB2	1.92	0.52
2:I:396:GLU:O	2:I:400:ALA:N	2.40	0.52
2:I:1679:ASN:HA	2:I:1682:ALA:HB3	1.92	0.52
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	1.91	0.52
2:B:4924:VAL:HG23	2:B:4925:ILE:HG12	1.90	0.52
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.43	0.52
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.92	0.52
2:B:1032:LYS:O	2:B:1036:ARG:N	2.40	0.51
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.92	0.51
2:G:1676:LEU:HD22	2:G:2167:ILE:HG13	1.93	0.51
2:G:1965:TYR:OH	2:G:2027:ILE:O	2.26	0.51
2:I:1865:MET:N	2:I:1865:MET:SD	2.83	0.51
2:I:2185:ILE:HA	2:I:2188:ASN:HD21	1.75	0.51
2:B:2128:TYR:OH	2:B:3676:ASP:OD2	2.28	0.51
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.43	0.51
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	1.92	0.51
2:G:4201:ASN:O	2:G:4205:TRP:N	2.43	0.51
2:I:647:ASN:ND2	2:I:820:ARG:O	2.39	0.51
2:B:3905:THR:HA	2:B:3912:THR:HG23	1.93	0.51
2:E:2128:TYR:OH	2:E:3676:ASP:OD2	2.28	0.51
2:G:264:PRO:HG2	2:G:270:SER:HB2	1.92	0.51
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.92	0.51
2:G:4577:LEU:HG	2:G:4580:TYR:HE2	1.75	0.51
2:I:4704:LEU:HD22	2:I:4778:TRP:HB2	1.92	0.51
2:B:261:ARG:HB3	2:B:283:ARG:HB3	1.91	0.51
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.93	0.51
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.93	0.51
2:G:3905:THR:HA	2:G:3912:THR:HG23	1.93	0.51
2:I:1196:PRO:O	2:I:1198:GLN:NE2	2.41	0.51
2:I:4201:ASN:O	2:I:4205:TRP:N	2.43	0.51
2:B:1865:MET:N	2:B:1865:MET:SD	2.84	0.51
2:B:2185:ILE:HA	2:B:2188:ASN:HD21	1.75	0.51
2:B:3990:VAL:HG13	2:B:4051:SER:HB2	1.92	0.51
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.93	0.51
2:E:2950:UNK:O	2:E:2954:UNK:N	2.43	0.51
2:I:772:ASN:ND2	2:I:774:ASP:OD2	2.44	0.51
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.93	0.51
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.44	0.51
2:I:3990:VAL:HG13	2:I:4051:SER:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.76	0.51
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.92	0.51
2:B:4237:PHE:O	2:B:4241:THR:OG1	2.22	0.51
2:G:1679:ASN:HA	2:G:1682:ALA:HB3	1.92	0.51
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	1.92	0.51
2:I:666:VAL:HG21	2:I:684:VAL:HG21	1.93	0.51
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.76	0.51
2:I:1240:LYS:O	2:I:1604:SER:N	2.43	0.51
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.92	0.51
2:E:666:VAL:HG21	2:E:684:VAL:HG21	1.93	0.51
2:E:831:ARG:HD2	2:E:1199:VAL:HG12	1.93	0.51
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.44	0.51
2:G:488:LEU:O	2:G:492:ASP:N	2.41	0.51
2:G:831:ARG:HD2	2:G:1199:VAL:HG12	1.93	0.51
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.92	0.51
2:G:2128:TYR:OH	2:G:3676:ASP:OD2	2.28	0.51
2:I:4843:LEU:HD22	2:I:4928:LEU:HD11	1.92	0.51
2:B:772:ASN:ND2	2:B:774:ASP:OD2	2.44	0.51
2:B:3552:UNK:O	2:B:3556:UNK:N	2.44	0.51
2:B:4843:LEU:HD22	2:B:4928:LEU:HD11	1.92	0.51
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.76	0.51
2:E:3674:ILE:HD11	2:E:3728:ILE:HG22	1.92	0.51
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.44	0.51
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.43	0.51
2:G:4843:LEU:HD22	2:G:4928:LEU:HD11	1.92	0.51
2:E:264:PRO:HG2	2:E:270:SER:HB2	1.92	0.51
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.93	0.51
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.93	0.51
2:G:666:VAL:HG21	2:G:684:VAL:HG21	1.93	0.51
2:G:772:ASN:ND2	2:G:774:ASP:OD2	2.44	0.51
2:G:1231:GLN:NE2	2:G:1821:ASP:O	2.44	0.51
2:G:1258:ALA:HB3	2:G:1271:ARG:HB3	1.93	0.51
2:G:4012:LEU:O	2:G:4016:LEU:N	2.43	0.51
2:I:1676:LEU:HD22	2:I:2167:ILE:HG13	1.92	0.51
2:I:3948:LYS:NZ	2:I:4008:SER:O	2.44	0.51
2:I:3992:PHE:O	2:I:3996:PHE:N	2.37	0.51
2:I:4577:LEU:HG	2:I:4580:TYR:HE2	1.75	0.51
2:B:645:ARG:N	2:B:824:GLU:O	2.39	0.51
2:B:1231:GLN:NE2	2:B:1821:ASP:O	2.44	0.51
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.44	0.51
2:B:4704:LEU:HD22	2:B:4778:TRP:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1865:MET:N	2:E:1865:MET:SD	2.84	0.51
2:E:2185:ILE:HA	2:E:2188:ASN:HD21	1.75	0.51
2:E:4024:VAL:HG23	2:E:4027:LEU:HD12	1.92	0.51
2:E:4843:LEU:HD22	2:E:4928:LEU:HD11	1.92	0.51
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.93	0.51
2:B:666:VAL:HG21	2:B:684:VAL:HG21	1.93	0.50
2:B:1258:ALA:HB3	2:B:1271:ARG:HB3	1.93	0.50
2:B:4012:LEU:O	2:B:4016:LEU:N	2.42	0.50
2:E:772:ASN:ND2	2:E:774:ASP:OD2	2.44	0.50
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	1.92	0.50
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.92	0.50
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.75	0.50
2:G:2185:ILE:HA	2:G:2188:ASN:HD21	1.75	0.50
2:G:3552:UNK:O	2:G:3556:UNK:N	2.44	0.50
2:G:3829:PHE:HA	2:G:3832:ILE:HD12	1.93	0.50
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.93	0.50
2:I:1258:ALA:HB3	2:I:1271:ARG:HB3	1.93	0.50
2:B:4201:ASN:O	2:B:4205:TRP:N	2.43	0.50
2:B:4577:LEU:HG	2:B:4580:TYR:HE2	1.75	0.50
2:E:1235:THR:OG1	2:E:1607:ARG:NE	2.45	0.50
2:E:1240:LYS:O	2:E:1604:SER:N	2.43	0.50
2:G:1865:MET:N	2:G:1865:MET:SD	2.84	0.50
2:G:3948:LYS:NZ	2:G:4008:SER:O	2.44	0.50
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.93	0.50
2:I:4813:LEU:HD12	2:I:4816:ILE:HD11	1.93	0.50
2:B:15:ARG:HD3	2:B:98:HIS:HB3	1.93	0.50
2:B:831:ARG:HD2	2:B:1199:VAL:HG12	1.93	0.50
2:B:1240:LYS:O	2:B:1604:SER:N	2.43	0.50
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.93	0.50
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.93	0.50
2:E:3948:LYS:NZ	2:E:4008:SER:O	2.44	0.50
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.76	0.50
2:I:3905:THR:HA	2:I:3912:THR:HG23	1.93	0.50
2:B:3948:LYS:NZ	2:B:4008:SER:O	2.44	0.50
2:E:488:LEU:O	2:E:492:ASP:N	2.41	0.50
2:I:831:ARG:HD2	2:I:1199:VAL:HG12	1.93	0.50
2:B:313:SER:HB3	2:B:351:VAL:HB	1.94	0.50
2:B:1676:LEU:HD22	2:B:2167:ILE:HG13	1.93	0.50
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.93	0.50
2:E:1258:ALA:HB3	2:E:1271:ARG:HB3	1.94	0.50
2:G:1203:ASN:ND2	2:G:1210:SER:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.93	0.50
2:I:1032:LYS:O	2:I:1036:ARG:N	2.40	0.50
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	1.92	0.50
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.92	0.50
2:B:914:PRO:O	2:B:918:ARG:N	2.42	0.50
2:B:1721:GLU:HG2	2:B:1725:ARG:HH12	1.77	0.50
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	1.92	0.50
2:E:313:SER:HB3	2:E:351:VAL:HB	1.94	0.50
2:E:3552:UNK:O	2:E:3556:UNK:N	2.44	0.50
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.43	0.50
2:G:15:ARG:HD3	2:G:98:HIS:HB3	1.93	0.50
2:G:396:GLU:O	2:G:400:ALA:N	2.40	0.50
2:G:683:ARG:NH1	2:G:707:VAL:O	2.40	0.50
2:I:1231:GLN:NE2	2:I:1821:ASP:O	2.44	0.50
2:I:3829:PHE:HA	2:I:3832:ILE:HD12	1.93	0.50
1:A:7:ILE:HG22	1:A:9:PRO:HD2	1.94	0.50
2:B:355:LEU:HB3	2:B:378:LEU:HB3	1.94	0.50
2:B:460:GLN:HG2	2:B:462:GLU:H	1.77	0.50
2:B:1235:THR:OG1	2:B:1607:ARG:NE	2.45	0.50
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.94	0.50
2:E:4088:ILE:HG23	2:E:4123:ILE:HB	1.94	0.50
2:G:645:ARG:N	2:G:824:GLU:O	2.39	0.50
2:G:4088:ILE:HG23	2:G:4123:ILE:HB	1.94	0.50
1:H:7:ILE:HG22	1:H:9:PRO:HD2	1.94	0.50
2:I:1865:MET:HB3	2:I:1926:LEU:HB2	1.94	0.50
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.94	0.50
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.93	0.50
2:I:4956:THR:O	2:I:4965:SER:N	2.42	0.50
1:J:7:ILE:HG22	1:J:9:PRO:HD2	1.94	0.50
2:E:838:HIS:HB3	2:E:1200:GLY:H	1.77	0.50
2:E:3990:VAL:HG13	2:E:4051:SER:HB2	1.93	0.50
1:F:7:ILE:HG22	1:F:9:PRO:HD2	1.94	0.50
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.45	0.50
2:G:1235:THR:OG1	2:G:1607:ARG:NE	2.44	0.50
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.93	0.50
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.93	0.50
2:B:4813:LEU:HD12	2:B:4816:ILE:HD11	1.93	0.50
2:E:914:PRO:O	2:E:918:ARG:N	2.42	0.50
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.94	0.50
2:E:4044:MET:HA	2:E:4047:MET:HG2	1.94	0.50
2:G:3674:ILE:HG13	2:G:3732:SER:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.94	0.50
2:G:4813:LEU:HD12	2:G:4816:ILE:HD11	1.93	0.50
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.43	0.50
2:I:4024:VAL:HG23	2:I:4027:LEU:HD12	1.93	0.50
2:B:264:PRO:HG2	2:B:270:SER:HB2	1.92	0.49
2:B:485:SER:O	2:B:489:ASN:N	2.44	0.49
2:B:1196:PRO:O	2:B:1198:GLN:NE2	2.41	0.49
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.93	0.49
2:G:728:ARG:NH2	2:G:1527:UNK:O	2.45	0.49
2:G:1196:PRO:O	2:G:1198:GLN:NE2	2.41	0.49
2:I:355:LEU:HB3	2:I:378:LEU:HB3	1.94	0.49
2:I:3552:UNK:O	2:I:3556:UNK:N	2.44	0.49
2:I:4012:LEU:O	2:I:4016:LEU:N	2.43	0.49
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.94	0.49
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.93	0.49
2:B:4088:ILE:HG23	2:B:4123:ILE:HB	1.94	0.49
2:E:355:LEU:HB3	2:E:378:LEU:HB3	1.94	0.49
2:E:1721:GLU:HG2	2:E:1725:ARG:HH12	1.77	0.49
2:E:3905:THR:HA	2:E:3912:THR:HG23	1.93	0.49
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.93	0.49
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.94	0.49
2:I:229:GLU:OE2	2:I:374:LYS:NZ	2.35	0.49
2:I:264:PRO:HG2	2:I:270:SER:HB2	1.92	0.49
2:I:1235:THR:OG1	2:I:1607:ARG:NE	2.44	0.49
2:I:1691:GLN:HG2	1:J:42:ARG:HG2	1.93	0.49
2:I:3674:ILE:HG13	2:I:3732:SER:HB3	1.94	0.49
2:I:4088:ILE:HG23	2:I:4123:ILE:HB	1.94	0.49
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.93	0.49
2:B:1865:MET:HB3	2:B:1926:LEU:HB2	1.94	0.49
2:B:2868:SER:O	2:B:2872:GLN:N	2.44	0.49
2:E:15:ARG:HD3	2:E:98:HIS:HB3	1.93	0.49
2:E:139:GLU:O	2:E:141:ALA:N	2.45	0.49
2:E:1231:GLN:NE2	2:E:1821:ASP:O	2.44	0.49
2:E:1676:LEU:HD22	2:E:2167:ILE:HG13	1.92	0.49
2:E:3674:ILE:HG13	2:E:3732:SER:HB3	1.94	0.49
2:G:139:GLU:O	2:G:141:ALA:N	2.45	0.49
2:G:1865:MET:HB3	2:G:1926:LEU:HB2	1.94	0.49
2:G:4024:VAL:HG23	2:G:4027:LEU:HD12	1.92	0.49
2:I:1269:CYS:HA	2:I:1473:UNK:HA	1.95	0.49
2:B:235:ALA:HA	2:B:257:ARG:HD3	1.95	0.49
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1271:ARG:HA	2:B:1471:UNK:HA	1.94	0.49
2:E:913:LEU:HD13	2:E:918:ARG:HA	1.94	0.49
2:G:838:HIS:HB3	2:G:1200:GLY:H	1.77	0.49
2:G:2336:ARG:HD3	2:G:2435:ARG:HD2	1.94	0.49
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.45	0.49
2:I:1163:THR:HA	2:I:1168:VAL:HA	1.95	0.49
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	1.95	0.49
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.95	0.49
2:B:2336:ARG:HD3	2:B:2435:ARG:HD2	1.94	0.49
2:B:4024:VAL:HG23	2:B:4027:LEU:HD12	1.93	0.49
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.95	0.49
2:E:682:LEU:HD13	2:E:787:VAL:HG11	1.94	0.49
2:E:2235:PHE:HA	2:E:2238:TYR:HD2	1.78	0.49
2:E:3829:PHE:HA	2:E:3832:ILE:HD12	1.93	0.49
2:E:4138:ASP:N	2:E:4138:ASP:OD1	2.45	0.49
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.94	0.49
2:I:15:ARG:HD3	2:I:98:HIS:HB3	1.93	0.49
2:I:682:LEU:HD13	2:I:787:VAL:HG11	1.94	0.49
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.94	0.49
2:I:2336:ARG:HD3	2:I:2435:ARG:HD2	1.94	0.49
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.94	0.49
2:B:3829:PHE:HA	2:B:3832:ILE:HD12	1.93	0.49
2:E:4813:LEU:HD12	2:E:4816:ILE:HD11	1.93	0.49
2:G:913:LEU:HD13	2:G:918:ARG:HA	1.94	0.49
2:G:914:PRO:O	2:G:918:ARG:N	2.42	0.49
2:G:3990:VAL:HG13	2:G:4051:SER:HB2	1.92	0.49
2:B:838:HIS:HB3	2:B:1200:GLY:H	1.77	0.49
2:B:3674:ILE:HG13	2:B:3732:SER:HB3	1.94	0.49
2:E:235:ALA:HA	2:E:257:ARG:HD3	1.95	0.49
2:E:460:GLN:HG2	2:E:462:GLU:H	1.77	0.49
1:F:26:TYR:OH	1:F:42:ARG:NH2	2.36	0.49
2:G:355:LEU:HB3	2:G:378:LEU:HB3	1.94	0.49
2:G:2868:SER:O	2:G:2872:GLN:N	2.44	0.49
2:G:4044:MET:HA	2:G:4047:MET:HG2	1.94	0.49
2:I:313:SER:HB3	2:I:351:VAL:HB	1.93	0.49
2:I:4044:MET:HA	2:I:4047:MET:HG2	1.94	0.49
2:B:229:GLU:OE2	2:B:374:LYS:NZ	2.35	0.49
2:B:1203:ASN:ND2	2:B:1210:SER:O	2.44	0.49
2:B:3882:GLN:HB2	2:B:3957:VAL:HG22	1.95	0.49
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.95	0.49
2:E:4560:TYR:O	2:E:4564:PHE:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:232:THR:HB	2:I:252:VAL:HG11	1.95	0.49
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.95	0.49
2:I:1684:ALA:HA	2:I:1782:PHE:HZ	1.77	0.49
