Full wwPDB EM Validation Report ⓘ

Nov 2, 2022 – 07:43 AM EDT

PDB ID	:	5TB1
EMDB ID	:	EMD-8392
Title	:	Structure of rabbit RyR1 (EGTA-only dataset, class 1)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-10
Resolution	:	4.60 Å(reported)

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

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

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

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

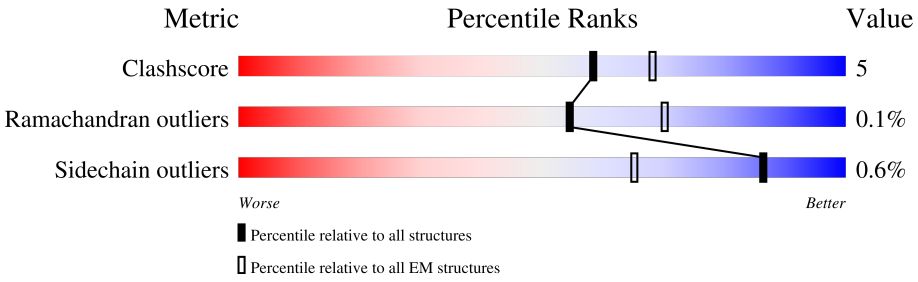
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.60 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	82% 74% 25% ·
1	F	108	83% 73% 26% ·
1	H	108	81% 76% 23% ·
1	J	108	82% 77% 22% ·
2	B	4416	70% 84% 11% 5%
2	E	4416	71% 84% 11% 5%
2	G	4416	70% 84% 11% 5%
2	I	4416	70% 84% 11% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 121272 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	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	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	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

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

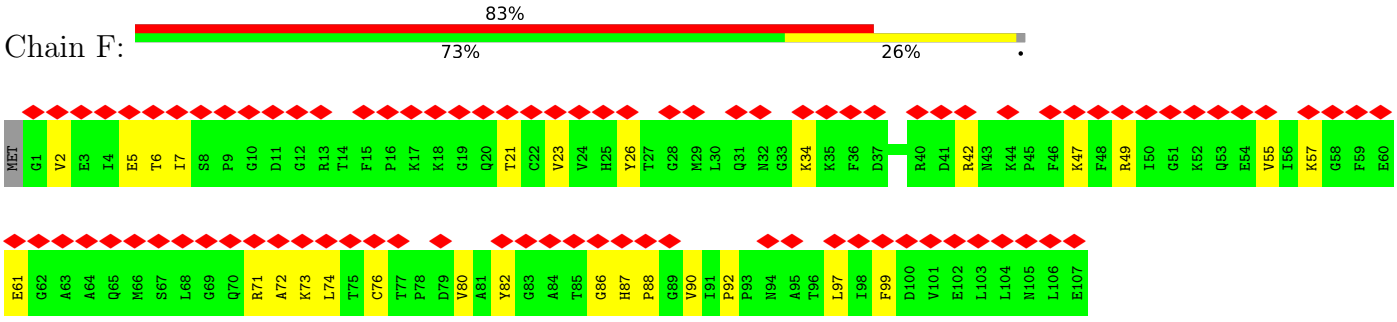
Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

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

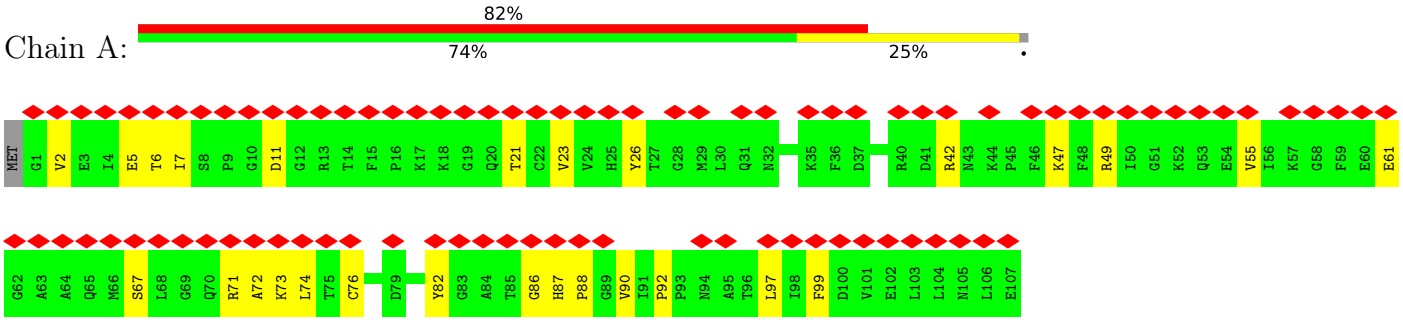
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



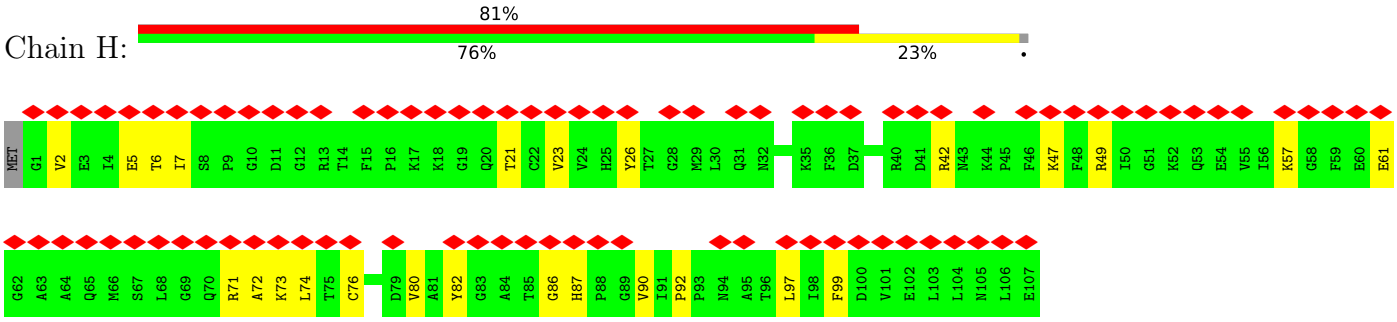
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



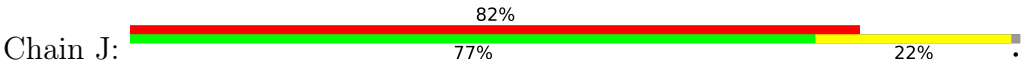
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

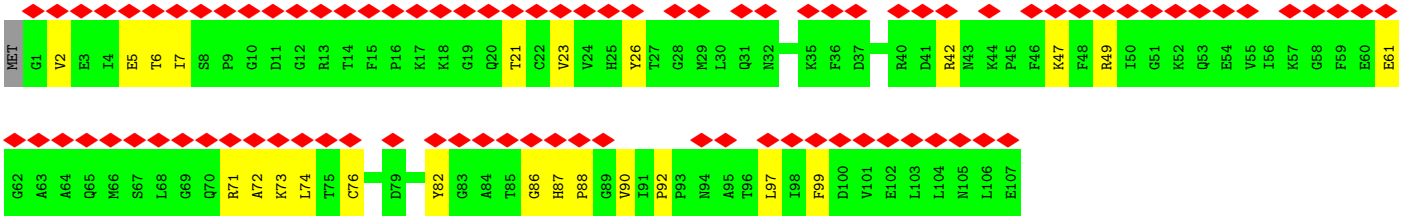
Chain H:



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

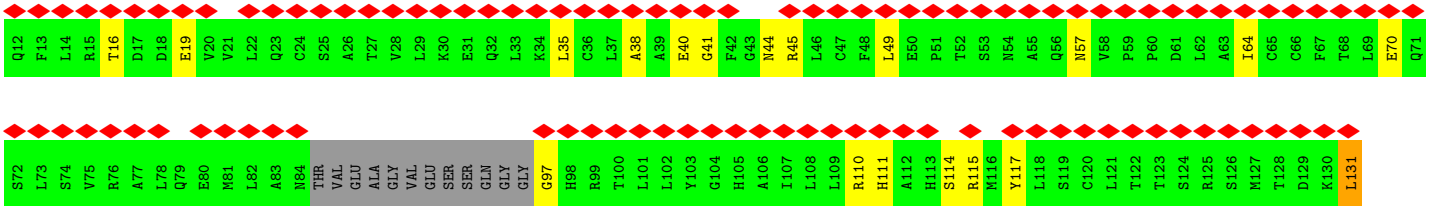
Chain J:

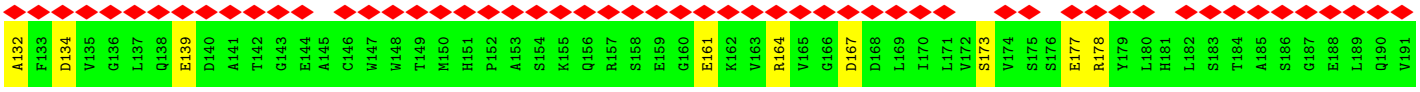


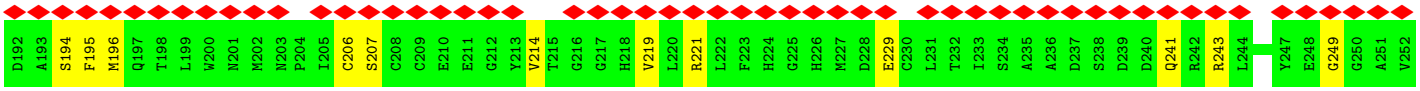


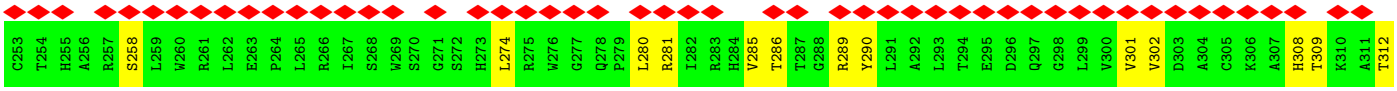
• Molecule 2: Ryanodine receptor 1

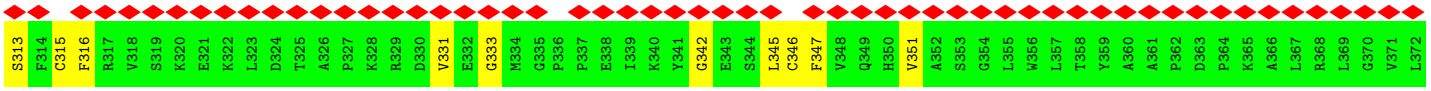
Chain B:

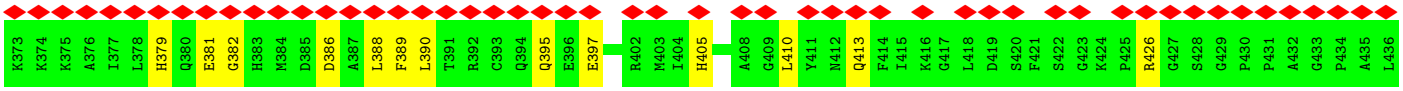


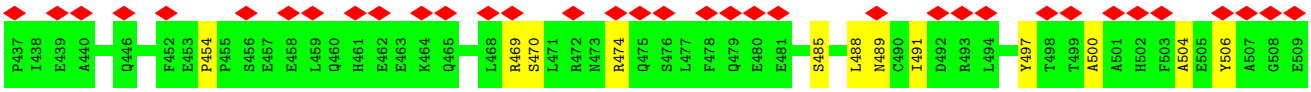


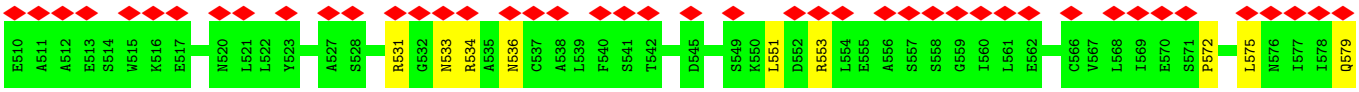


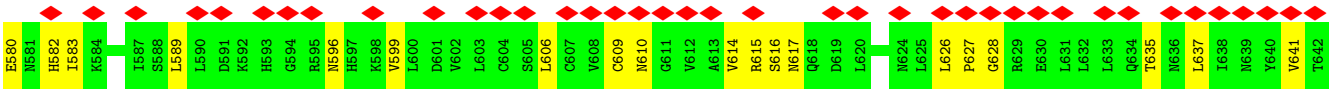


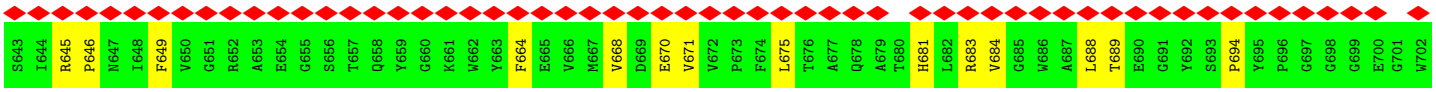


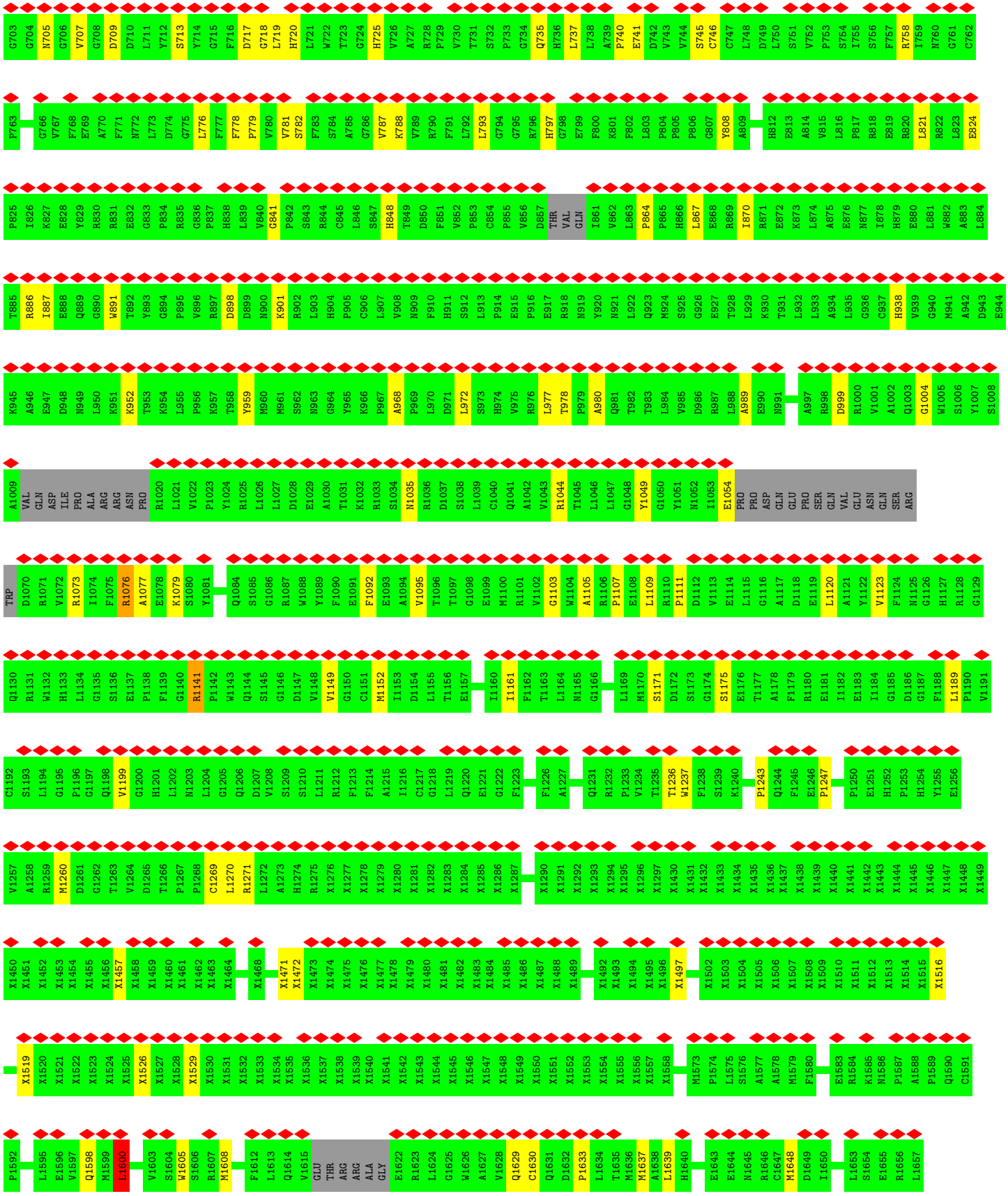








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P763 G766 V767 F768 E769 A770 F771 N772 L773 D774 G775 L776 F777 F778 P779 V780 V781 S782 F783 S784 A785 G786 V787 K788 V789 R790 F791 L792 L793 G794 G795 R796 H797 G798 E799 F800 K801 F802 L803 P804 P805 P806 G807 Y808 A809 H812 E813 A814 V815 L816 P817 R818 E819 R820 L821 R822 L823 E824
P825 I826 K827 E828 Y829 R830 R831 E832 G833 P834 R835 G836 P837 H838 L839 V840 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 E868 R869 I870 R871 E872 K873 L874 A875 E876 N877 I878 H879 E880 L881 W882 A883 L884
T885 R886 I887 E888 Q889 N949 G890 W891 T892 Y893 G894 P895 V896 R897 D898 D899 N900 K901 R902 L903 H904 P905 C906 L907 V908 N909 P910 H911 S912 L913 P914 E915 P916 E917 R918 N919 Y920 N921 L922 Q923 M924 S925 G926 E927 T928 L929 K930 T931 L932 L933 A934 L935 G936 C937 H938 V939 G940 M941 A942 D943 E944