2:G:1240:LYS:O	2:G:1604:SER:N	2.43	0.49
2:G:1979:LEU:HA	2:G:1983:ALA:HB3	1.95	0.49
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	1.95	0.49
2:I:1721:GLU:HG2	2:I:1725:ARG:HH12	1.77	0.49
1:A:62:GLY:HA3	1:A:74:LEU:HD21	1.93	0.49
2:B:139:GLU:O	2:B:141:ALA:N	2.45	0.49
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	1.95	0.49
2:B:2257:LEU:O	2:B:2261:SER:N	2.46	0.49
2:E:1203:ASN:ND2	2:E:1210:SER:O	2.44	0.49
2:E:1865:MET:HB3	2:E:1926:LEU:HB2	1.94	0.49
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	1.95	0.49
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.94	0.49
2:E:4201:ASN:O	2:E:4205:TRP:N	2.43	0.49
2:G:1684:ALA:HA	2:G:1782:PHE:HZ	1.77	0.49
2:G:2235:PHE:HA	2:G:2238:TYR:HD2	1.78	0.49
2:I:139:GLU:O	2:I:141:ALA:N	2.45	0.49
2:I:235:ALA:HA	2:I:257:ARG:HD3	1.95	0.49
2:B:4044:MET:HA	2:B:4047:MET:HG2	1.94	0.48
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.94	0.48
1:F:62:GLY:HA3	1:F:74:LEU:HD21	1.94	0.48
2:G:313:SER:HB3	2:G:351:VAL:HB	1.93	0.48
2:G:1721:GLU:HG2	2:G:1725:ARG:HH12	1.77	0.48
2:I:793:LEU:HD12	2:I:797:HIS:HB2	1.95	0.48
2:B:682:LEU:HD13	2:B:787:VAL:HG11	1.94	0.48
2:E:1684:ALA:HA	2:E:1782:PHE:HZ	1.77	0.48
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	1.95	0.48
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.95	0.48
1:H:62:GLY:HA3	1:H:74:LEU:HD21	1.94	0.48
1:J:62:GLY:HA3	1:J:74:LEU:HD21	1.94	0.48
2:E:652:ARG:HB3	2:E:773:LEU:HD13	1.95	0.48
2:E:2013:LYS:HA	2:E:2028:ARG:HB2	1.95	0.48
2:G:235:ALA:HA	2:G:257:ARG:HD3	1.95	0.48
2:G:4795:TYR:HE1	2:G:4812:HIS:HA	1.79	0.48
2:I:460:GLN:HG2	2:I:462:GLU:H	1.77	0.48
2:I:838:HIS:HB3	2:I:1200:GLY:H	1.77	0.48
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	1.95	0.48
2:I:3882:GLN:HB2	2:I:3957:VAL:HG22	1.95	0.48
2:B:652:ARG:HB3	2:B:773:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:793:LEU:HD12	2:B:797:HIS:HB2	1.95	0.48
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	1.95	0.48
2:B:1931:LEU:HD22	2:B:1935:VAL:HG11	1.96	0.48
2:B:4795:TYR:HE1	2:B:4812:HIS:HA	1.79	0.48
2:E:111:HIS:CD2	2:E:114:SER:H	2.26	0.48
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.45	0.48
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.95	0.48
2:G:232:THR:HB	2:G:252:VAL:HG11	1.95	0.48
2:G:460:GLN:HG2	2:G:462:GLU:H	1.77	0.48
2:G:652:ARG:HB3	2:G:773:LEU:HD13	1.96	0.48
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.94	0.48
2:G:2257:LEU:O	2:G:2261:SER:N	2.46	0.48
2:G:4837:LEU:HD11	2:G:4936:ILE:HD11	1.96	0.48
2:G:4849:TYR:OH	2:I:4574:ASN:O	2.29	0.48
2:I:652:ARG:HB3	2:I:773:LEU:HD13	1.96	0.48
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	1.95	0.48
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	1.95	0.48
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.96	0.48
2:B:1778:SER:N	2:B:1799:SER:O	2.46	0.48
2:E:3994:HIS:O	2:E:3998:HIS:ND1	2.39	0.48
2:E:4837:LEU:HD11	2:E:4936:ILE:HD11	1.96	0.48
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.96	0.48
2:I:4105:GLY:HA2	2:I:4108:ILE:HD12	1.95	0.48
2:I:4837:LEU:HD11	2:I:4936:ILE:HD11	1.96	0.48
2:B:1684:ALA:HA	2:B:1782:PHE:HZ	1.77	0.48
2:E:880:GLU:OE1	2:E:968:ALA:N	2.47	0.48
2:G:682:LEU:HD13	2:G:787:VAL:HG11	1.94	0.48
2:G:793:LEU:HD12	2:G:797:HIS:HB2	1.95	0.48
2:G:1032:LYS:O	2:G:1036:ARG:N	2.40	0.48
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	1.95	0.48
2:I:1713:ASP:O	2:I:1717:SER:N	2.46	0.48
2:I:1931:LEU:HD22	2:I:1935:VAL:HG11	1.96	0.48
2:I:2235:PHE:HA	2:I:2238:TYR:HD2	1.78	0.48
1:A:57:LYS:HB2	1:A:80:VAL:HB	1.96	0.48
2:B:215:THR:HG22	2:B:273:HIS:HA	1.95	0.48
2:B:1163:THR:HA	2:B:1168:VAL:HA	1.95	0.48
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.49	0.48
2:B:1979:LEU:HA	2:B:1983:ALA:HB3	1.95	0.48
2:B:2235:PHE:HA	2:B:2238:TYR:HD2	1.78	0.48
2:E:2336:ARG:HD3	2:E:2435:ARG:HD2	1.94	0.48
2:G:1075:PHE:HB2	2:G:1192:CYS:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1647:CYS:SG	2:G:1648:MET:N	2.87	0.48
2:I:3729:MET:HB3	2:I:3770:LEU:HD21	1.96	0.48
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.94	0.48
2:B:1659:LEU:O	2:B:1663:HIS:N	2.44	0.48
2:B:1952:GLN:HA	2:B:1955:VAL:HG12	1.96	0.48
2:B:4956:THR:O	2:B:4965:SER:N	2.42	0.48
2:E:3882:GLN:HB2	2:E:3957:VAL:HG22	1.95	0.48
2:G:215:THR:HG22	2:G:273:HIS:HA	1.95	0.48
1:H:57:LYS:HB2	1:H:80:VAL:HB	1.96	0.48
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.49	0.48
1:J:57:LYS:HB2	1:J:80:VAL:HB	1.96	0.48
1:J:87:HIS:N	1:J:91:ILE:O	2.47	0.48
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.94	0.48
2:E:1647:CYS:SG	2:E:1648:MET:N	2.87	0.48
2:E:1848:LEU:HB3	2:E:1853:ILE:HB	1.95	0.48
2:E:1979:LEU:HA	2:E:1983:ALA:HB3	1.95	0.48
2:E:4795:TYR:HE1	2:E:4812:HIS:HA	1.79	0.48
2:G:988:LEU:O	2:G:992:GLY:N	2.46	0.48
2:G:1931:LEU:HD22	2:G:1935:VAL:HG11	1.96	0.48
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.79	0.48
2:B:913:LEU:HD13	2:B:918:ARG:HA	1.95	0.48
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	1.95	0.48
2:B:1854:PHE:HD1	2:B:1858:ASP:HB3	1.79	0.48
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.79	0.48
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	1.95	0.48
2:E:1163:THR:HA	2:E:1168:VAL:HA	1.95	0.48
2:E:2257:LEU:O	2:E:2261:SER:N	2.46	0.48
1:F:57:LYS:HB2	1:F:80:VAL:HB	1.96	0.48
2:G:731:THR:OG1	2:G:1519:UNK:O	2.27	0.48
2:G:4105:GLY:HA2	2:G:4108:ILE:HD12	1.95	0.48
2:G:4956:THR:O	2:G:4965:SER:N	2.42	0.48
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.94	0.48
1:H:87:HIS:N	1:H:91:ILE:O	2.47	0.48
2:I:1952:GLN:HA	2:I:1955:VAL:HG12	1.96	0.48
2:I:2257:LEU:O	2:I:2261:SER:N	2.46	0.48
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.94	0.48
2:B:1848:LEU:HB3	2:B:1853:ILE:HB	1.95	0.47
2:B:2950:UNK:O	2:B:2954:UNK:N	2.47	0.47
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.96	0.47
2:E:4105:GLY:HA2	2:E:4108:ILE:HD12	1.95	0.47
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3806:ASN:HA	2:G:3890:LEU:HD13	1.96	0.47
2:G:3882:GLN:HB2	2:G:3957:VAL:HG22	1.95	0.47
2:G:3981:ALA:HA	2:G:3986:TRP:HE1	1.79	0.47
2:G:4138:ASP:OD1	2:G:4138:ASP:N	2.45	0.47
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.96	0.47
2:I:645:ARG:N	2:I:824:GLU:O	2.39	0.47
2:I:913:LEU:HD13	2:I:918:ARG:HA	1.95	0.47
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.79	0.47
2:I:4795:TYR:HE1	2:I:4812:HIS:HA	1.79	0.47
2:B:488:LEU:O	2:B:492:ASP:N	2.41	0.47
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.96	0.47
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.95	0.47
2:B:2013:LYS:HA	2:B:2028:ARG:HB2	1.95	0.47
2:E:1931:LEU:HD22	2:E:1935:VAL:HG11	1.96	0.47
1:F:87:HIS:N	1:F:91:ILE:O	2.47	0.47
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.49	0.47
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	1.95	0.47
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.96	0.47
2:I:1647:CYS:SG	2:I:1648:MET:N	2.87	0.47
2:B:1647:CYS:SG	2:B:1648:MET:N	2.87	0.47
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	1.96	0.47
2:E:1232:ARG:HD3	2:E:1702:HIS:HB3	1.96	0.47
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.95	0.47
2:E:3806:ASN:HA	2:E:3890:LEU:HD13	1.96	0.47
2:G:3729:MET:HB3	2:G:3770:LEU:HD21	1.96	0.47
2:I:4003:LEU:HB2	2:I:4013:LEU:HD13	1.96	0.47
2:B:3992:PHE:O	2:B:3996:PHE:N	2.38	0.47
2:B:4571:PHE:O	2:B:4575:PHE:N	2.48	0.47
2:B:4837:LEU:HD11	2:B:4936:ILE:HD11	1.96	0.47
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	1.95	0.47
2:E:4571:PHE:O	2:E:4575:PHE:N	2.48	0.47
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	1.96	0.47
2:G:1163:THR:HA	2:G:1168:VAL:HA	1.95	0.47
2:G:1232:ARG:HD3	2:G:1702:HIS:HB3	1.96	0.47
2:G:1848:LEU:HB3	2:G:1853:ILE:HB	1.95	0.47
2:I:1232:ARG:HD3	2:I:1702:HIS:HB3	1.96	0.47
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.95	0.47
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.48	0.47
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.96	0.47
2:B:1516:UNK:N	2:B:1529:UNK:O	2.47	0.47
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4003:LEU:HB2	2:B:4013:LEU:HD13	1.96	0.47
2:E:232:THR:HB	2:E:252:VAL:HG11	1.95	0.47
2:E:1075:PHE:HB2	2:E:1192:CYS:HB2	1.95	0.47
2:E:1713:ASP:O	2:E:1717:SER:N	2.46	0.47
2:E:2868:SER:O	2:E:2872:GLN:N	2.44	0.47
2:E:4116:GLU:H	2:E:4128:PHE:HZ	1.63	0.47
2:G:637:LEU:HG	2:G:1693:GLN:HB3	1.96	0.47
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.95	0.47
2:G:2347:GLU:O	2:G:2351:ASN:N	2.43	0.47
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.80	0.47
2:B:3806:ASN:HA	2:B:3890:LEU:HD13	1.96	0.47
2:E:215:THR:HG22	2:E:273:HIS:HA	1.95	0.47
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.49	0.47
2:E:3920:VAL:O	2:E:3924:LEU:N	2.44	0.47
2:I:215:THR:HG22	2:I:273:HIS:HA	1.95	0.47
2:I:637:LEU:HG	2:I:1693:GLN:HB3	1.96	0.47
2:I:2013:LYS:HA	2:I:2028:ARG:HB2	1.96	0.47
2:I:2950:UNK:O	2:I:2954:UNK:N	2.48	0.47
2:I:4138:ASP:OD1	2:I:4138:ASP:N	2.45	0.47
2:B:988:LEU:O	2:B:992:GLY:N	2.46	0.47
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	1.97	0.47
2:B:3729:MET:HB3	2:B:3770:LEU:HD21	1.96	0.47
2:E:793:LEU:HD12	2:E:797:HIS:HB2	1.95	0.47
2:E:988:LEU:O	2:E:992:GLY:N	2.46	0.47
2:E:1032:LYS:O	2:E:1036:ARG:N	2.40	0.47
2:E:1778:SER:N	2:E:1799:SER:O	2.46	0.47
2:E:1854:PHE:HD1	2:E:1858:ASP:HB3	1.79	0.47
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	1.97	0.47
2:G:2013:LYS:HA	2:G:2028:ARG:HB2	1.95	0.47
2:G:4116:GLU:H	2:G:4128:PHE:HZ	1.63	0.47
2:I:379:HIS:CD2	2:I:382:GLY:H	2.33	0.47
2:I:880:GLU:OE1	2:I:968:ALA:N	2.47	0.47
2:I:1075:PHE:HB2	2:I:1192:CYS:HB2	1.95	0.47
2:I:1659:LEU:O	2:I:1663:HIS:N	2.44	0.47
2:I:1854:PHE:HD1	2:I:1858:ASP:HB3	1.79	0.47
2:I:1979:LEU:HA	2:I:1983:ALA:HB3	1.95	0.47
2:I:3889:GLN:HE22	2:I:3963:ASN:HB3	1.79	0.47
2:I:3994:HIS:O	2:I:3998:HIS:ND1	2.39	0.47
2:I:4824:ARG:HA	2:I:4827:LEU:HB3	1.97	0.47
1:A:87:HIS:N	1:A:91:ILE:O	2.47	0.47
2:B:1075:PHE:HB2	2:B:1192:CYS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	1.97	0.47
2:E:2347:GLU:O	2:E:2351:ASN:N	2.43	0.47
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.96	0.47
2:G:120:CYS:H	2:G:145:ALA:HB1	1.80	0.47
2:G:485:SER:O	2:G:489:ASN:N	2.44	0.47
2:G:880:GLU:OE1	2:G:968:ALA:N	2.47	0.47
2:G:2950:UNK:O	2:G:2954:UNK:N	2.48	0.47
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	1.97	0.47
2:I:3981:ALA:HA	2:I:3986:TRP:HE1	1.79	0.47
1:A:34:LYS:NZ	2:B:635:THR:O	2.47	0.47
2:B:232:THR:HB	2:B:252:VAL:HG11	1.95	0.47
2:B:4105:GLY:HA2	2:B:4108:ILE:HD12	1.95	0.47
2:E:1952:GLN:HA	2:E:1955:VAL:HG12	1.96	0.47
2:G:1713:ASP:O	2:G:1717:SER:N	2.46	0.47
2:I:1848:LEU:HB3	2:I:1853:ILE:HB	1.95	0.47
2:E:120:CYS:H	2:E:145:ALA:HB1	1.80	0.47
2:E:2871:LEU:HD22	2:E:2927:LEU:HD22	1.97	0.47
2:I:485:SER:O	2:I:489:ASN:N	2.44	0.47
2:I:1286:UNK:HA	2:I:1461:UNK:HA	1.96	0.47
2:B:4560:TYR:O	2:B:4564:PHE:N	2.43	0.46
2:B:4824:ARG:HA	2:B:4827:LEU:HB3	1.97	0.46
2:I:4634:GLU:HG3	2:I:4636:THR:H	1.81	0.46
2:I:5012:LYS:O	2:I:5016:GLU:N	2.43	0.46
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.96	0.46
2:B:379:HIS:CD2	2:B:382:GLY:H	2.33	0.46
2:B:1232:ARG:HD3	2:B:1702:HIS:HB3	1.97	0.46
2:B:2231:SER:HA	2:B:2234:ARG:HG2	1.98	0.46
2:B:4634:GLU:HG3	2:B:4636:THR:H	1.80	0.46
2:B:5012:LYS:O	2:B:5016:GLU:N	2.43	0.46
2:E:3729:MET:HB3	2:E:3770:LEU:HD21	1.96	0.46
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.79	0.46
2:E:3889:GLN:HE22	2:E:3963:ASN:HB3	1.80	0.46
2:E:3981:ALA:HA	2:E:3986:TRP:HE1	1.79	0.46
2:E:4003:LEU:HB2	2:E:4013:LEU:HD13	1.96	0.46
2:G:733:PRO:HD2	2:G:763:PRO:HD2	1.97	0.46
2:G:1854:PHE:HD1	2:G:1858:ASP:HB3	1.79	0.46
2:G:1952:GLN:HA	2:G:1955:VAL:HG12	1.96	0.46
2:G:2871:LEU:HD22	2:G:2927:LEU:HD22	1.97	0.46
2:G:4003:LEU:HB2	2:G:4013:LEU:HD13	1.96	0.46
2:I:1778:SER:N	2:I:1799:SER:O	2.46	0.46
2:I:4571:PHE:O	2:I:4575:PHE:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4116:GLU:H	2:B:4128:PHE:HZ	1.63	0.46
2:E:733:PRO:HD2	2:E:763:PRO:HD2	1.97	0.46
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.96	0.46
2:G:4560:TYR:O	2:G:4564:PHE:N	2.43	0.46
2:G:4571:PHE:O	2:G:4575:PHE:N	2.48	0.46
2:I:865:PRO:O	2:I:869:ARG:N	2.49	0.46
2:I:1855:GLY:O	2:I:1859:VAL:N	2.45	0.46
2:B:637:LEU:HG	2:B:1693:GLN:HB3	1.96	0.46
2:E:164:ARG:N	2:E:167:ASP:OD2	2.48	0.46
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.96	0.46
2:E:2231:SER:HA	2:E:2234:ARG:HG2	1.98	0.46
2:G:164:ARG:N	2:G:167:ASP:OD2	2.48	0.46
2:G:1778:SER:N	2:G:1799:SER:O	2.46	0.46
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.96	0.46
2:I:120:CYS:H	2:I:145:ALA:HB1	1.80	0.46
2:I:2231:SER:HA	2:I:2234:ARG:HG2	1.98	0.46
2:I:3806:ASN:HA	2:I:3890:LEU:HD13	1.96	0.46
2:B:120:CYS:H	2:B:145:ALA:HB1	1.80	0.46
2:B:731:THR:OG1	2:B:1519:UNK:O	2.27	0.46
2:E:637:LEU:HG	2:E:1693:GLN:HB3	1.96	0.46
2:E:1229:ASN:O	2:E:1827:ARG:N	2.43	0.46
2:E:1729:SER:O	2:E:2163:ARG:NH1	2.49	0.46
2:G:1779:PRO:HG2	1:H:44:LYS:HE3	1.98	0.46
2:G:2231:SER:HA	2:G:2234:ARG:HG2	1.98	0.46
2:G:4634:GLU:HG3	2:G:4636:THR:H	1.81	0.46
2:I:69:LEU:HD22	2:I:107:ILE:HD11	1.98	0.46
2:B:38:ALA:HB1	2:B:64:ILE:HG13	1.97	0.46
2:B:880:GLU:OE1	2:B:968:ALA:N	2.47	0.46
2:E:731:THR:OG1	2:E:1519:UNK:O	2.34	0.46
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.97	0.46
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.48	0.46
2:G:1229:ASN:O	2:G:1827:ARG:N	2.43	0.46
2:G:4824:ARG:HA	2:G:4827:LEU:HB3	1.97	0.46
2:B:69:LEU:HD22	2:B:107:ILE:HD11	1.98	0.46
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.98	0.46
2:B:1713:ASP:O	2:B:1717:SER:N	2.46	0.46
2:B:3981:ALA:HA	2:B:3986:TRP:HE1	1.79	0.46
2:E:379:HIS:CD2	2:E:382:GLY:H	2.33	0.46
2:E:4824:ARG:HA	2:E:4827:LEU:HB3	1.97	0.46
2:G:1729:SER:O	2:G:2163:ARG:NH1	2.49	0.46
2:I:838:HIS:CE1	2:I:1201:HIS:HD2	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.97	0.46
2:B:838:HIS:CE1	2:B:1201:HIS:HD2	2.34	0.46
2:B:3758:MET:O	2:B:3762:ARG:NE	2.46	0.46
2:B:4051:SER:HG	2:B:4054:ASN:HB2	1.80	0.46
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.98	0.46
2:I:733:PRO:HD2	2:I:763:PRO:HD2	1.97	0.46
1:A:83:GLY:O	1:A:94:ASN:N	2.48	0.46
2:E:3927:GLN:O	2:E:3931:SER:N	2.45	0.46
2:E:4634:GLU:HG3	2:E:4636:THR:H	1.81	0.46
2:I:4942:GLU:O	2:I:4946:GLN:N	2.44	0.46
2:B:629:ARG:HB3	2:B:634:GLN:NE2	2.32	0.45
2:B:733:PRO:HD2	2:B:763:PRO:HD2	1.97	0.45
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.80	0.45
2:B:4697:VAL:O	2:B:4701:TRP:N	2.49	0.45
2:G:629:ARG:HB3	2:G:634:GLN:NE2	2.32	0.45
2:G:4998:LYS:NZ	2:G:5007:GLU:OE1	2.42	0.45
2:I:1203:ASN:ND2	2:I:1210:SER:O	2.44	0.45
2:I:2871:LEU:HD22	2:I:2927:LEU:HD22	1.97	0.45
2:I:4116:GLU:H	2:I:4128:PHE:HZ	1.63	0.45
1:J:83:GLY:O	1:J:94:ASN:N	2.48	0.45
2:B:1729:SER:O	2:B:2163:ARG:NH1	2.49	0.45
2:B:2336:ARG:NH2	2:B:2428:ALA:O	2.49	0.45
2:E:709:ASP:HB3	2:E:725:HIS:CE1	2.51	0.45
2:E:4934:GLY:O	2:E:4938:ASP:N	2.47	0.45
1:F:23:VAL:HB	1:F:105:ASN:HA	1.99	0.45
2:I:38:ALA:HB1	2:I:64:ILE:HG13	1.97	0.45
2:I:1729:SER:O	2:I:2163:ARG:NH1	2.49	0.45
1:A:23:VAL:HB	1:A:105:ASN:HA	1.99	0.45
2:B:4942:GLU:O	2:B:4946:GLN:N	2.43	0.45
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.98	0.45
2:G:38:ALA:HB1	2:G:64:ILE:HG13	1.97	0.45
2:G:865:PRO:O	2:G:869:ARG:N	2.49	0.45
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.97	0.45
2:I:2868:SER:O	2:I:2872:GLN:N	2.44	0.45
2:I:2880:GLU:O	2:I:2884:ASN:N	2.45	0.45
2:B:124:SER:HA	2:B:132:ALA:HB3	1.99	0.45
2:B:709:ASP:HB3	2:B:725:HIS:CE1	2.52	0.45
2:E:38:ALA:HB1	2:E:64:ILE:HG13	1.97	0.45
2:E:2286:LEU:HA	2:E:2289:ALA:HB3	1.99	0.45
2:E:4697:VAL:O	2:E:4701:TRP:N	2.49	0.45
2:G:838:HIS:CE1	2:G:1201:HIS:HD2	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4791:TYR:HD2	2:G:4792:LEU:HD22	1.82	0.45
2:I:709:ASP:HB3	2:I:725:HIS:CE1	2.52	0.45
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.98	0.45
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.97	0.45
2:B:2871:LEU:HD22	2:B:2927:LEU:HD22	1.97	0.45
2:B:2880:GLU:O	2:B:2884:ASN:N	2.45	0.45
2:E:124:SER:HA	2:E:132:ALA:HB3	1.99	0.45
2:E:629:ARG:HB3	2:E:634:GLN:NE2	2.32	0.45
2:E:838:HIS:CE1	2:E:1201:HIS:HD2	2.34	0.45
2:G:709:ASP:HB3	2:G:725:HIS:CE1	2.52	0.45
1:H:23:VAL:HB	1:H:105:ASN:HA	1.99	0.45
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.98	0.45
2:I:2347:GLU:O	2:I:2351:ASN:N	2.43	0.45
1:J:23:VAL:HB	1:J:105:ASN:HA	1.99	0.45
2:B:546:TRP:O	2:B:550:LYS:NZ	2.38	0.45
2:B:2132:GLY:O	2:B:2136:ARG:N	2.50	0.45
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.99	0.45
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.98	0.45
2:E:1659:LEU:O	2:E:1663:HIS:N	2.44	0.45
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.98	0.45
2:G:124:SER:HA	2:G:132:ALA:HB3	1.99	0.45
2:G:4109:GLN:O	2:G:4113:SER:N	2.45	0.45
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	1.99	0.45
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.99	0.45
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.98	0.45
2:B:4138:ASP:OD1	2:B:4138:ASP:N	2.45	0.45
2:B:4961:CYS:SG	2:B:4978:HIS:NE2	2.90	0.45
2:E:1577:ALA:HB1	2:E:1584:ARG:HA	1.99	0.45
2:G:69:LEU:HD22	2:G:107:ILE:HD11	1.98	0.45
2:G:2286:LEU:HA	2:G:2289:ALA:HB3	1.99	0.45
2:G:4705:VAL:HB	2:G:4778:TRP:CG	2.52	0.45
1:H:83:GLY:O	1:H:94:ASN:N	2.48	0.45
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.99	0.45
2:I:124:SER:HA	2:I:132:ALA:HB3	1.99	0.45
2:B:2286:LEU:HA	2:B:2289:ALA:HB3	1.99	0.45
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	1.98	0.45
2:B:4853:VAL:HA	2:B:4856:PHE:HB3	1.98	0.45
2:E:69:LEU:HD22	2:E:107:ILE:HD11	1.98	0.45
2:E:485:SER:O	2:E:489:ASN:N	2.44	0.45
2:E:1041:GLN:O	2:E:1045:THR:OG1	2.29	0.45
1:F:83:GLY:O	1:F:94:ASN:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	1.97	0.45
2:I:629:ARG:HB3	2:I:634:GLN:NE2	2.31	0.45
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.99	0.45
2:I:3920:VAL:O	2:I:3924:LEU:N	2.44	0.45
2:I:4961:CYS:SG	2:I:4978:HIS:NE2	2.90	0.45
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.99	0.45
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.48	0.45
2:E:732:SER:HB3	2:E:764:VAL:HA	1.99	0.45
2:G:732:SER:HB3	2:G:764:VAL:HA	1.99	0.45
2:G:2132:GLY:O	2:G:2136:ARG:N	2.50	0.45
2:G:2758:PHE:O	2:G:2762:THR:N	2.47	0.45
2:G:4853:VAL:HA	2:G:4856:PHE:HB3	1.98	0.45
2:I:180:LEU:HD22	2:I:200:TRP:NE1	2.32	0.45
2:I:233:ILE:HD12	2:I:242:ARG:HB3	1.99	0.45
2:I:2132:GLY:O	2:I:2136:ARG:N	2.50	0.45
2:I:3758:MET:O	2:I:3762:ARG:NE	2.46	0.45
1:J:29:MET:HB3	1:J:98:ILE:HB	1.99	0.45
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.99	0.45
2:B:865:PRO:O	2:B:869:ARG:N	2.49	0.45
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.50	0.45
2:E:4791:TYR:HD2	2:E:4792:LEU:HD22	1.81	0.45
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.99	0.45
2:G:233:ILE:HD12	2:G:242:ARG:HB3	1.99	0.45
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.99	0.45
2:G:1577:ALA:HB1	2:G:1584:ARG:HA	1.99	0.45
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.48	0.45
2:G:2869:ARG:HH12	2:G:2945:UNK:C	2.30	0.45
2:G:3773:ARG:HG2	2:G:3815:LYS:HD3	1.99	0.45
2:I:4560:TYR:O	2:I:4564:PHE:N	2.43	0.45
2:I:4791:TYR:HD2	2:I:4792:LEU:HD22	1.82	0.45
2:I:4989:MET:O	2:I:4993:MET:N	2.42	0.45
2:B:1294:UNK:HA	2:B:1455:UNK:HA	1.99	0.44
2:B:4791:TYR:HD2	2:B:4792:LEU:HD22	1.82	0.44
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.98	0.44
1:F:29:MET:HB3	1:F:98:ILE:HB	1.99	0.44
2:G:4885:PHE:HE2	2:G:4901:ILE:HD11	1.82	0.44
2:G:4961:CYS:SG	2:G:4978:HIS:NE2	2.90	0.44
2:I:2286:LEU:HA	2:I:2289:ALA:HB3	1.99	0.44
2:I:4853:VAL:HA	2:I:4856:PHE:HB3	1.98	0.44
2:B:3765:TYR:O	2:B:3769:ARG:N	2.48	0.44
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4705:VAL:HB	2:E:4778:TRP:CG	2.52	0.44
2:E:5012:LYS:O	2:E:5016:GLU:N	2.43	0.44
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	1.98	0.44
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.99	0.44
2:I:1497:UNK:HA	2:I:1535:UNK:HA	1.98	0.44
2:I:4885:PHE:HE2	2:I:4901:ILE:HD11	1.82	0.44
2:B:1229:ASN:O	2:B:1827:ARG:N	2.43	0.44
2:E:59:PRO:HG3	2:E:307:ALA:HB3	1.99	0.44
2:E:233:ILE:HD12	2:E:242:ARG:HB3	1.99	0.44
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.99	0.44
2:G:78:LEU:O	2:G:82:LEU:N	2.49	0.44
2:G:379:HIS:CD2	2:G:382:GLY:H	2.33	0.44
2:G:978:THR:HB	2:G:980:ALA:H	1.83	0.44
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.50	0.44
2:I:164:ARG:N	2:I:167:ASP:OD2	2.48	0.44
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.83	0.44
2:B:59:PRO:HG3	2:B:307:ALA:HB3	1.99	0.44
2:B:233:ILE:HD12	2:B:242:ARG:HB3	1.99	0.44
2:E:639:ASN:HD22	2:E:1635:THR:HA	1.83	0.44
2:G:1659:LEU:O	2:G:1663:HIS:N	2.44	0.44
2:G:2142:TYR:CG	2:G:2197:LEU:HD13	2.53	0.44
2:G:3649:ALA:O	2:G:3653:PHE:N	2.46	0.44
2:G:4237:PHE:O	2:G:4241:THR:OG1	2.22	0.44
2:I:59:PRO:HG3	2:I:307:ALA:HB3	2.00	0.44
2:I:4705:VAL:HB	2:I:4778:TRP:CG	2.52	0.44
1:A:29:MET:HB3	1:A:98:ILE:HB	1.99	0.44
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.83	0.44
2:B:3713:LYS:HG2	2:B:3715:LYS:H	1.83	0.44
2:B:4109:GLN:O	2:B:4113:SER:N	2.45	0.44
2:B:4885:PHE:HE2	2:B:4901:ILE:HD11	1.82	0.44
2:E:546:TRP:O	2:E:550:LYS:NZ	2.39	0.44
2:E:870:ILE:HD11	2:E:1049:TYR:CG	2.53	0.44
2:E:1817:GLU:O	2:E:1821:ASP:N	2.44	0.44
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.99	0.44
2:G:3927:GLN:O	2:G:3931:SER:N	2.45	0.44
2:G:5012:LYS:O	2:G:5016:GLU:N	2.43	0.44
2:I:357:LEU:HD21	2:I:376:ALA:HB1	1.99	0.44
2:I:1649:ASP:OD1	2:I:1650:ILE:N	2.51	0.44
2:I:3773:ARG:HG2	2:I:3815:LYS:HD3	2.00	0.44
2:B:639:ASN:HD22	2:B:1635:THR:HA	1.83	0.44
2:B:870:ILE:HD11	2:B:1049:TYR:CG	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1577:ALA:HB1	2:B:1584:ARG:HA	1.99	0.44
2:B:4705:VAL:HB	2:B:4778:TRP:CG	2.52	0.44
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.99	0.44
2:E:3773:ARG:HG2	2:E:3815:LYS:HD3	1.99	0.44
2:E:4782:VAL:O	2:E:4785:THR:OG1	2.34	0.44
2:E:4885:PHE:HE2	2:E:4901:ILE:HD11	1.82	0.44
2:E:4961:CYS:SG	2:E:4978:HIS:NE2	2.90	0.44
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.45	0.44
2:G:1991:THR:O	2:G:1995:THR:OG1	2.30	0.44
2:I:1516:UNK:N	2:I:1529:UNK:O	2.51	0.44
2:I:1577:ALA:HB1	2:I:1584:ARG:HA	1.99	0.44
2:I:3927:GLN:NE2	2:I:3988:ALA:O	2.47	0.44
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.99	0.44
2:E:3998:HIS:CE1	2:E:4054:ASN:HD21	2.36	0.44
2:G:180:LEU:HD22	2:G:200:TRP:NE1	2.32	0.44
2:G:639:ASN:HD22	2:G:1635:THR:HA	1.83	0.44
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.98	0.44
2:G:3880:PHE:O	2:G:3884:LEU:N	2.51	0.44
2:G:4702:ASP:HA	2:G:4778:TRP:HE1	1.83	0.44
2:I:639:ASN:HD22	2:I:1635:THR:HA	1.83	0.44
2:I:978:THR:HB	2:I:980:ALA:H	1.83	0.44
2:I:2142:TYR:CG	2:I:2197:LEU:HD13	2.53	0.44
2:B:732:SER:HB3	2:B:764:VAL:HA	1.99	0.44
2:E:316:PHE:HB3	2:E:346:CYS:HB3	2.00	0.44
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.50	0.44
2:E:4853:VAL:HA	2:E:4856:PHE:HB3	1.98	0.44
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.99	0.44
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.98	0.44
2:G:546:TRP:O	2:G:550:LYS:NZ	2.38	0.44
2:G:867:LEU:HD22	2:G:929:LEU:HD22	2.00	0.44
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.98	0.44
2:I:2758:PHE:O	2:I:2762:THR:N	2.47	0.44
2:B:17:ASP:HB2	2:B:98:HIS:CE1	2.53	0.44
2:B:180:LEU:HD22	2:B:200:TRP:NE1	2.32	0.44
2:B:2347:GLU:O	2:B:2351:ASN:N	2.43	0.44
2:E:865:PRO:O	2:E:869:ARG:N	2.49	0.44
2:E:1516:UNK:N	2:E:1529:UNK:O	2.51	0.44
2:G:663:TYR:HB2	2:G:808:TYR:HB3	2.00	0.44
2:G:1245:PHE:HE1	2:G:1600:LEU:HD23	1.83	0.44
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.83	0.44
1:H:29:MET:HB3	1:H:98:ILE:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:709:ASP:O	2:I:725:HIS:ND1	2.51	0.44
2:I:3713:LYS:HG2	2:I:3715:LYS:H	1.83	0.44
2:B:111:HIS:CD2	2:B:114:SER:H	2.26	0.43
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.83	0.43
2:E:663:TYR:HB2	2:E:808:TYR:HB3	2.00	0.43
2:E:829:TYR:HB3	2:E:1073:ARG:HH11	1.83	0.43
2:E:3880:PHE:O	2:E:3884:LEU:N	2.51	0.43
2:E:4109:GLN:O	2:E:4113:SER:N	2.45	0.43
2:G:59:PRO:HG3	2:G:307:ALA:HB3	2.00	0.43
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.83	0.43
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.99	0.43
2:I:1663:HIS:O	2:I:1667:LEU:N	2.50	0.43
2:B:316:PHE:HB3	2:B:346:CYS:HB3	2.00	0.43
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.99	0.43
2:B:867:LEU:HD22	2:B:929:LEU:HD22	2.00	0.43
2:B:1965:TYR:OH	2:B:2027:ILE:O	2.26	0.43
2:B:3880:PHE:O	2:B:3884:LEU:N	2.51	0.43
2:E:357:LEU:HD21	2:E:376:ALA:HB1	2.00	0.43