K945 A946 E947 D948 L950 K951 K952 T953 K954 L955 P956 K957 T958 Y959 M960 M961 S962 N963 G964 Y965 K966 P967 A968 P969 L970 D971 L972 S973 H974 V975 R976 L977 T978 P979 A980 Q981 T982 T983 L984 V985 D986 R987 L988 A989 E990 N991 A997 R998 D999 R1000 V1001 A1002 Q1003 G1004 W1005 S1006 Y1007 S1008
A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 L1021 V1022 P1023 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 Q1084 S1085 G1086 R1087 W1088 Y1089 F1090 E1091 F1092 E1093 A1094 A1095 V1096 T1096 T1097 G1098 E1099 M1100 R1101 V1102 G1103 W1104 A1105 R1106 P1107 E1108 L1109 R1110 P1111 D1112 V1113 E1114 L1115 G1116 A1117 D1118 E1119 L1120 A1121 Y1122 V1123 F1124 N1125 G1126 H1127 R1128 G1129
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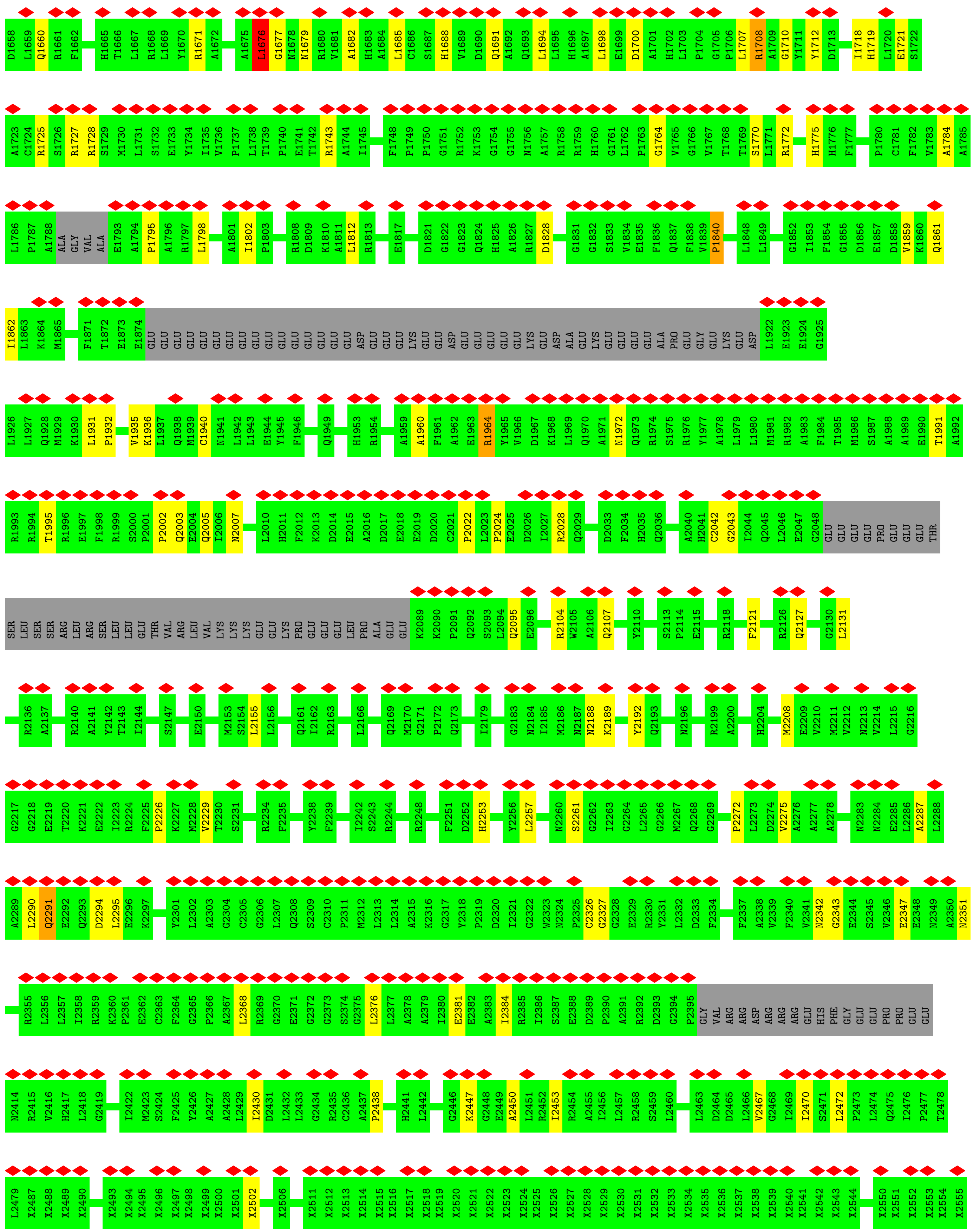
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I1862 L1863 K1864 M1865 F1871 T1872 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 G1925
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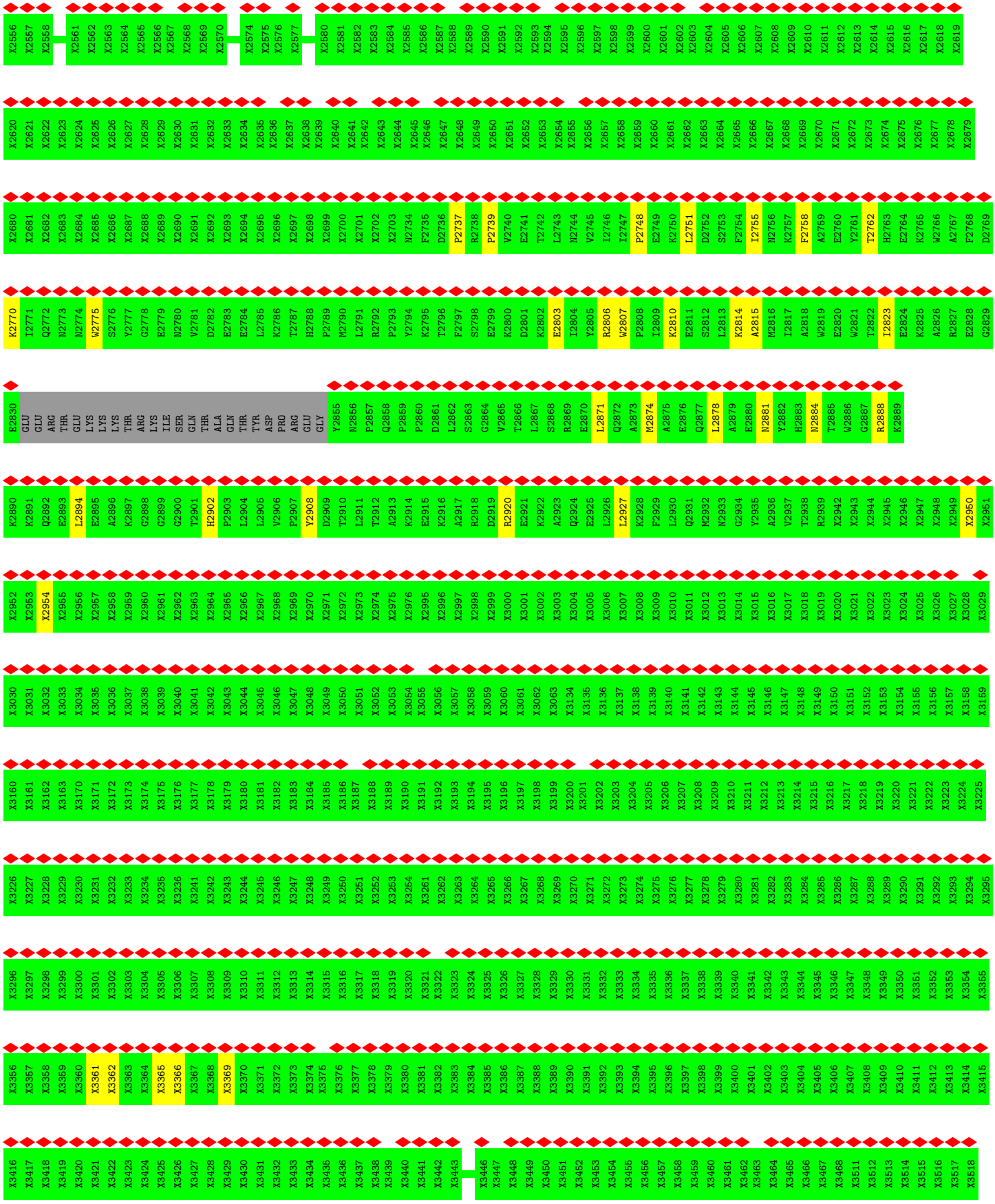
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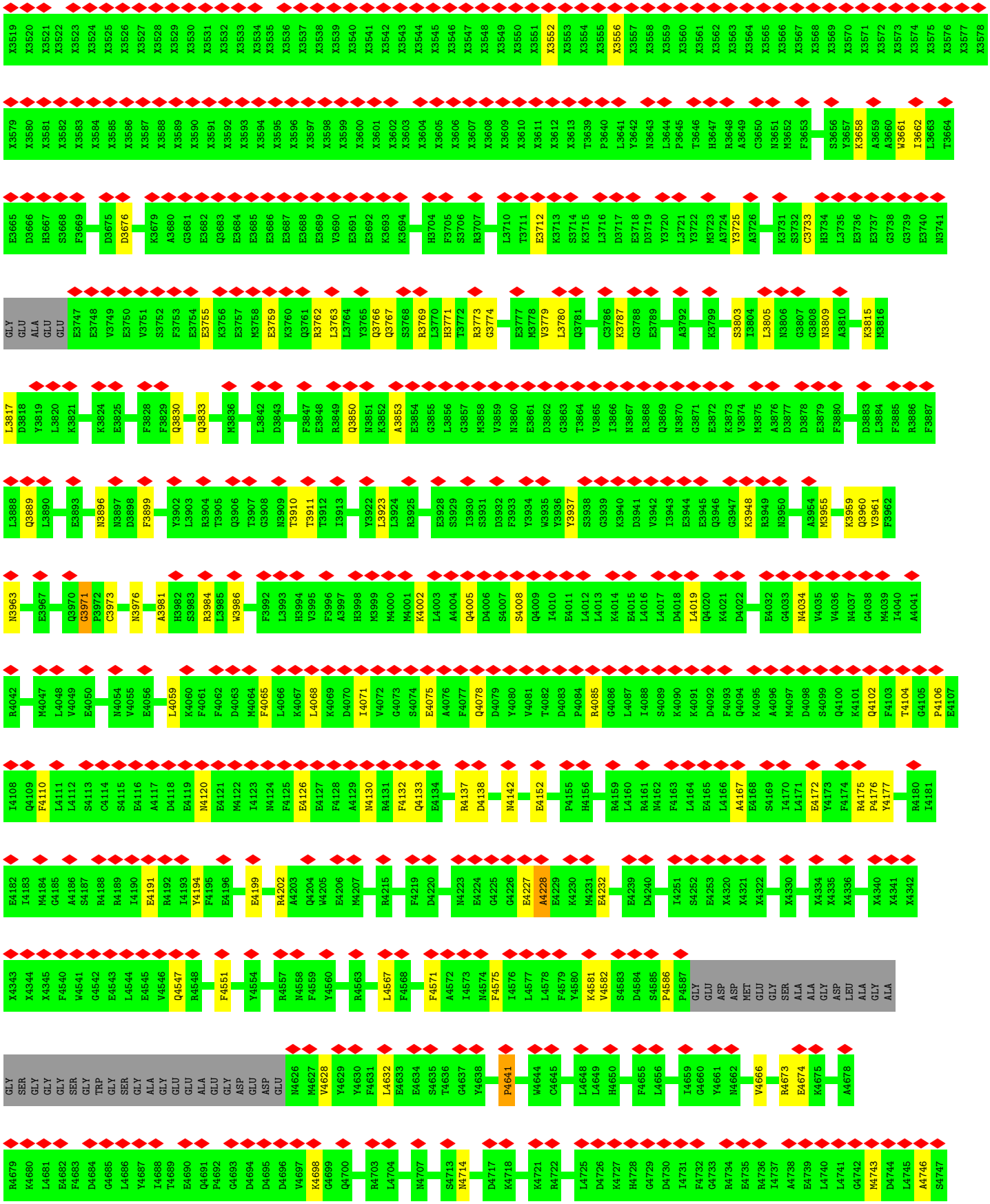
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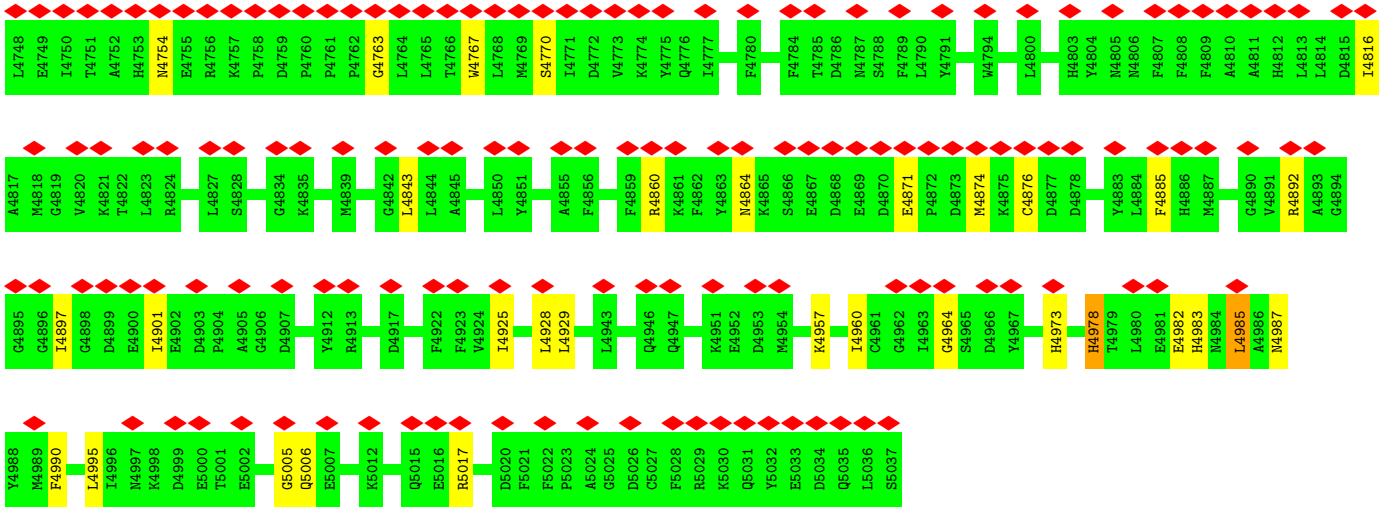