2:E:709:ASP:O	2:E:725:HIS:ND1	2.51	0.43
2:E:1245:PHE:HE1	2:E:1600:LEU:HD23	1.83	0.43
2:E:1649:ASP:OD1	2:E:1650:ILE:N	2.51	0.43
2:E:2142:TYR:CG	2:E:2197:LEU:HD13	2.53	0.43
2:E:2327:GLY:HA2	2:E:2330:ARG:HD3	2.00	0.43
2:G:357:LEU:HD21	2:G:376:ALA:HB1	1.99	0.43
2:G:1817:GLU:O	2:G:1821:ASP:N	2.44	0.43
2:G:3974:THR:HA	2:G:3977:GLN:HB2	2.00	0.43
2:G:4782:VAL:O	2:G:4785:THR:OG1	2.34	0.43
2:I:78:LEU:O	2:I:82:LEU:N	2.49	0.43
2:B:709:ASP:O	2:B:725:HIS:ND1	2.51	0.43
2:B:1991:THR:O	2:B:1995:THR:OG1	2.30	0.43
2:B:2142:TYR:CG	2:B:2197:LEU:HD13	2.53	0.43
2:B:2758:PHE:O	2:B:2762:THR:N	2.47	0.43
2:E:3974:THR:HA	2:E:3977:GLN:HB2	2.00	0.43
2:E:4745:LEU:O	2:E:4749:GLU:N	2.50	0.43
2:G:1663:HIS:O	2:G:1667:LEU:N	2.50	0.43
2:G:3758:MET:O	2:G:3762:ARG:NE	2.46	0.43
2:G:4989:MET:O	2:G:4993:MET:N	2.42	0.43
2:I:870:ILE:HD11	2:I:1049:TYR:CG	2.53	0.43
2:I:1077:ALA:HB3	2:I:1189:LEU:HD11	2.01	0.43
2:I:2207:VAL:HG13	2:I:2232:CYS:HB2	2.00	0.43
2:I:4697:VAL:O	2:I:4701:TRP:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:ARG:N	2:B:167:ASP:OD2	2.48	0.43
2:B:2361:PRO:HA	2:B:2364:PHE:HD2	1.83	0.43
2:E:978:THR:HB	2:E:980:ALA:H	1.83	0.43
2:G:1649:ASP:OD1	2:G:1650:ILE:N	2.51	0.43
2:G:2361:PRO:HA	2:G:2364:PHE:HD2	1.83	0.43
2:I:732:SER:HB3	2:I:764:VAL:HA	1.99	0.43
2:I:3676:ASP:N	2:I:3676:ASP:OD1	2.51	0.43
2:B:709:ASP:HA	2:B:725:HIS:H	1.84	0.43
2:B:1649:ASP:OD1	2:B:1650:ILE:N	2.51	0.43
2:B:1679:ASN:O	2:B:1683:HIS:ND1	2.38	0.43
2:B:2207:VAL:HG13	2:B:2232:CYS:HB2	2.00	0.43
2:B:3773:ARG:HG2	2:B:3815:LYS:HD3	1.99	0.43
2:B:3974:THR:HA	2:B:3977:GLN:HB2	2.00	0.43
2:B:3998:HIS:CE1	2:B:4054:ASN:HD21	2.36	0.43
2:E:180:LEU:HD22	2:E:200:TRP:NE1	2.32	0.43
2:E:867:LEU:HD22	2:E:929:LEU:HD22	2.00	0.43
2:E:1077:ALA:HB3	2:E:1189:LEU:HD11	2.01	0.43
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	1.99	0.43
2:I:709:ASP:HA	2:I:725:HIS:H	1.84	0.43
2:I:765:GLN:NE2	2:I:1522:UNK:O	2.51	0.43
2:I:1095:VAL:HA	2:I:1146:GLY:H	1.84	0.43
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.50	0.43
2:I:4957:LYS:HB3	2:I:4957:LYS:HE3	1.83	0.43
2:B:151:HIS:HB2	2:B:170:ILE:HB	2.01	0.43
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	2.01	0.43
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.51	0.43
2:B:4702:ASP:HA	2:B:4778:TRP:HE1	1.83	0.43
2:E:1092:PHE:O	2:E:1149:VAL:N	2.48	0.43
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.83	0.43
2:E:2144:ILE:H	2:E:2144:ILE:HG13	1.75	0.43
2:E:3713:LYS:HG2	2:E:3715:LYS:H	1.83	0.43
2:G:252:VAL:HA	2:G:255:HIS:CG	2.54	0.43
2:G:1095:VAL:HA	2:G:1146:GLY:H	1.84	0.43
2:G:4697:VAL:O	2:G:4701:TRP:N	2.49	0.43
2:I:634:GLN:HB3	1:J:34:LYS:HZ2	1.84	0.43
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.83	0.43
2:I:2361:PRO:HA	2:I:2364:PHE:HD2	1.83	0.43
2:I:3880:PHE:O	2:I:3884:LEU:N	2.51	0.43
2:I:4702:ASP:HA	2:I:4778:TRP:HE1	1.83	0.43
2:B:357:LEU:HD21	2:B:376:ALA:HB1	1.99	0.43
2:B:4745:LEU:O	2:B:4749:GLU:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:809:ALA:O	2:E:811:CYS:N	2.50	0.43
2:E:2207:VAL:HG13	2:E:2232:CYS:HB2	2.00	0.43
2:E:4702:ASP:HA	2:E:4778:TRP:HE1	1.83	0.43
2:G:316:PHE:HB3	2:G:346:CYS:HB3	2.00	0.43
2:I:546:TRP:O	2:I:550:LYS:NZ	2.38	0.43
2:B:79:GLN:HA	2:B:82:LEU:HB2	2.01	0.43
2:B:1077:ALA:HB3	2:B:1189:LEU:HD11	2.01	0.43
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.84	0.43
2:B:2869:ARG:HH12	2:B:2945:UNK:C	2.32	0.43
2:B:4934:GLY:O	2:B:4938:ASP:N	2.47	0.43
2:E:79:GLN:HA	2:E:82:LEU:HB2	2.01	0.43
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	2.01	0.43
2:E:3765:TYR:O	2:E:3769:ARG:N	2.48	0.43
2:G:685:GLY:N	2:G:780:VAL:O	2.39	0.43
2:G:709:ASP:O	2:G:725:HIS:ND1	2.51	0.43
2:G:829:TYR:HB3	2:G:1073:ARG:HH11	1.84	0.43
2:G:1077:ALA:HB3	2:G:1189:LEU:HD11	2.01	0.43
2:G:1105:ALA:O	2:G:1189:LEU:N	2.52	0.43
2:G:1516:UNK:N	2:G:1529:UNK:O	2.51	0.43
2:G:3998:HIS:CE1	2:G:4054:ASN:HD21	2.36	0.43
2:I:401:ALA:HA	2:I:404:ILE:HD12	2.01	0.43
2:I:3974:THR:HA	2:I:3977:GLN:HB2	2.00	0.43
2:B:583:ILE:HA	2:B:586:ILE:HD12	2.01	0.43
2:B:1497:UNK:HA	2:B:1535:UNK:HA	2.01	0.43
2:B:2327:GLY:HA2	2:B:2330:ARG:HD3	2.00	0.43
2:B:3927:GLN:O	2:B:3931:SER:N	2.45	0.43
2:E:151:HIS:HB2	2:E:170:ILE:HB	2.00	0.43
2:E:583:ILE:HA	2:E:586:ILE:HD12	2.01	0.43
2:E:4857:ASN:HB2	2:G:4807:PHE:CE1	2.53	0.43
2:G:533:ASN:HB3	2:G:536:ASN:HB2	2.01	0.43
2:G:870:ILE:HD11	2:G:1049:TYR:CG	2.53	0.43
2:G:1866:ILE:HG13	2:G:1926:LEU:HB3	2.01	0.43
2:I:379:HIS:CD2	2:I:381:GLU:H	2.37	0.43
2:I:829:TYR:HB3	2:I:1073:ARG:HH11	1.84	0.43
2:I:867:LEU:HD22	2:I:929:LEU:HD22	2.00	0.43
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.84	0.43
2:I:1268:PRO:HB2	2:I:1591:CYS:HB2	2.01	0.43
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	2.00	0.43
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.84	0.43
2:B:663:TYR:HB2	2:B:808:TYR:HB3	2.00	0.43
2:B:1095:VAL:HA	2:B:1146:GLY:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3927:GLN:NE2	2:B:3988:ALA:O	2.48	0.43
2:E:2880:GLU:O	2:E:2884:ASN:N	2.45	0.43
2:G:709:ASP:HA	2:G:725:HIS:H	1.84	0.43
2:G:731:THR:OG1	2:G:1520:UNK:O	2.37	0.43
2:G:1149:VAL:HG22	2:G:1164:LEU:HD13	2.01	0.43
2:G:3713:LYS:HG2	2:G:3715:LYS:H	1.83	0.43
2:I:1046:LEU:HB3	2:I:1051:TYR:HB2	2.01	0.43
2:I:1092:PHE:O	2:I:1149:VAL:N	2.48	0.43
2:I:1777:PHE:HA	2:I:1799:SER:HB2	2.01	0.43
2:I:2021:CYS:HA	2:I:2022:PRO:HD3	1.91	0.43
2:I:2327:GLY:HA2	2:I:2330:ARG:HD3	2.00	0.43
2:E:2132:GLY:O	2:E:2136:ARG:N	2.50	0.42
2:E:4956:THR:O	2:E:4965:SER:N	2.42	0.42
2:E:5026:ASP:OD1	2:E:5027:CYS:N	2.52	0.42
2:G:176:SER:HB2	2:G:178:ARG:HH21	1.84	0.42
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.45	0.42
2:I:663:TYR:HB2	2:I:808:TYR:HB3	2.00	0.42
2:I:2185:ILE:HA	2:I:2188:ASN:ND2	2.34	0.42
2:I:3842:LEU:O	2:I:3929:SER:OG	2.37	0.42
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	2.01	0.42
2:I:4791:TYR:OH	2:I:4815:ASP:HB2	2.19	0.42
2:B:379:HIS:CD2	2:B:381:GLU:H	2.37	0.42
2:B:684:VAL:HA	2:B:781:VAL:HA	2.01	0.42
2:B:978:THR:HB	2:B:980:ALA:H	1.83	0.42
2:B:4208:PRO:HA	2:B:4211:LYS:HB3	2.02	0.42
2:E:17:ASP:HB2	2:E:98:HIS:CE1	2.53	0.42
2:E:401:ALA:HA	2:E:404:ILE:HD12	2.01	0.42
2:G:809:ALA:O	2:G:811:CYS:N	2.50	0.42
2:G:932:LEU:HD23	2:G:935:LEU:HD12	2.02	0.42
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	2.01	0.42
2:G:3663:LEU:H	2:G:3663:LEU:HG	1.64	0.42
2:G:4208:PRO:HA	2:G:4211:LYS:HB3	2.01	0.42
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.84	0.42
2:I:176:SER:HB2	2:I:178:ARG:HH21	1.84	0.42
2:I:731:THR:OG1	2:I:1519:UNK:O	2.28	0.42
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	2.01	0.42
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	2.01	0.42
2:B:1268:PRO:HB2	2:B:1591:CYS:HB2	2.01	0.42
2:E:932:LEU:HD23	2:E:935:LEU:HD12	2.02	0.42
2:E:1095:VAL:HA	2:E:1146:GLY:H	1.84	0.42
2:E:1663:HIS:O	2:E:1667:LEU:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1777:PHE:HA	2:G:1799:SER:HB2	2.01	0.42
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.51	0.42
2:I:316:PHE:HB3	2:I:346:CYS:HB3	2.00	0.42
2:I:684:VAL:HA	2:I:781:VAL:HA	2.01	0.42
2:I:4237:PHE:O	2:I:4241:THR:OG1	2.22	0.42
2:I:4934:GLY:O	2:I:4938:ASP:N	2.47	0.42
1:A:91:ILE:HD12	1:A:97:LEU:HD11	2.02	0.42
2:B:252:VAL:HA	2:B:255:HIS:CG	2.54	0.42
2:B:3842:LEU:O	2:B:3929:SER:OG	2.37	0.42
2:B:4791:TYR:OH	2:B:4815:ASP:HB2	2.19	0.42
2:E:252:VAL:HA	2:E:255:HIS:CG	2.54	0.42
2:E:315:CYS:SG	2:E:316:PHE:N	2.93	0.42
2:E:1149:VAL:HG22	2:E:1164:LEU:HD13	2.01	0.42
2:E:2361:PRO:HA	2:E:2364:PHE:HD2	1.83	0.42
2:E:4928:LEU:HA	2:E:4931:ILE:HD12	2.01	0.42
2:G:79:GLN:HA	2:G:82:LEU:HB2	2.01	0.42
2:G:379:HIS:CD2	2:G:381:GLU:H	2.37	0.42
2:G:583:ILE:HA	2:G:586:ILE:HD12	2.01	0.42
2:G:2265:LEU:HD22	2:G:2330:ARG:HB3	2.01	0.42
2:G:2327:GLY:HA2	2:G:2330:ARG:HD3	2.00	0.42
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	2.01	0.42
2:G:3927:GLN:NE2	2:G:3988:ALA:O	2.48	0.42
2:I:426:ARG:HG2	2:I:431:PRO:HA	2.02	0.42
2:I:3765:TYR:O	2:I:3769:ARG:N	2.48	0.42
2:I:4208:PRO:HA	2:I:4211:LYS:HB3	2.01	0.42
2:I:4945:ASP:HA	2:I:4948:GLU:HB2	2.02	0.42
2:B:176:SER:HB2	2:B:178:ARG:HH21	1.84	0.42
2:B:876:GLU:O	2:B:880:GLU:N	2.48	0.42
2:B:1105:ALA:O	2:B:1189:LEU:N	2.52	0.42
2:B:4945:ASP:HA	2:B:4948:GLU:HB2	2.02	0.42
2:B:5026:ASP:OD1	2:B:5027:CYS:N	2.52	0.42
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.84	0.42
2:E:3840:SER:OG	2:E:3875:MET:O	2.30	0.42
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.84	0.42
2:G:627:PRO:HB2	1:H:92:PRO:HD3	2.02	0.42
2:G:684:VAL:HA	2:G:781:VAL:HA	2.01	0.42
2:G:1268:PRO:HB2	2:G:1591:CYS:HB2	2.01	0.42
2:G:2207:VAL:HG13	2:G:2232:CYS:HB2	2.00	0.42
2:G:3842:LEU:O	2:G:3929:SER:OG	2.38	0.42
2:G:4051:SER:HG	2:G:4054:ASN:HB2	1.83	0.42
2:G:4568:PHE:HA	2:G:4571:PHE:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:79:GLN:HA	2:I:82:LEU:HB2	2.01	0.42
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.84	0.42
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	2.01	0.42
2:I:3998:HIS:CE1	2:I:4054:ASN:HD21	2.36	0.42
2:B:1046:LEU:HB3	2:B:1051:TYR:HB2	2.01	0.42
2:B:1703:LEU:HD21	2:B:1830:VAL:HG13	2.01	0.42
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	2.01	0.42
2:B:1866:ILE:HG13	2:B:1926:LEU:HB3	2.01	0.42
2:E:426:ARG:HG2	2:E:431:PRO:HA	2.02	0.42
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.84	0.42
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	2.01	0.42
2:E:4208:PRO:HA	2:E:4211:LYS:HB3	2.01	0.42
2:G:426:ARG:HG2	2:G:431:PRO:HA	2.02	0.42
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.84	0.42
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	2.01	0.42
2:G:4063:ASP:HB3	2:G:4170:ILE:HG13	2.02	0.42
2:G:5026:ASP:OD1	2:G:5027:CYS:N	2.52	0.42
2:I:288:GLY:HA3	2:I:405:HIS:CE1	2.55	0.42
2:I:583:ILE:HA	2:I:586:ILE:HD12	2.01	0.42
2:I:3915:ILE:O	2:I:3919:THR:N	2.51	0.42
2:I:4051:SER:HG	2:I:4054:ASN:HB2	1.83	0.42
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.84	0.42
2:B:426:ARG:HG2	2:B:431:PRO:HA	2.02	0.42
2:B:533:ASN:HB3	2:B:536:ASN:HB2	2.01	0.42
2:B:1092:PHE:O	2:B:1149:VAL:N	2.48	0.42
2:B:2185:ILE:HA	2:B:2188:ASN:ND2	2.34	0.42
2:B:2265:LEU:HD22	2:B:2330:ARG:HB3	2.01	0.42
2:E:684:VAL:HA	2:E:781:VAL:HA	2.01	0.42
2:E:3842:LEU:O	2:E:3929:SER:OG	2.37	0.42
1:F:91:ILE:HD12	1:F:97:LEU:HD11	2.02	0.42
2:G:488:LEU:HA	2:G:491:ILE:HB	2.02	0.42
2:G:2185:ILE:HA	2:G:2188:ASN:ND2	2.34	0.42
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	2.01	0.42
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	2.02	0.42
2:I:533:ASN:HB3	2:I:536:ASN:HB2	2.01	0.42
2:I:1105:ALA:O	2:I:1189:LEU:N	2.52	0.42
2:I:1970:GLN:HB2	2:I:3642:TYR:HA	2.01	0.42
2:B:317:ARG:N	2:B:347:PHE:O	2.52	0.42
2:B:1149:VAL:HG22	2:B:1164:LEU:HD13	2.01	0.42
2:E:379:HIS:CD2	2:E:381:GLU:H	2.37	0.42
2:E:2265:LEU:HD22	2:E:2330:ARG:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3649:ALA:O	2:E:3653:PHE:N	2.46	0.42
2:E:3676:ASP:OD1	2:E:3676:ASP:N	2.51	0.42
2:E:4051:SER:HG	2:E:4054:ASN:HB2	1.83	0.42
2:G:315:CYS:SG	2:G:316:PHE:N	2.93	0.42
2:G:4928:LEU:HA	2:G:4931:ILE:HD12	2.01	0.42
2:I:278:GLN:N	2:I:315:CYS:SG	2.90	0.42
2:I:932:LEU:HD23	2:I:935:LEU:HD12	2.02	0.42
2:I:1245:PHE:HE1	2:I:1600:LEU:HD23	1.83	0.42
2:I:1951:LEU:HD13	2:I:2126:ARG:HH21	1.85	0.42
2:B:932:LEU:HD23	2:B:935:LEU:HD12	2.02	0.42
2:B:1245:PHE:HE1	2:B:1600:LEU:HD23	1.83	0.42
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	2.01	0.42
2:E:709:ASP:HA	2:E:725:HIS:H	1.83	0.42
2:E:1777:PHE:HA	2:E:1799:SER:HB2	2.01	0.42
2:E:1970:GLN:HB2	2:E:3642:TYR:HA	2.01	0.42
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	2.02	0.42
2:G:401:ALA:HA	2:G:404:ILE:HD12	2.01	0.42
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.84	0.42
2:G:4942:GLU:O	2:G:4946:GLN:N	2.44	0.42
2:I:151:HIS:HB2	2:I:170:ILE:HB	2.01	0.42
2:I:634:GLN:HB3	1:J:34:LYS:NZ	2.35	0.42
2:I:809:ALA:O	2:I:811:CYS:N	2.50	0.42
2:I:2265:LEU:HD22	2:I:2330:ARG:HB3	2.01	0.42
2:I:4182:GLU:HA	2:I:4192:ARG:HA	2.02	0.42
2:I:4568:PHE:HA	2:I:4571:PHE:HD2	1.85	0.42
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	2.02	0.42
2:B:313:SER:HB2	2:B:350:HIS:CE1	2.55	0.42
2:B:315:CYS:SG	2:B:316:PHE:N	2.93	0.42
2:B:401:ALA:HA	2:B:404:ILE:HD12	2.01	0.42
2:E:176:SER:HB2	2:E:178:ARG:HH21	1.84	0.42
2:E:288:GLY:HA3	2:E:405:HIS:CE1	2.55	0.42
2:E:2185:ILE:HA	2:E:2188:ASN:ND2	2.34	0.42
2:G:151:HIS:HB2	2:G:170:ILE:HB	2.01	0.42
2:G:288:GLY:HA3	2:G:405:HIS:CE1	2.55	0.42
2:G:2829:GLY:HA3	2:G:2933:ASN:H	1.85	0.42
2:G:2880:GLU:O	2:G:2884:ASN:N	2.45	0.42
2:I:17:ASP:HB2	2:I:98:HIS:CE1	2.53	0.42
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	2.01	0.42
2:I:3927:GLN:O	2:I:3931:SER:N	2.45	0.42
2:B:204:PRO:HG2	2:B:268:SER:HB3	2.02	0.41
2:B:947:GLU:HG3	2:B:1049:TYR:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	2.02	0.41
2:E:317:ARG:N	2:E:347:PHE:O	2.52	0.41
2:E:1268:PRO:HB2	2:E:1591:CYS:HB2	2.01	0.41
2:E:1693:GLN:HA	2:E:1696:HIS:HB3	2.02	0.41
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	2.00	0.41
2:E:4945:ASP:HA	2:E:4948:GLU:HB2	2.02	0.41
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	2.02	0.41
2:G:3932:ASP:HA	2:G:3935:TRP:HD1	1.85	0.41
2:I:252:VAL:HA	2:I:255:HIS:CG	2.54	0.41
2:I:313:SER:HB2	2:I:350:HIS:CE1	2.55	0.41
2:I:947:GLU:HG3	2:I:1049:TYR:HD1	1.85	0.41
2:E:1866:ILE:HG13	2:E:1926:LEU:HB3	2.01	0.41
2:E:2869:ARG:HH12	2:E:2945:UNK:C	2.33	0.41
2:E:4942:GLU:O	2:E:4946:GLN:N	2.43	0.41
2:G:1046:LEU:HB3	2:G:1051:TYR:HB2	2.01	0.41
2:G:1693:GLN:HA	2:G:1696:HIS:HB3	2.02	0.41
2:G:4791:TYR:OH	2:G:4815:ASP:HB2	2.19	0.41
2:G:4945:ASP:HA	2:G:4948:GLU:HB2	2.02	0.41
2:I:204:PRO:HG2	2:I:268:SER:HB3	2.02	0.41
2:I:350:HIS:CG	2:I:353:SER:HG	2.38	0.41
2:I:1866:ILE:HG13	2:I:1926:LEU:HB3	2.01	0.41
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	2.03	0.41
2:B:288:GLY:HA3	2:B:405:HIS:CE1	2.55	0.41
2:B:4182:GLU:HA	2:B:4192:ARG:HA	2.02	0.41
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.84	0.41
2:E:1046:LEU:HB3	2:E:1051:TYR:HB2	2.01	0.41
2:E:1105:ALA:O	2:E:1189:LEU:N	2.52	0.41
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	2.02	0.41
2:E:4568:PHE:HA	2:E:4571:PHE:HD2	1.85	0.41
2:E:4989:MET:O	2:E:4993:MET:N	2.42	0.41
2:G:317:ARG:N	2:G:347:PHE:O	2.52	0.41
2:G:1703:LEU:HD21	2:G:1830:VAL:HG13	2.01	0.41
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	2.02	0.41
2:G:2336:ARG:NH2	2:G:2428:ALA:O	2.49	0.41
2:G:4176:PRO:O	2:G:4202:ARG:NH1	2.54	0.41
2:I:1708:ARG:HG2	2:I:1711:TYR:CE2	2.56	0.41
1:A:55:VAL:HG23	1:A:60:GLU:HB2	2.03	0.41
2:B:668:VAL:HG22	2:B:789:VAL:HG23	2.03	0.41
2:B:790:ARG:HG2	2:B:1627:ALA:HA	2.01	0.41
2:B:3662:ILE:H	2:B:3662:ILE:HG13	1.71	0.41
2:E:204:PRO:HG2	2:E:268:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2829:GLY:HA3	2:E:2933:ASN:H	1.85	0.41
2:E:3663:LEU:H	2:E:3663:LEU:HG	1.64	0.41
2:E:5013:MET:HA	2:E:5016:GLU:HB3	2.02	0.41
2:G:1951:LEU:HD13	2:G:2126:ARG:HH21	1.85	0.41
2:I:1149:VAL:HG22	2:I:1164:LEU:HD13	2.01	0.41
2:I:1679:ASN:O	2:I:1683:HIS:ND1	2.38	0.41
2:I:2874:MET:HA	2:I:2877:GLN:HB3	2.03	0.41
2:B:1951:LEU:HD13	2:B:2126:ARG:HH21	1.85	0.41
2:B:4568:PHE:HA	2:B:4571:PHE:HD2	1.85	0.41
2:B:4928:LEU:HA	2:B:4931:ILE:HD12	2.01	0.41
2:E:790:ARG:HG2	2:E:1627:ALA:HA	2.01	0.41
2:E:1703:LEU:HD21	2:E:1830:VAL:HG13	2.01	0.41
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	2.01	0.41
2:E:4791:TYR:OH	2:E:4815:ASP:HB2	2.19	0.41
2:G:17:ASP:HB2	2:G:98:HIS:CE1	2.53	0.41
2:G:204:PRO:HG2	2:G:268:SER:HB3	2.02	0.41
2:G:290:TYR:O	2:G:302:VAL:N	2.53	0.41
2:G:790:ARG:HG2	2:G:1627:ALA:HA	2.01	0.41
2:G:1694:LEU:O	2:G:1712:TYR:OH	2.27	0.41
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	2.02	0.41
2:G:4182:GLU:HA	2:G:4192:ARG:HA	2.02	0.41
2:I:315:CYS:SG	2:I:316:PHE:N	2.93	0.41
2:I:488:LEU:HA	2:I:491:ILE:HB	2.02	0.41
2:I:668:VAL:HG22	2:I:789:VAL:HG23	2.03	0.41
2:I:1703:LEU:HD21	2:I:1830:VAL:HG13	2.01	0.41
2:I:4928:LEU:HA	2:I:4931:ILE:HD12	2.01	0.41
1:J:91:ILE:HD12	1:J:97:LEU:HD11	2.02	0.41
2:B:404:ILE:HG21	2:B:481:GLU:HG3	2.03	0.41
2:B:792:LEU:HD22	2:B:799:GLU:H	1.85	0.41
2:B:809:ALA:O	2:B:811:CYS:N	2.50	0.41
2:B:829:TYR:HB3	2:B:1073:ARG:HH11	1.84	0.41
2:B:1777:PHE:HA	2:B:1799:SER:HB2	2.01	0.41
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	2.02	0.41
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	2.01	0.41
2:E:385:ASP:N	2:E:385:ASP:OD1	2.54	0.41
2:E:3927:GLN:NE2	2:E:3988:ALA:O	2.47	0.41
2:E:4182:GLU:HA	2:E:4192:ARG:HA	2.02	0.41
2:G:530:ILE:HA	2:G:536:ASN:HB3	2.02	0.41
2:G:1970:GLN:HB2	2:G:3642:TYR:HA	2.01	0.41
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	2.03	0.41
1:J:55:VAL:HG23	1:J:60:GLU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:PRO:HD3	2:B:627:PRO:HB2	2.02	0.41
2:B:42:PHE:HD1	2:B:447:ASP:HB3	1.86	0.41
2:B:2874:MET:HA	2:B:2877:GLN:HB3	2.03	0.41
2:E:947:GLU:HG3	2:E:1049:TYR:HD1	1.85	0.41
2:E:3932:ASP:HA	2:E:3935:TRP:HD1	1.85	0.41
1:F:55:VAL:HG23	1:F:60:GLU:HB2	2.03	0.41
2:G:313:SER:HB2	2:G:350:HIS:CE1	2.55	0.41
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	2.02	0.41
2:I:3663:LEU:H	2:I:3663:LEU:HG	1.64	0.41
2:I:4745:LEU:O	2:I:4749:GLU:N	2.50	0.41
2:I:5026:ASP:OD1	2:I:5027:CYS:N	2.52	0.41
2:B:218:HIS:HB3	2:B:392:ARG:HD3	2.03	0.41
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	2.03	0.41
2:B:2032:GLN:O	2:B:2036:GLN:N	2.49	0.41
2:B:4176:PRO:O	2:B:4202:ARG:NH1	2.54	0.41
2:B:5013:MET:HA	2:B:5016:GLU:HB3	2.02	0.41
2:E:313:SER:HB2	2:E:350:HIS:CE1	2.55	0.41
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.45	0.41
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.56	0.41
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	2.02	0.41
2:E:3758:MET:O	2:E:3762:ARG:NE	2.46	0.41
2:E:4710:SER:OG	2:E:4772:ASP:OD2	2.31	0.41
2:G:4843:LEU:HA	2:G:4846:VAL:HG12	2.03	0.41
1:H:91:ILE:HD12	1:H:97:LEU:HD11	2.02	0.41
2:I:218:HIS:HB3	2:I:392:ARG:HD3	2.03	0.41
2:I:988:LEU:O	2:I:992:GLY:N	2.47	0.41
2:B:290:TYR:O	2:B:302:VAL:N	2.53	0.41
2:B:530:ILE:HA	2:B:536:ASN:HB3	2.02	0.41
2:B:688:LEU:HB3	2:B:777:PHE:CE1	2.56	0.41
2:B:1189:LEU:HD12	2:B:1190:PRO:HD2	2.03	0.41
2:B:1694:LEU:HD23	2:B:1715:LEU:HD13	2.03	0.41
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.56	0.41
2:B:1721:GLU:O	2:B:1725:ARG:NH2	2.54	0.41
2:B:2437:ALA:HA	2:B:2438:PRO:HD3	1.94	0.41
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	2.02	0.41
2:B:3932:ASP:HA	2:B:3935:TRP:HD1	1.85	0.41
2:E:42:PHE:HD1	2:E:447:ASP:HB3	1.86	0.41
2:E:290:TYR:O	2:E:302:VAL:N	2.53	0.41
2:E:379:HIS:NE2	2:E:381:GLU:OE1	2.54	0.41
2:E:392:ARG:HH12	2:E:398:SER:HB2	1.86	0.41
2:E:488:LEU:HA	2:E:491:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:533:ASN:HB3	2:E:536:ASN:HB2	2.01	0.41
2:E:1679:ASN:O	2:E:1683:HIS:ND1	2.38	0.41
2:E:1965:TYR:OH	2:E:2027:ILE:O	2.26	0.41
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	2.03	0.41
2:E:2255:SER:HA	2:E:2258:LEU:HB3	2.03	0.41
2:E:2874:MET:HA	2:E:2877:GLN:HB3	2.03	0.41
2:E:4176:PRO:O	2:E:4202:ARG:NH1	2.54	0.41
2:E:4833:ASN:HD22	2:E:4936:ILE:HD13	1.86	0.41
2:G:218:HIS:HB3	2:G:392:ARG:HD3	2.03	0.41
2:G:379:HIS:NE2	2:G:381:GLU:OE1	2.54	0.41
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.45	0.41
2:G:668:VAL:HG22	2:G:789:VAL:HG23	2.03	0.41
2:G:876:GLU:O	2:G:880:GLU:N	2.48	0.41
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.56	0.41
2:G:1721:GLU:O	2:G:1725:ARG:NH2	2.54	0.41
2:G:3920:VAL:O	2:G:3924:LEU:N	2.44	0.41
2:G:3994:HIS:O	2:G:3998:HIS:ND1	2.39	0.41
2:G:5013:MET:HA	2:G:5016:GLU:HB3	2.02	0.41
1:H:55:VAL:HG23	1:H:60:GLU:HB2	2.03	0.41
2:I:379:HIS:NE2	2:I:381:GLU:OE1	2.54	0.41
2:I:404:ILE:HG21	2:I:481:GLU:HG3	2.03	0.41
2:I:1739:THR:H	2:I:1742:THR:HB	1.86	0.41
2:I:3901:ASN:OD1	2:I:3904:ARG:NH1	2.43	0.41
2:I:3932:ASP:HA	2:I:3935:TRP:HD1	1.85	0.41
2:I:4558:ASN:OD1	2:I:4558:ASN:N	2.52	0.41
2:B:758:ARG:NH2	2:B:803:LEU:O	2.54	0.41
2:B:2318:TYR:HA	2:B:2319:PRO:HD3	1.89	0.41
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.54	0.41
2:E:792:LEU:HD22	2:E:799:GLU:H	1.85	0.41
2:E:3901:ASN:OD1	2:E:3904:ARG:NH1	2.43	0.41
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.54	0.41
2:G:792:LEU:HD22	2:G:799:GLU:H	1.85	0.41
2:G:3953:LYS:O	2:G:3956:SER:OG	2.32	0.41
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.54	0.41
2:G:4833:ASN:HD21	2:G:4939:ALA:HB2	1.86	0.41
2:G:4934:GLY:O	2:G:4938:ASP:N	2.48	0.41
2:I:42:PHE:HD1	2:I:447:ASP:HB3	1.86	0.41
2:I:758:ARG:NH2	2:I:803:LEU:O	2.54	0.41
2:I:2336:ARG:NH2	2:I:2428:ALA:O	2.49	0.41
2:I:2829:GLY:HA3	2:I:2933:ASN:H	1.85	0.41
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4971:THR:HG21	2:I:5029:ARG:HH12	1.86	0.41
2:I:5013:MET:HA	2:I:5016:GLU:HB3	2.02	0.41
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	2.03	0.40
2:B:4989:MET:O	2:B:4993:MET:N	2.42	0.40
2:E:241:GLN:O	2:E:289:ARG:NH1	2.49	0.40
2:E:758:ARG:NH2	2:E:803:LEU:O	2.54	0.40
2:E:1721:GLU:O	2:E:1725:ARG:NH2	2.54	0.40
2:E:1950:GLU:OE2	2:E:1954:ARG:NH2	2.54	0.40
2:E:1951:LEU:HD13	2:E:2126:ARG:HH21	1.85	0.40
2:G:42:PHE:HD1	2:G:447:ASP:HB3	1.86	0.40
2:G:1497:UNK:HA	2:G:1535:UNK:HA	2.03	0.40
2:I:290:TYR:O	2:I:302:VAL:N	2.53	0.40
2:I:545:ASP:HA	2:I:582:HIS:CE1	2.56	0.40
2:I:688:LEU:HB3	2:I:777:PHE:CE1	2.56	0.40
2:I:2039:LEU:HA	2:I:2042:CYS:HB3	2.03	0.40
2:I:4097:MET:HB3	2:I:4108:ILE:HG12	2.03	0.40
2:B:392:ARG:HH12	2:B:398:SER:HB2	1.86	0.40
2:E:218:HIS:HB3	2:E:392:ARG:HD3	2.03	0.40
2:E:688:LEU:HB3	2:E:777:PHE:CE1	2.56	0.40
2:E:2758:PHE:O	2:E:2762:THR:N	2.47	0.40
2:E:4833:ASN:HD21	2:E:4939:ALA:HB2	1.87	0.40
2:G:545:ASP:HA	2:G:582:HIS:CE1	2.56	0.40
2:G:758:ARG:NH2	2:G:803:LEU:O	2.54	0.40
2:G:1071:ARG:HD3	2:G:1241:SER:HB3	2.03	0.40
2:I:317:ARG:N	2:I:347:PHE:O	2.52	0.40
2:I:385:ASP:OD1	2:I:385:ASP:N	2.54	0.40
2:I:1694:LEU:HD23	2:I:1715:LEU:HD13	2.03	0.40
2:I:1950:GLU:OE2	2:I:1954:ARG:NH2	2.54	0.40
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.55	0.40
2:B:78:LEU:O	2:B:82:LEU:N	2.49	0.40
2:B:1663:HIS:O	2:B:1667:LEU:N	2.50	0.40
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.86	0.40
2:B:2587:UNK:O	2:B:2591:UNK:N	2.55	0.40
2:E:404:ILE:HG21	2:E:481:GLU:HG3	2.03	0.40
2:E:2336:ARG:NH2	2:E:2428:ALA:O	2.49	0.40
2:E:4971:THR:HG21	2:E:5029:ARG:HH12	1.86	0.40
2:G:688:LEU:HB3	2:G:777:PHE:CE1	2.56	0.40
2:G:947:GLU:HG3	2:G:1049:TYR:HD1	1.85	0.40
2:G:3765:TYR:O	2:G:3769:ARG:N	2.48	0.40
2:G:4826:ILE:O	2:G:4829:SER:OG	2.33	0.40
2:G:4833:ASN:HD22	2:G:4936:ILE:HD13	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:790:ARG:HG2	2:I:1627:ALA:HA	2.02	0.40
2:I:2144:ILE:H	2:I:2144:ILE:HG13	1.76	0.40
2:I:4176:PRO:O	2:I:4202:ARG:NH1	2.54	0.40
2:I:4833:ASN:HD21	2:I:4939:ALA:HB2	1.86	0.40
2:B:379:HIS:NE2	2:B:381:GLU:OE1	2.54	0.40
2:B:1693:GLN:HA	2:B:1696:HIS:HB3	2.02	0.40
2:B:3229:UNK:HA	2:B:3302:UNK:HA	2.03	0.40
2:B:4192:ARG:HH12	2:B:4982:GLU:HG2	1.87	0.40
2:E:530:ILE:HA	2:E:536:ASN:HB3	2.02	0.40
2:E:668:VAL:HG22	2:E:789:VAL:HG23	2.03	0.40
2:E:2039:LEU:HA	2:E:2042:CYS:HB3	2.04	0.40
2:E:2212:VAL:O	2:E:2216:GLY:N	2.53	0.40
2:G:404:ILE:HG21	2:G:481:GLU:HG3	2.03	0.40
2:G:2255:SER:HA	2:G:2258:LEU:HB3	2.03	0.40
2:G:2874:MET:HA	2:G:2877:GLN:HB3	2.03	0.40
2:G:3361:UNK:O	2:G:3365:UNK:N	2.55	0.40
2:G:3915:ILE:O	2:G:3919:THR:N	2.51	0.40
2:G:4192:ARG:HH12	2:G:4982:GLU:HG2	1.87	0.40
2:I:530:ILE:HA	2:I:536:ASN:HB3	2.02	0.40
2:I:792:LEU:HD22	2:I:799:GLU:H	1.85	0.40
2:I:1693:GLN:HA	2:I:1696:HIS:HB3	2.02	0.40
2:I:4833:ASN:HD22	2:I:4936:ILE:HD13	1.86	0.40
2:B:1829:PRO:HB2	2:B:1837:GLN:HB2	2.04	0.40
2:B:1970:GLN:HB2	2:B:3642:TYR:HA	2.01	0.40
2:B:3649:ALA:O	2:B:3653:PHE:N	2.46	0.40
2:E:176:SER:HB2	2:E:178:ARG:HD3	2.04	0.40
2:E:635:THR:O	1:F:34:LYS:NZ	2.51	0.40
2:E:870:ILE:HD12	2:E:870:ILE:HA	1.89	0.40
2:E:1189:LEU:HD12	2:E:1190:PRO:HD2	2.04	0.40
2:E:4978:HIS:ND1	2:E:4982:GLU:OE1	2.43	0.40
2:G:4971:THR:HG21	2:G:5029:ARG:HH12	1.86	0.40
2:I:392:ARG:HH12	2:I:398:SER:HB2	1.86	0.40
2:I:4782:VAL:O	2:I:4785:THR:OG1	2.34	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	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	H	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	J	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	B	3235/4687 (69%)	2862 (88%)	367 (11%)	6 (0%)	47	81
2	E	3235/4687 (69%)	2861 (88%)	367 (11%)	7 (0%)	47	81
2	G	3235/4687 (69%)	2863 (88%)	365 (11%)	7 (0%)	47	81
2	I	3235/4687 (69%)	2863 (88%)	365 (11%)	7 (0%)	47	81
All	All	13360/19180 (70%)	11833 (89%)	1500 (11%)	27 (0%)	50	81