- Molecule 2: Ryanodine receptor 1

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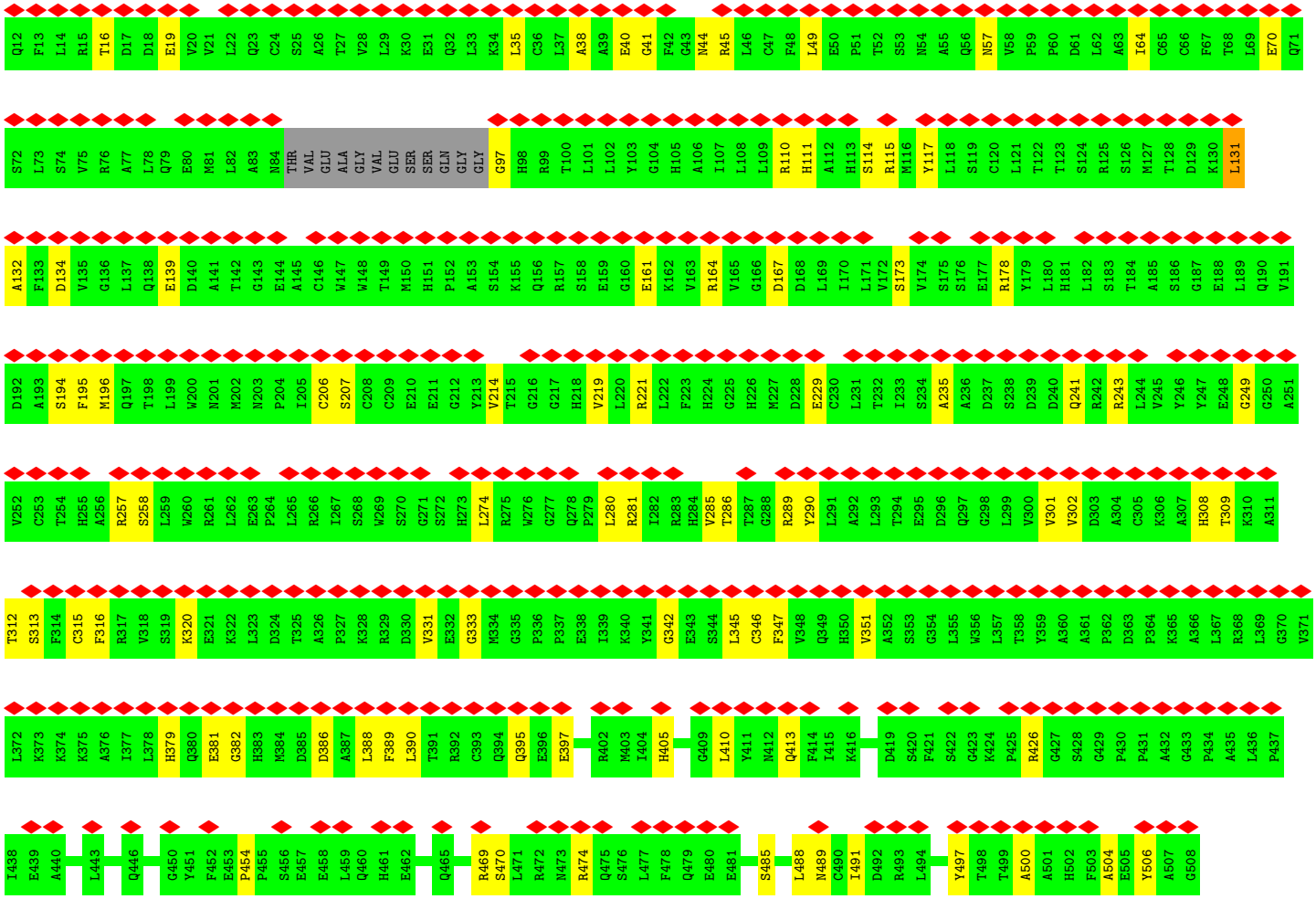