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1829	PRO
2	B	1932	PRO
2	E	1829	PRO
2	G	1829	PRO
2	I	1829	PRO
2	B	1708	ARG
2	B	4667	PRO
2	E	1708	ARG
2	E	1932	PRO
2	E	4667	PRO
2	G	1708	ARG
2	G	1932	PRO
2	G	4667	PRO
2	I	1708	ARG
2	I	1932	PRO
2	I	4667	PRO
2	B	2343	GLY

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Mol	Chain	Res	Type
2	E	2343	GLY
2	I	2343	GLY
2	G	2343	GLY
2	B	4641	PRO
2	E	1840	PRO
2	E	4641	PRO
2	G	1840	PRO
2	G	4641	PRO
2	I	1840	PRO
2	I	4641	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3209 (78%)	2475 (99%)	18 (1%)	84	90
2	E	2493/3209 (78%)	2475 (99%)	18 (1%)	84	90
2	G	2493/3209 (78%)	2475 (99%)	18 (1%)	84	90
2	I	2493/3209 (78%)	2475 (99%)	18 (1%)	84	90
All	All	10324/13192 (78%)	10252 (99%)	72 (1%)	84	90

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	688	LEU
2	B	978	THR

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Mol	Chain	Res	Type
2	B	1076	ARG
2	B	1141	ARG
2	B	1964	ARG
2	B	3663	LEU
2	B	3762	ARG
2	B	3787	LYS
2	B	3805	LEU
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4957	LYS
2	B	4984	ASN
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	688	LEU
2	E	978	THR
2	E	1076	ARG
2	E	1141	ARG
2	E	1964	ARG
2	E	3663	LEU
2	E	3762	ARG
2	E	3787	LYS
2	E	3805	LEU
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4957	LYS
2	E	4984	ASN
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	688	LEU
2	G	978	THR
2	G	1076	ARG
2	G	1141	ARG
2	G	1964	ARG
2	G	3663	LEU
2	G	3762	ARG
2	G	3787	LYS

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Mol	Chain	Res	Type
2	G	3805	LEU
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4957	LYS
2	G	4984	ASN
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	688	LEU
2	I	978	THR
2	I	1076	ARG
2	I	1141	ARG
2	I	1964	ARG
2	I	3663	LEU
2	I	3762	ARG
2	I	3787	LYS
2	I	3805	LEU
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4957	LYS
2	I	4984	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (157) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	23	GLN
2	B	57	ASN
2	B	111	HIS
2	B	113	HIS
2	B	203	ASN
2	B	224	HIS
2	B	273	HIS
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	405	HIS
2	B	639	ASN
2	B	838	HIS

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Mol	Chain	Res	Type
2	B	1035	ASN
2	B	1158	ASN
2	B	1231	GLN
2	B	1598	GLN
2	B	1679	ASN
2	B	1691	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	2127	GLN
2	B	2858	GLN
2	B	3809	ASN
2	B	3882	GLN
2	B	3889	GLN
2	B	3896	ASN
2	B	3960	GLN
2	B	4034	ASN
2	B	4054	ASN
2	B	4120	ASN
2	B	4130	ASN
2	B	4142	ASN
2	B	4691	GLN
2	B	4833	ASN
2	B	4886	HIS
2	B	4984	ASN
2	B	4987	ASN
2	E	23	GLN
2	E	57	ASN
2	E	111	HIS
2	E	113	HIS
2	E	203	ASN
2	E	224	HIS
2	E	273	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	405	HIS
2	E	639	ASN
2	E	838	HIS
2	E	1035	ASN
2	E	1158	ASN
2	E	1231	GLN
2	E	1598	GLN