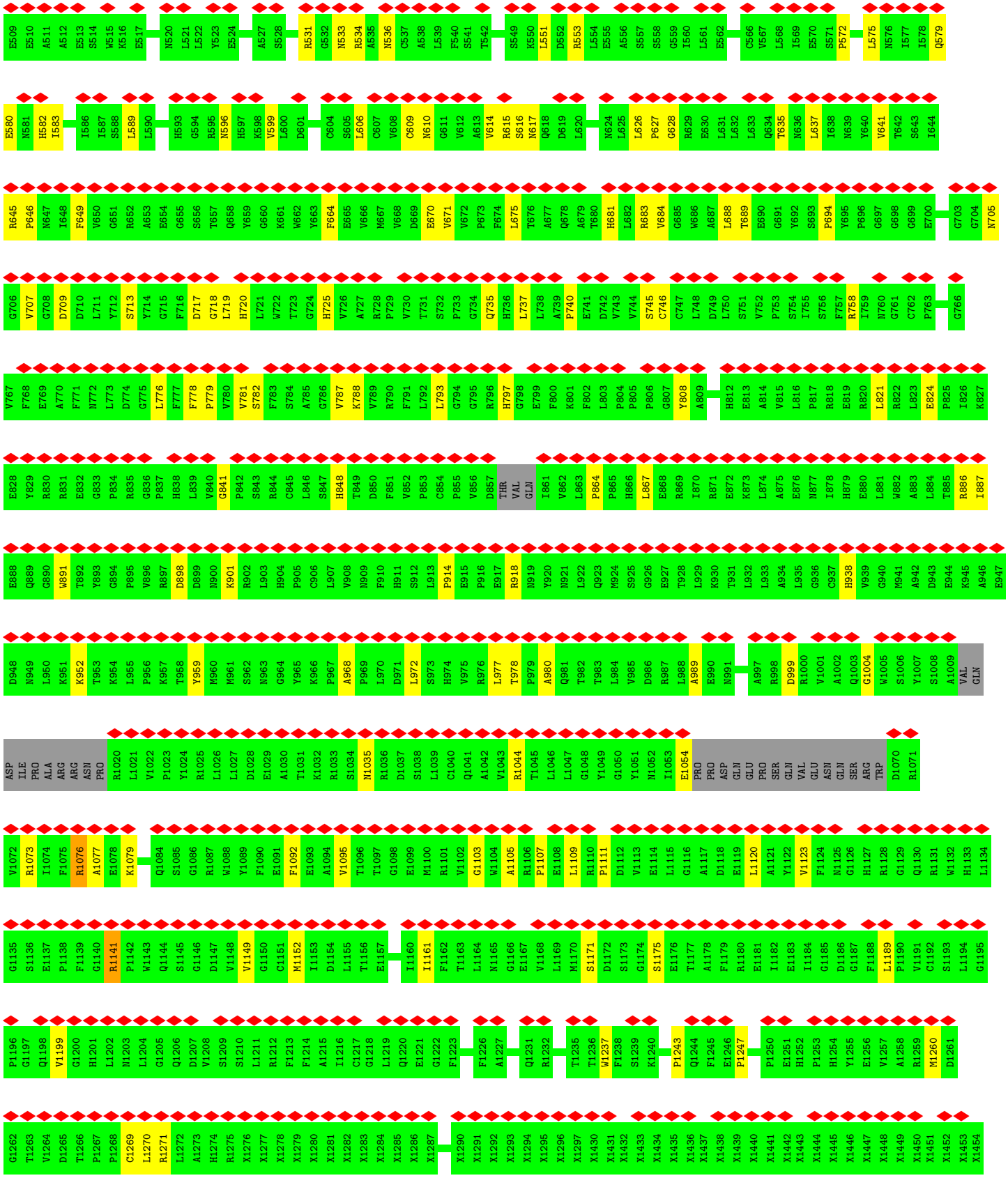
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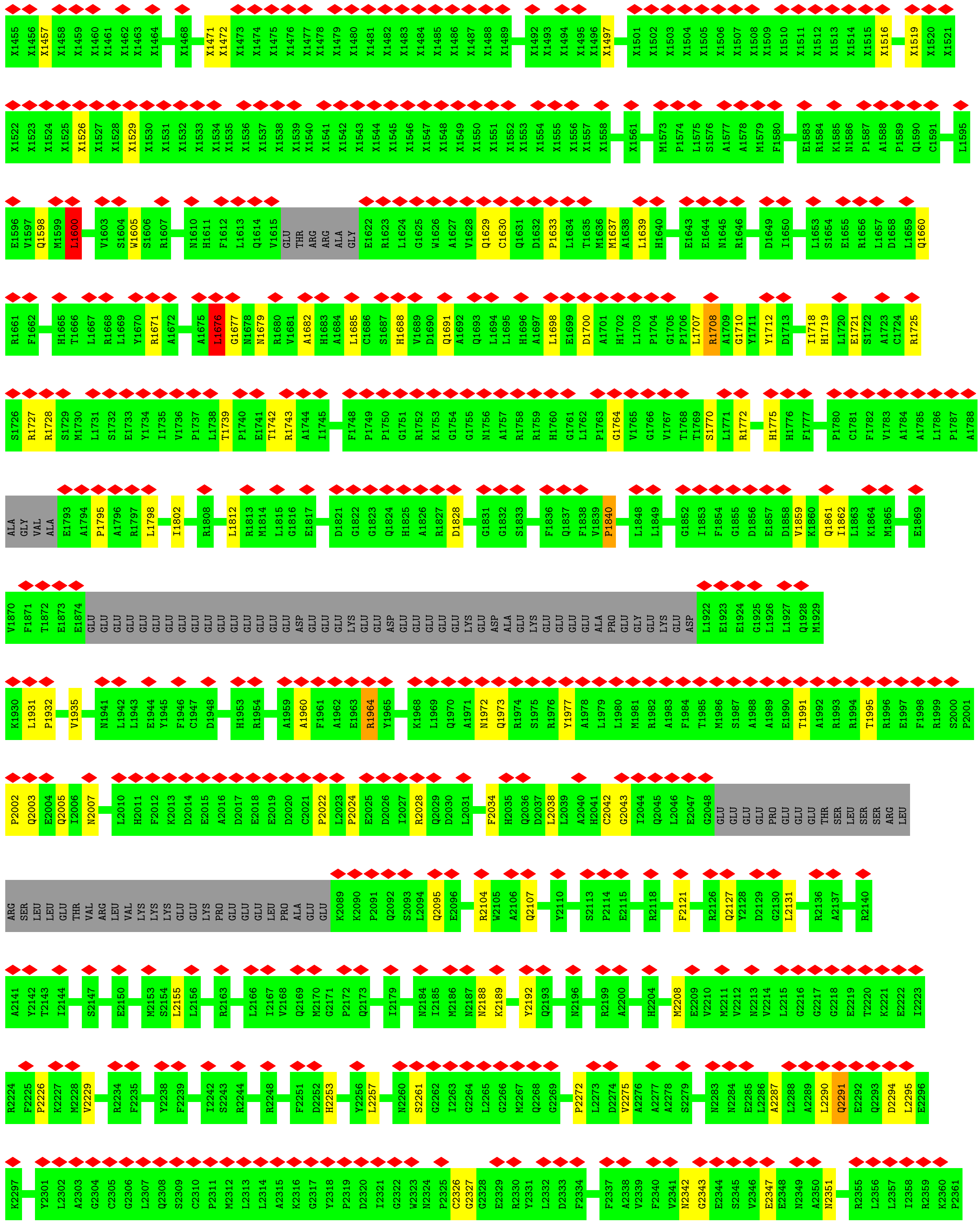
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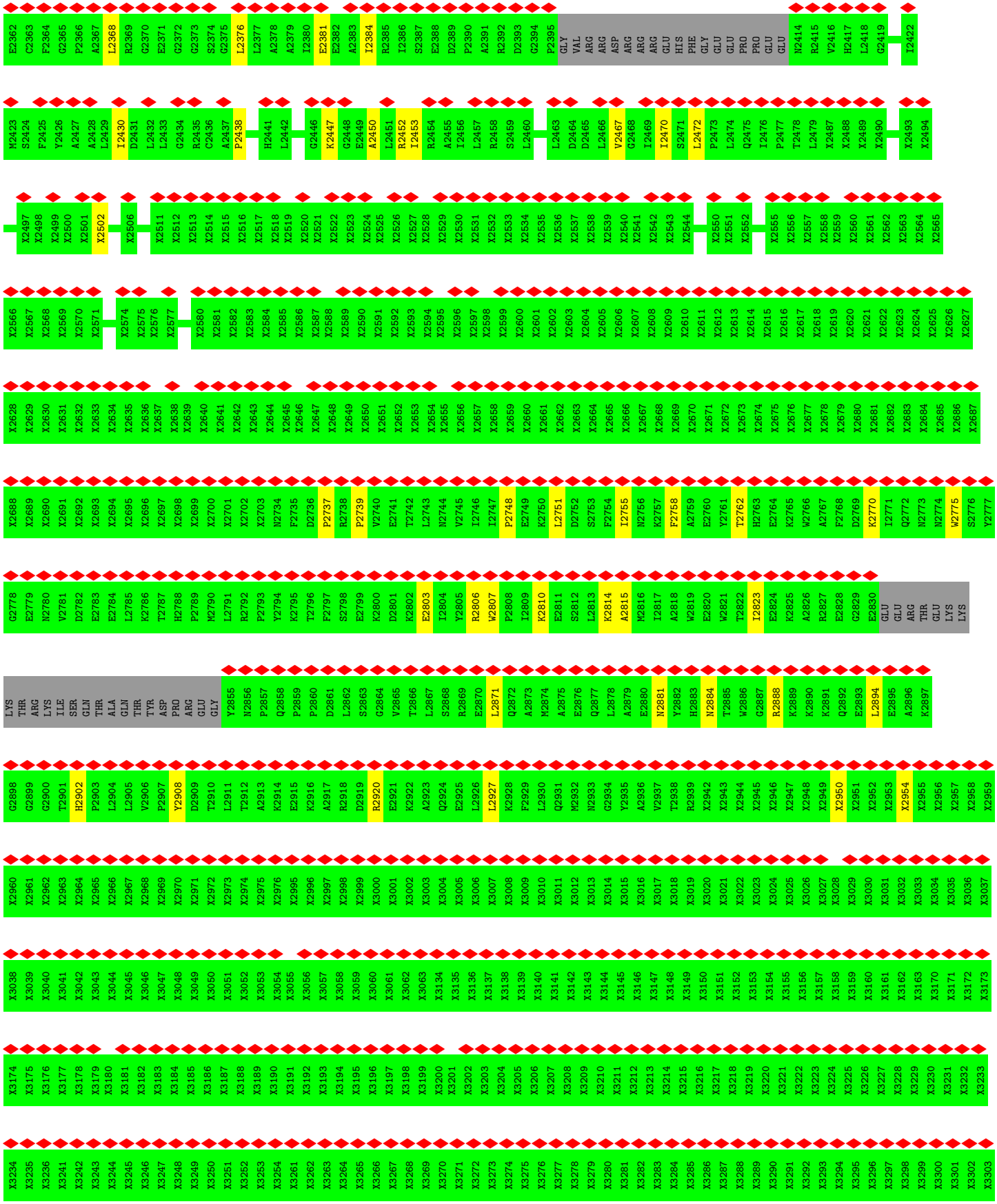
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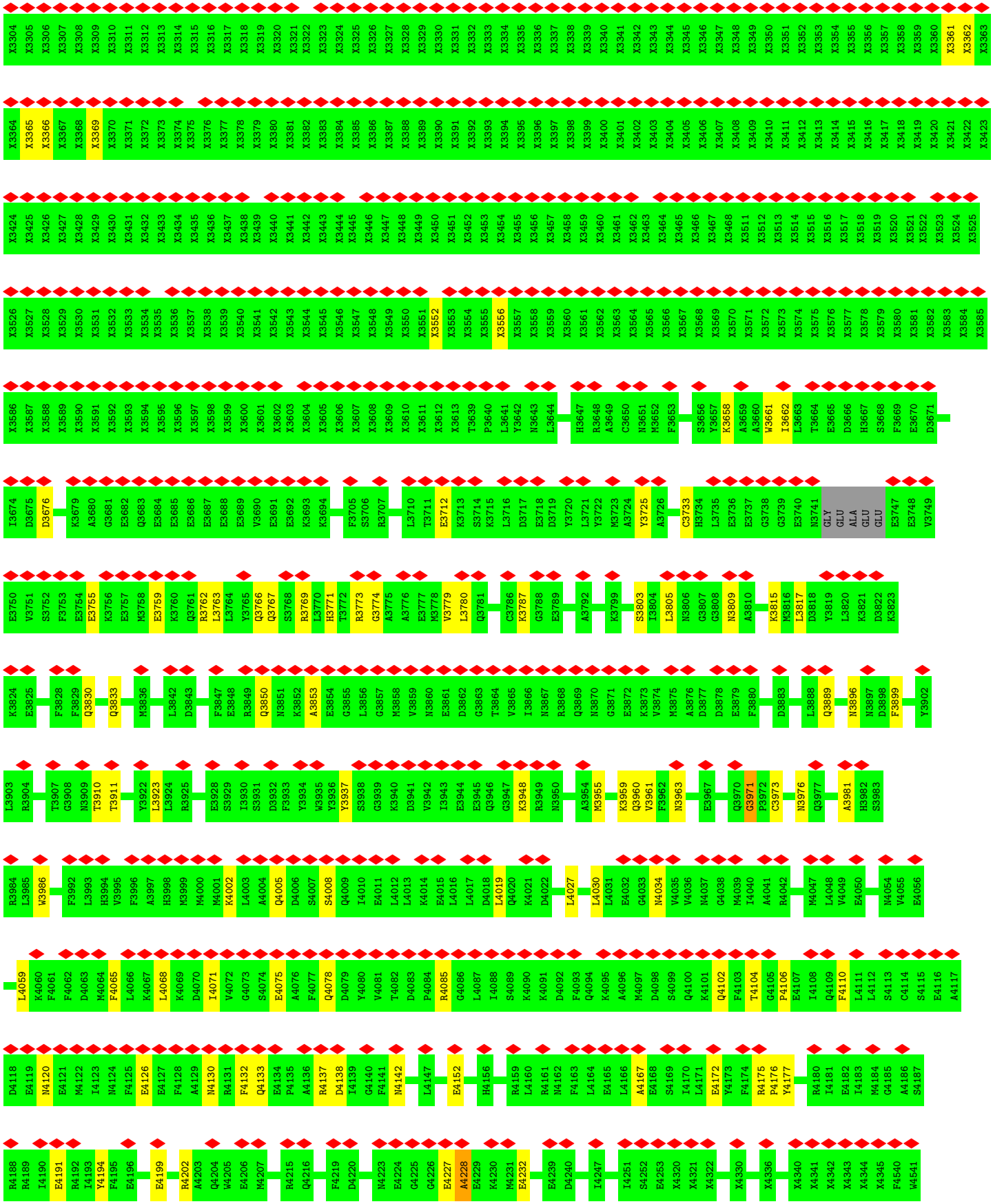
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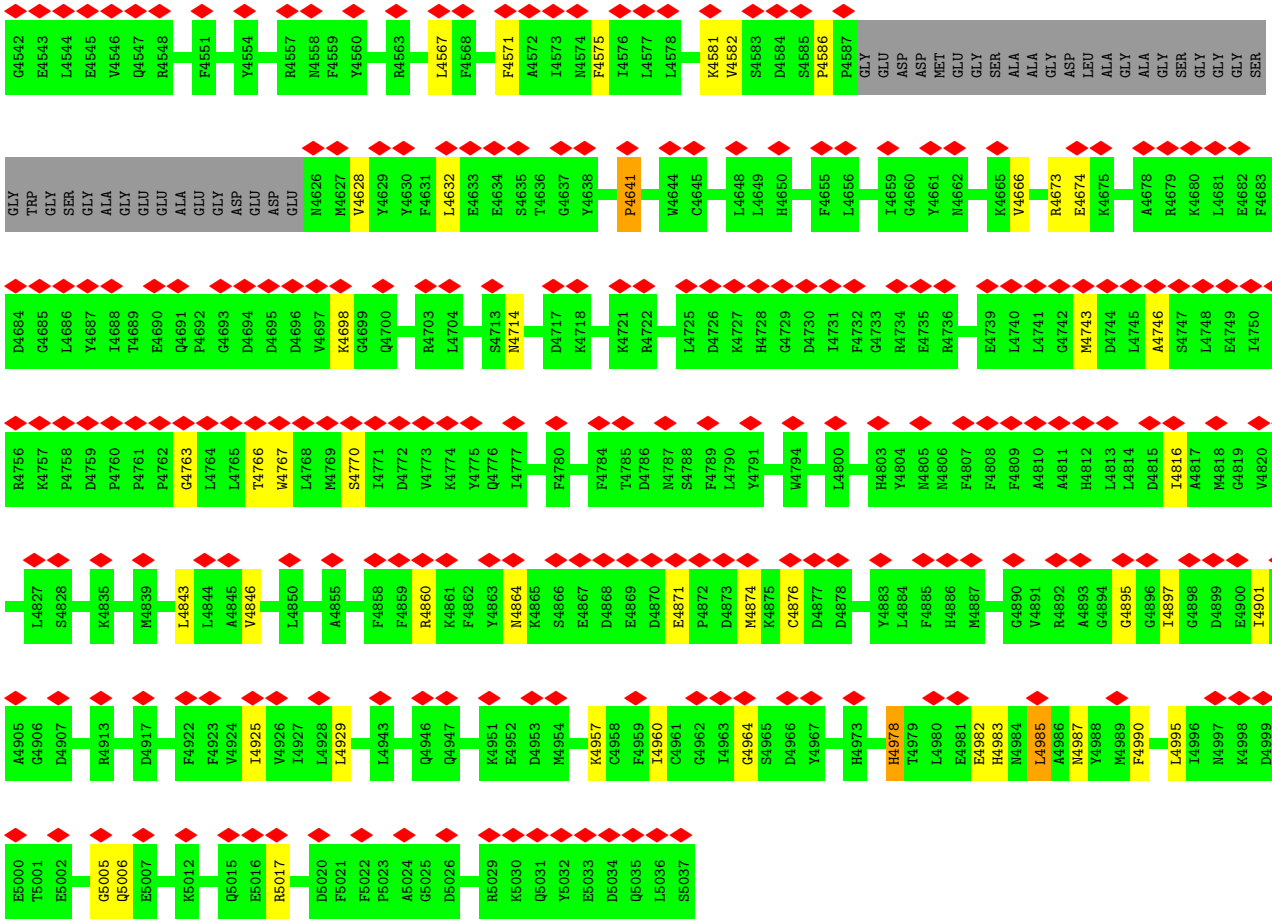
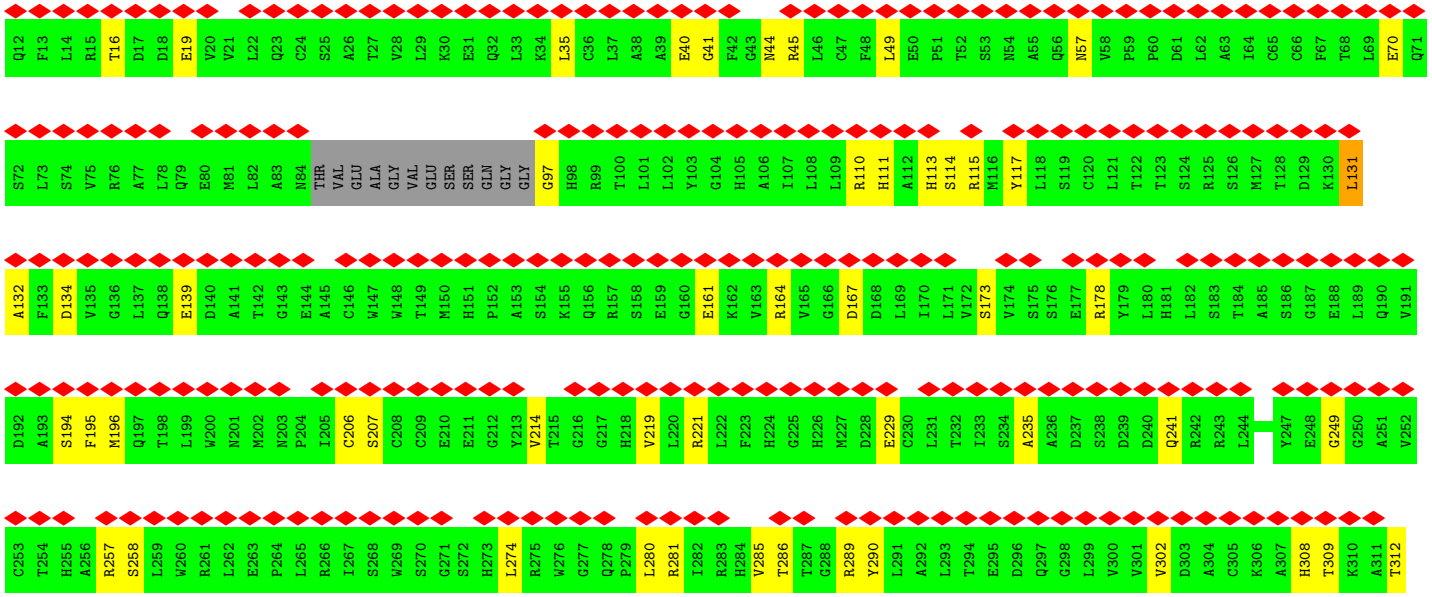
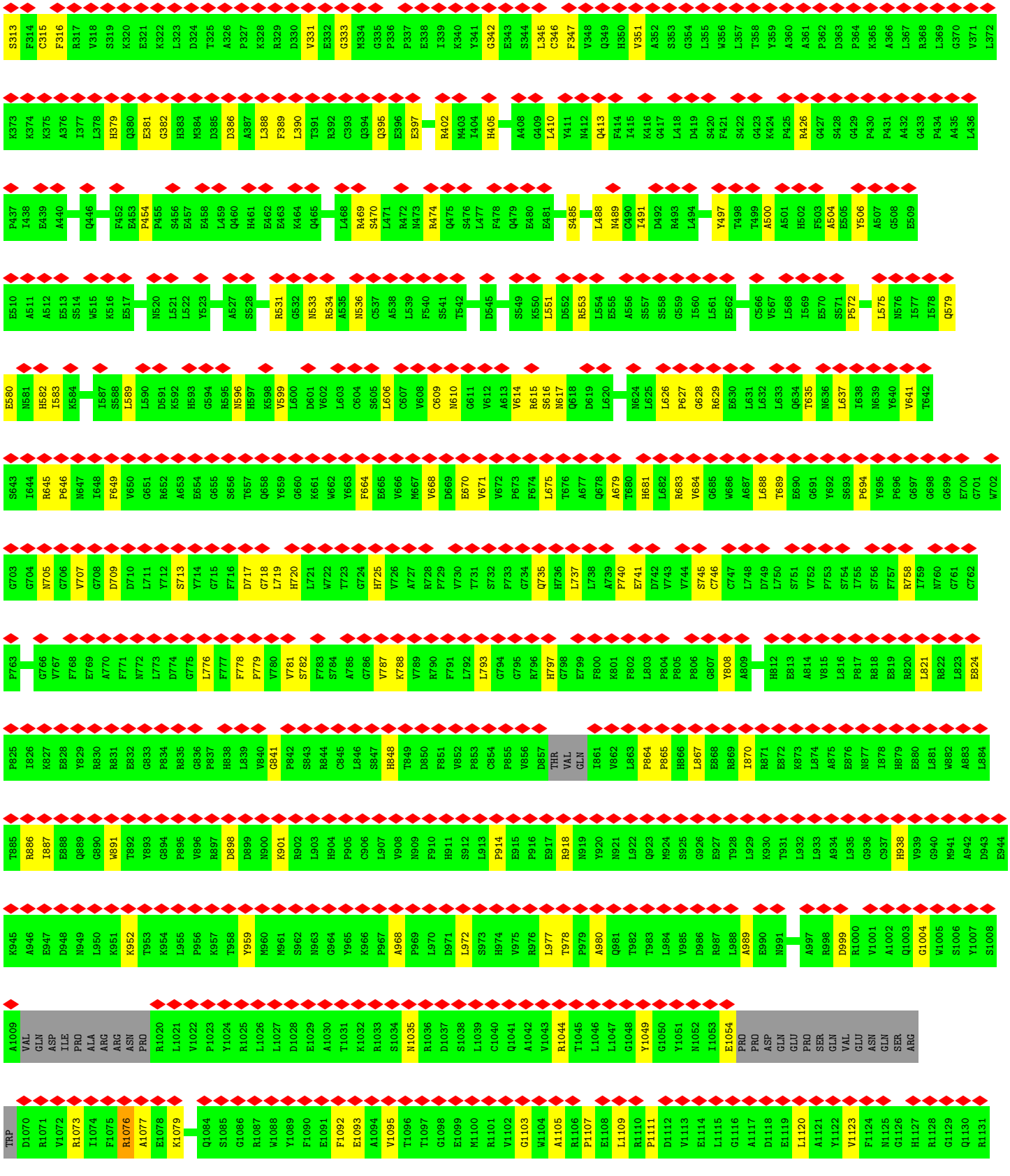