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Mol	Chain	Res	Type
2	E	1679	ASN
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	1973	GLN
2	E	2005	GLN
2	E	2127	GLN
2	E	2858	GLN
2	E	3809	ASN
2	E	3882	GLN
2	E	3889	GLN
2	E	3896	ASN
2	E	3960	GLN
2	E	4034	ASN
2	E	4054	ASN
2	E	4120	ASN
2	E	4130	ASN
2	E	4142	ASN
2	E	4691	GLN
2	E	4833	ASN
2	E	4886	HIS
2	E	4984	ASN
2	E	4987	ASN
2	G	23	GLN
2	G	57	ASN
2	G	111	HIS
2	G	113	HIS
2	G	203	ASN
2	G	224	HIS
2	G	273	HIS
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	405	HIS
2	G	639	ASN
2	G	838	HIS
2	G	1035	ASN
2	G	1158	ASN
2	G	1231	GLN
2	G	1598	GLN
2	G	1679	ASN
2	G	1691	GLN

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Mol	Chain	Res	Type
2	G	1719	HIS
2	G	1775	HIS
2	G	1973	GLN
2	G	2005	GLN
2	G	2127	GLN
2	G	2858	GLN
2	G	3809	ASN
2	G	3882	GLN
2	G	3889	GLN
2	G	3896	ASN
2	G	3960	GLN
2	G	4034	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4130	ASN
2	G	4142	ASN
2	G	4691	GLN
2	G	4833	ASN
2	G	4886	HIS
2	G	4984	ASN
2	G	4987	ASN
2	I	23	GLN
2	I	57	ASN
2	I	111	HIS
2	I	113	HIS
2	I	203	ASN
2	I	224	HIS
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	405	HIS
2	I	639	ASN
2	I	765	GLN
2	I	838	HIS
2	I	1035	ASN
2	I	1158	ASN
2	I	1231	GLN
2	I	1598	GLN
2	I	1679	ASN
2	I	1691	GLN
2	I	1719	HIS

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Mol	Chain	Res	Type
2	I	1775	HIS
2	I	2127	GLN
2	I	2858	GLN
2	I	3809	ASN
2	I	3882	GLN
2	I	3889	GLN
2	I	3896	ASN
2	I	3960	GLN
2	I	4034	ASN
2	I	4054	ASN
2	I	4120	ASN
2	I	4130	ASN
2	I	4142	ASN
2	I	4691	GLN
2	I	4833	ASN
2	I	4886	HIS
2	I	4984	ASN
2	I	4987	ASN

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	I	12
2	B	12
2	G	12
2	E	12

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	3613:UNK	C	3639:THR	N	43.91
1	B	3613:UNK	C	3639:THR	N	43.68
1	G	3613:UNK	C	3639:THR	N	43.62
1	E	3613:UNK	C	3639:THR	N	43.61
1	I	3163:UNK	C	3170:UNK	N	16.30
1	B	3163:UNK	C	3170:UNK	N	16.29
1	E	3163:UNK	C	3170:UNK	N	16.26
1	G	3163:UNK	C	3170:UNK	N	16.24
1	G	3468:UNK	C	3511:UNK	N	15.09
1	I	3468:UNK	C	3511:UNK	N	15.04
1	E	3468:UNK	C	3511:UNK	N	15.02
1	B	3468:UNK	C	3511:UNK	N	15.00
1	I	2703:UNK	C	2734:ASN	N	14.81
1	E	2703:UNK	C	2734:ASN	N	14.71
1	B	2703:UNK	C	2734:ASN	N	14.67
1	G	2703:UNK	C	2734:ASN	N	14.61
1	I	3063:UNK	C	3134:UNK	N	14.51
1	G	3063:UNK	C	3134:UNK	N	14.50
1	E	3063:UNK	C	3134:UNK	N	14.48
1	B	3063:UNK	C	3134:UNK	N	14.47
1	I	3236:UNK	C	3241:UNK	N	13.17
1	G	3236:UNK	C	3241:UNK	N	13.16
1	E	3236:UNK	C	3241:UNK	N	13.07

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3236:UNK	C	3241:UNK	N	13.05
1	B	1564:UNK	C	1573:MET	N	12.84
1	E	1564:UNK	C	1573:MET	N	12.81
1	I	1564:UNK	C	1573:MET	N	12.73
1	G	1564:UNK	C	1573:MET	N	12.72
1	B	2976:UNK	C	2995:UNK	N	12.10
1	E	2976:UNK	C	2995:UNK	N	12.09
1	G	2976:UNK	C	2995:UNK	N	12.09
1	I	2976:UNK	C	2995:UNK	N	12.07
1	G	3254:UNK	C	3261:UNK	N	8.66
1	E	3254:UNK	C	3261:UNK	N	8.62
1	I	3254:UNK	C	3261:UNK	N	8.62
1	B	3254:UNK	C	3261:UNK	N	8.56
1	B	1297:UNK	C	1430:UNK	N	5.73
1	G	1297:UNK	C	1430:UNK	N	5.70
1	E	1297:UNK	C	1430:UNK	N	5.67
1	I	1297:UNK	C	1430:UNK	N	5.44
1	B	2939:ARG	C	2942:UNK	N	3.59
1	I	2939:ARG	C	2942:UNK	N	3.56
1	G	2479:LEU	C	2487:UNK	N	3.55
1	I	2479:LEU	C	2487:UNK	N	3.55
1	E	2479:LEU	C	2487:UNK	N	3.47
1	G	2939:ARG	C	2942:UNK	N	3.46
1	B	2479:LEU	C	2487:UNK	N	3.45
1	E	2939:ARG	C	2942:UNK	N	3.34

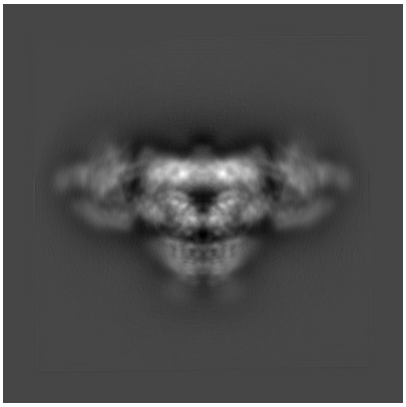
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22392. These allow visual inspection of the internal detail of the map and identification of artifacts.

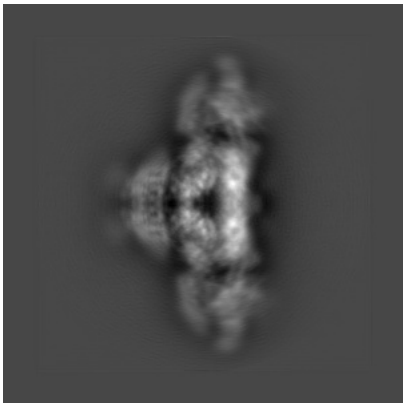
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

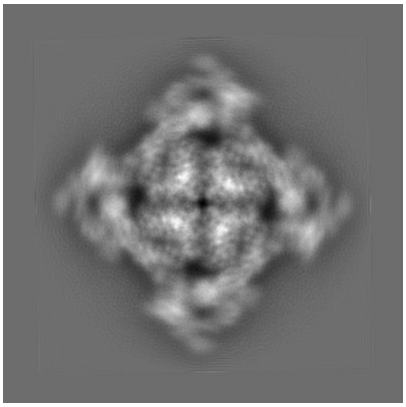
6.1.1 Primary map



X



Y

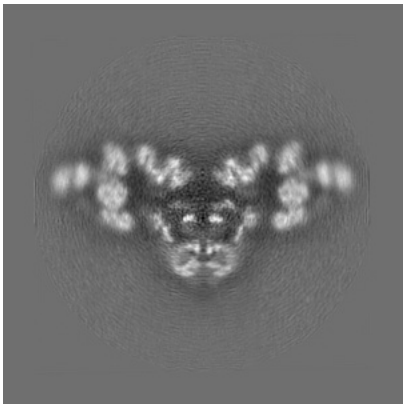


Z

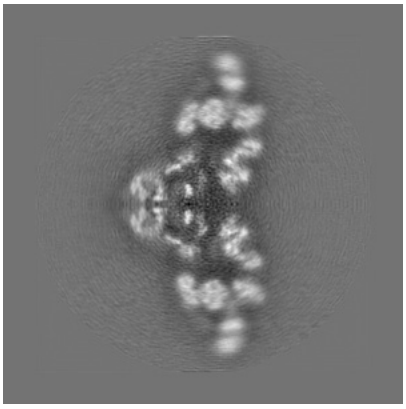
The images above show the map projected in three orthogonal directions.

6.2 Central slices

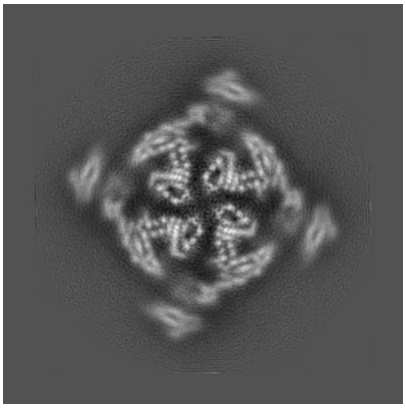
6.2.1 Primary map



X Index: 200



Y Index: 200

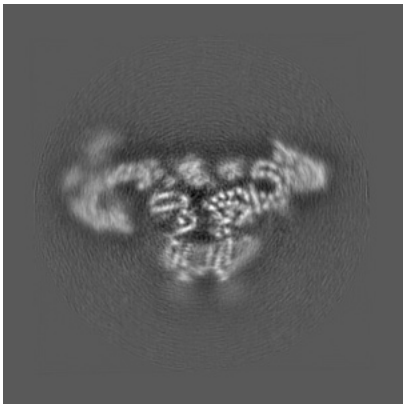


Z Index: 200

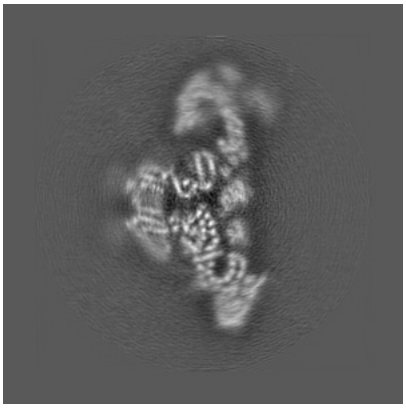
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

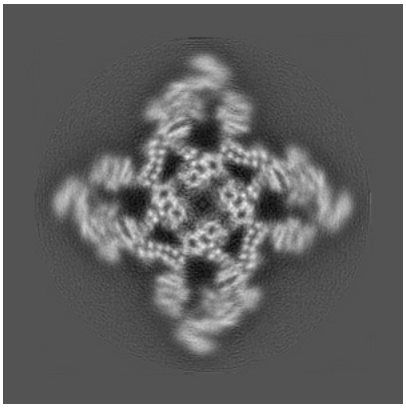
6.3.1 Primary map



X Index: 177



Y Index: 177



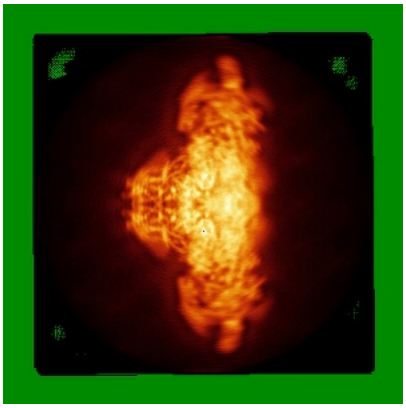
Z Index: 226

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

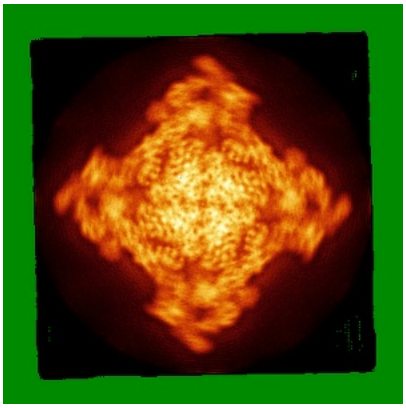
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

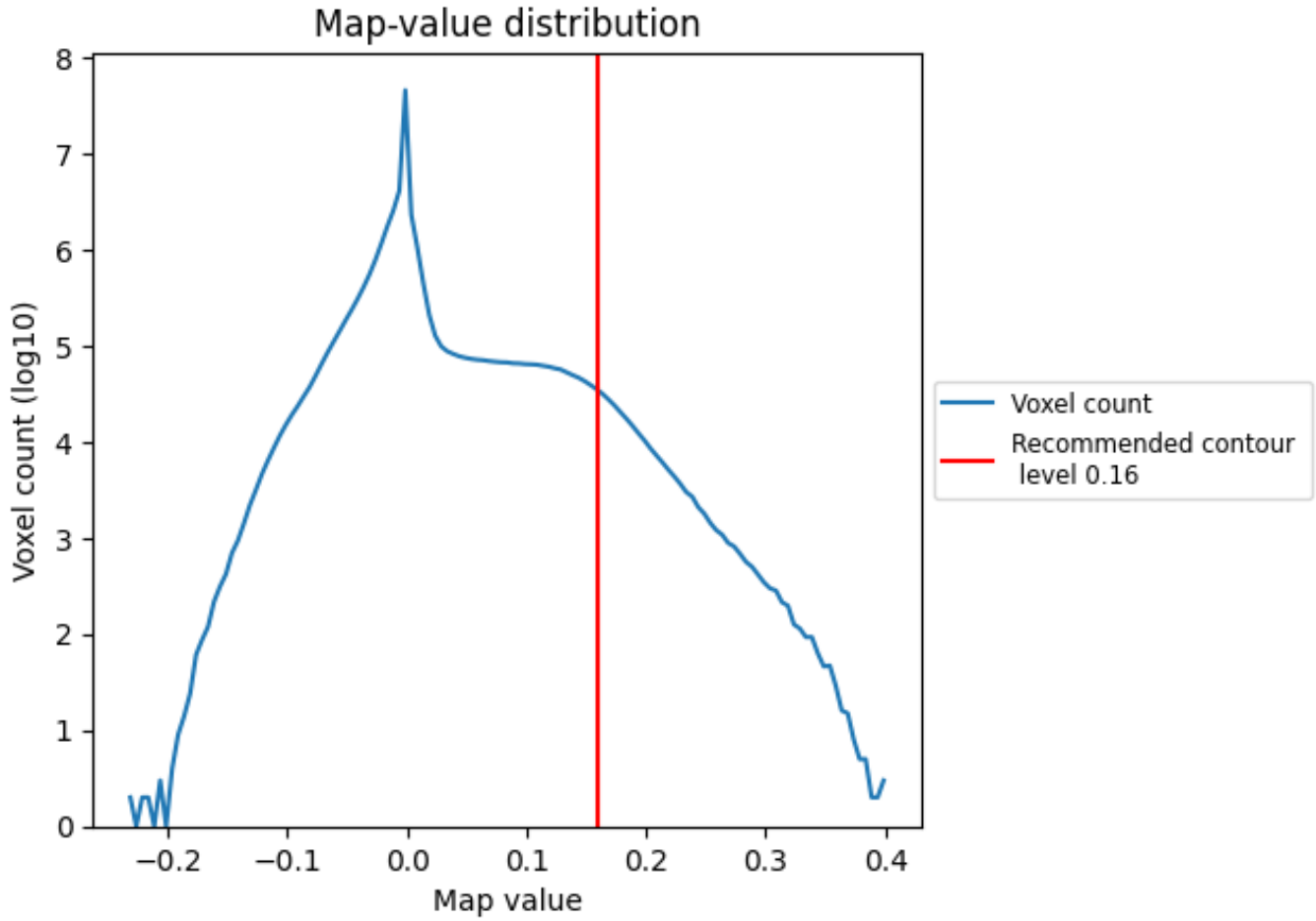
6.6 Mask visualisation (i)

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

7 Map analysis

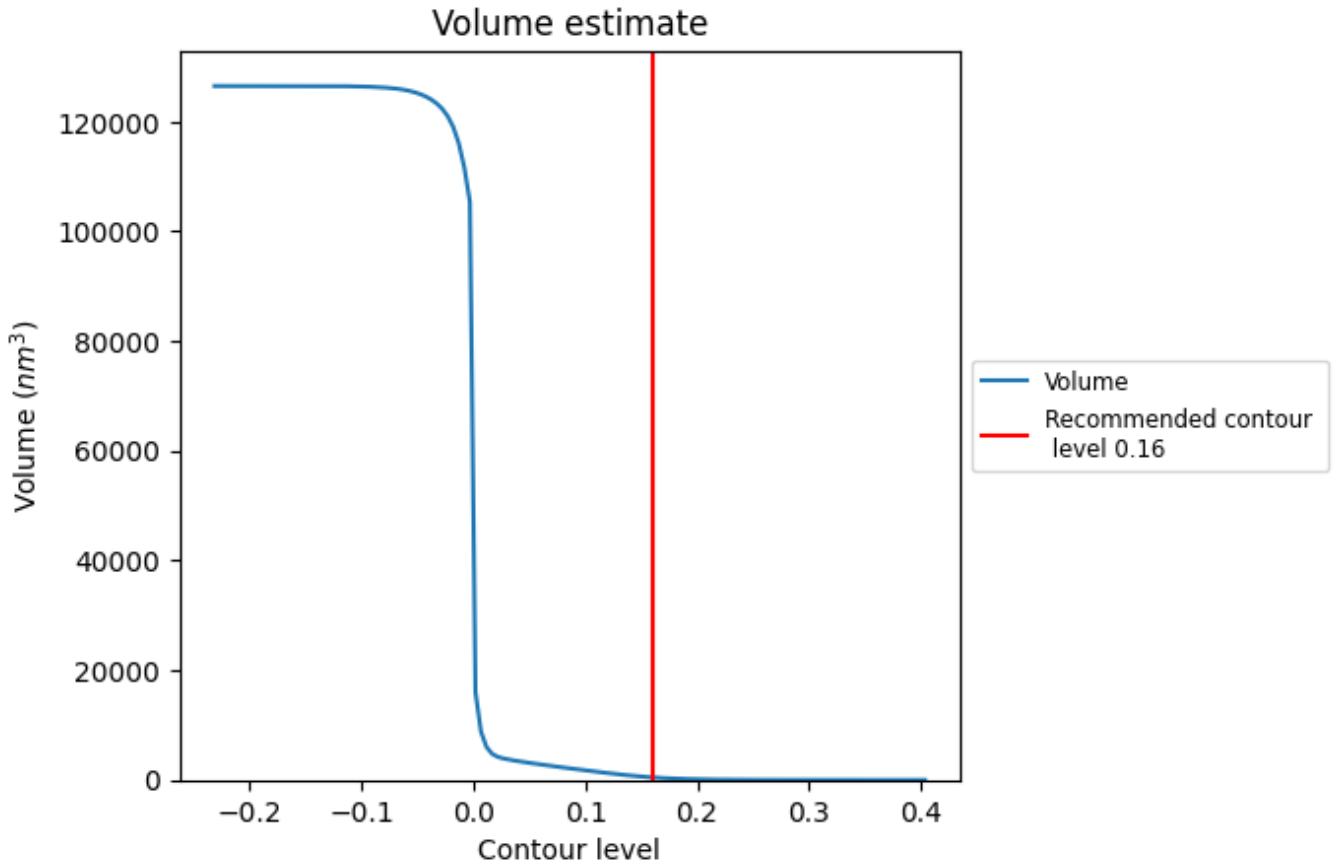
This section contains the results of statistical analysis of the map.

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.

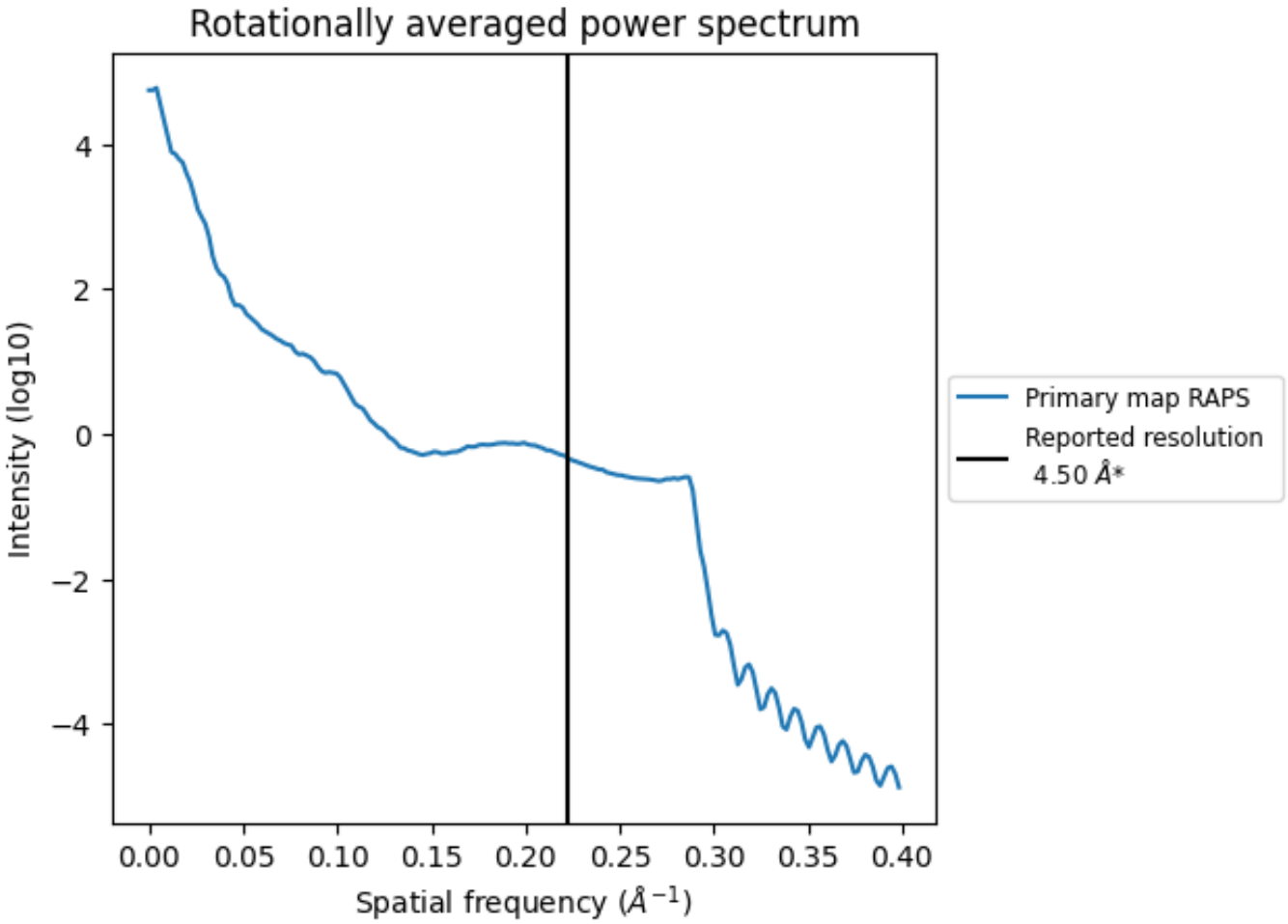
7.2 Volume estimate



The volume at the recommended contour level is 469 nm^3; this corresponds to an approximate mass of 423 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 0.222 Å^{-1}

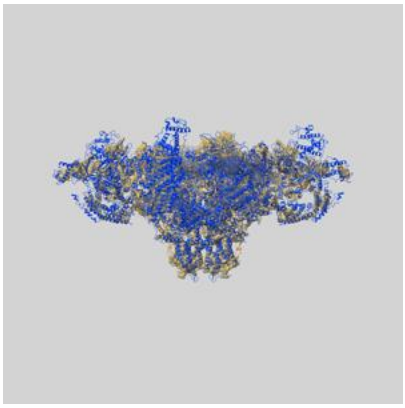
8 Fourier-Shell correlation

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

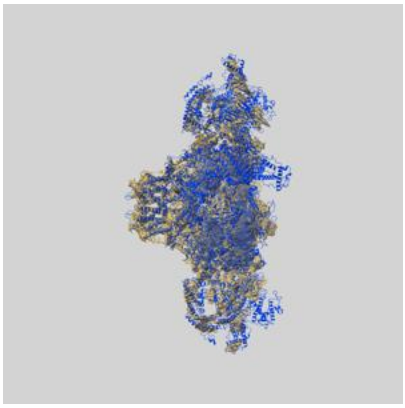
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22392 and PDB model 7JMF. Per-residue inclusion information can be found in section 3 on page 5.

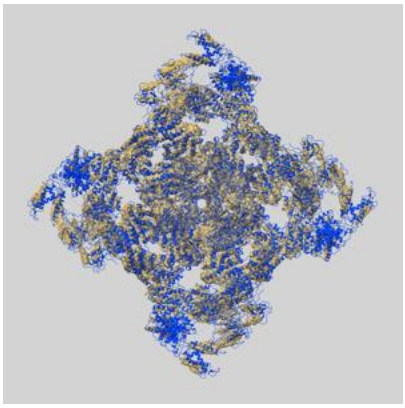
9.1 Map-model overlay



X



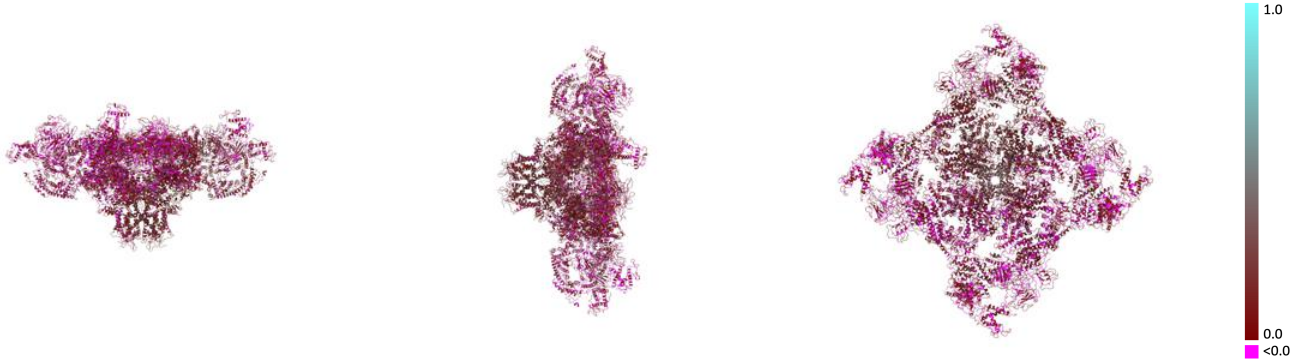
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16 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.

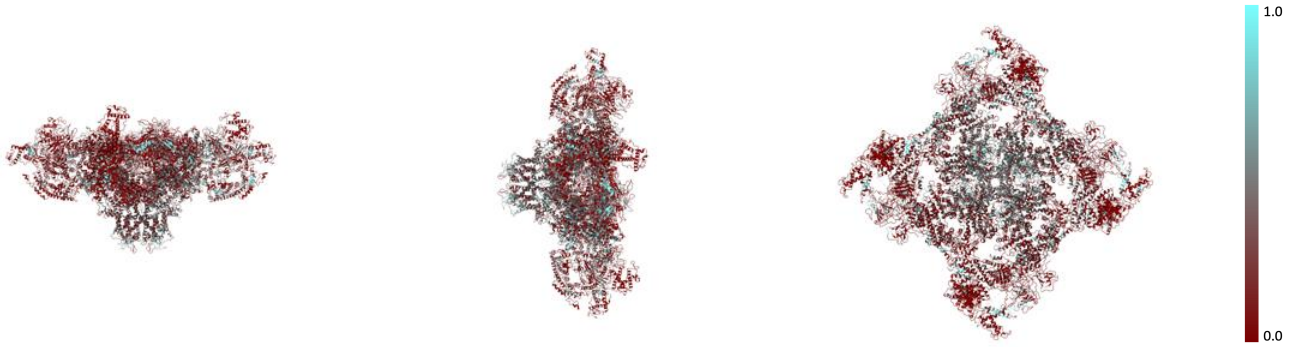
9.2 Q-score mapped to coordinate model



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.

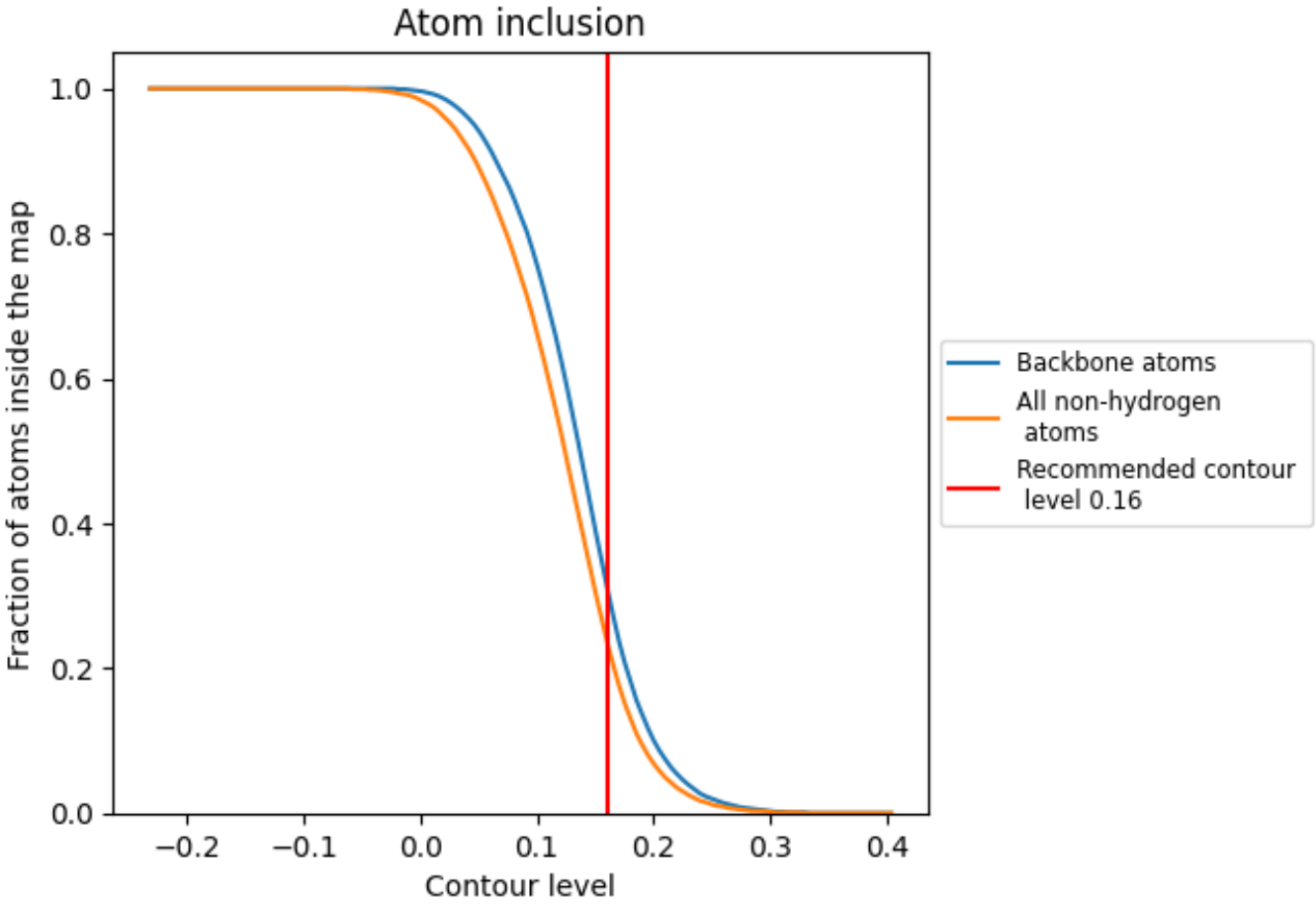
9.3 Atom inclusion mapped to coordinate model



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 (0.16).

9.4 Atom inclusion (i)



At the recommended contour level, 31% of all backbone atoms, 24% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2380	0.1100
A	0.1450	0.1330
B	0.2720	0.1490
E	0.2580	0.1200
F	0.1430	0.0750
G	0.2200	0.0820
H	0.1090	0.0850
I	0.2150	0.0890
J	0.1250	0.0820