• Molecule 2: Ryanodine receptor 1

Chain E:

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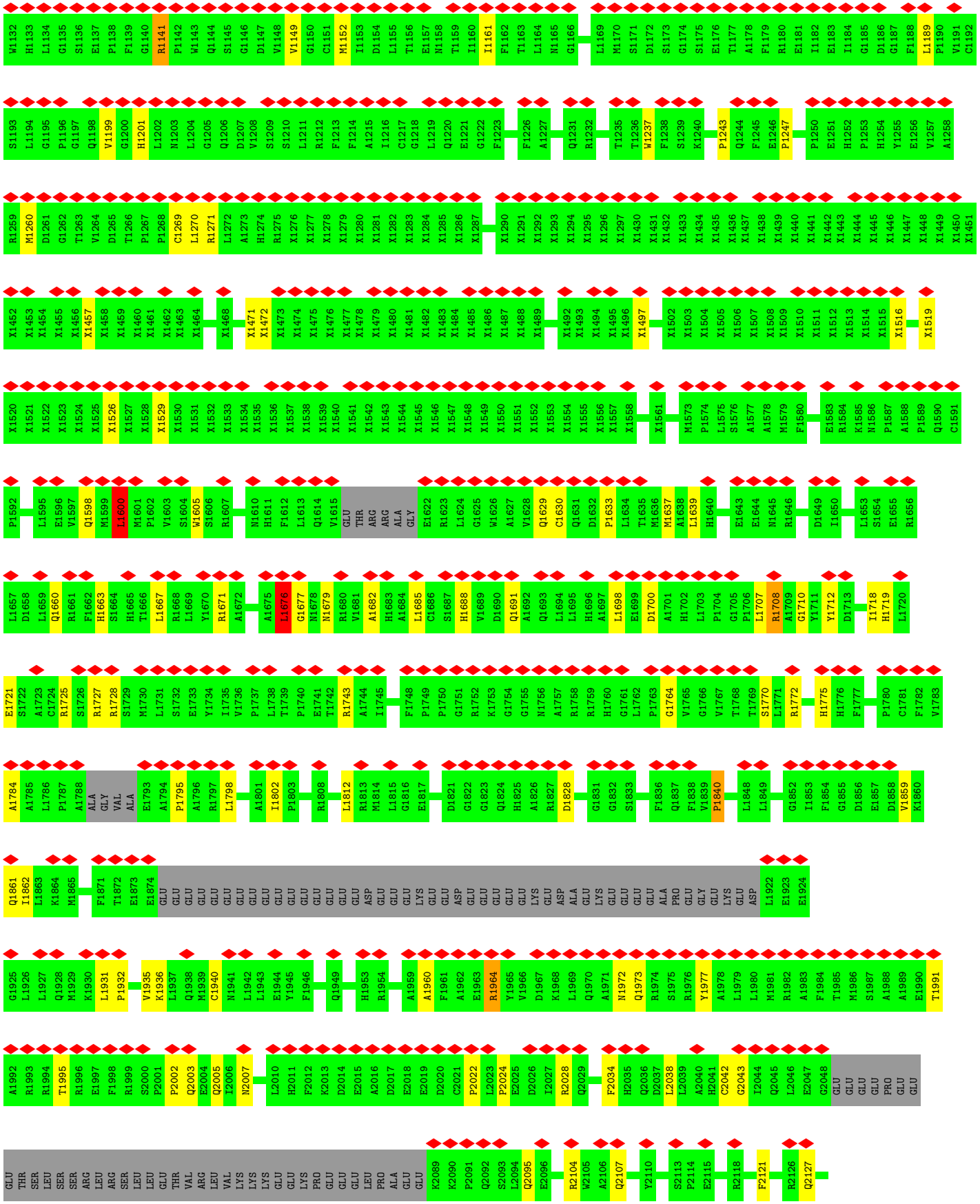
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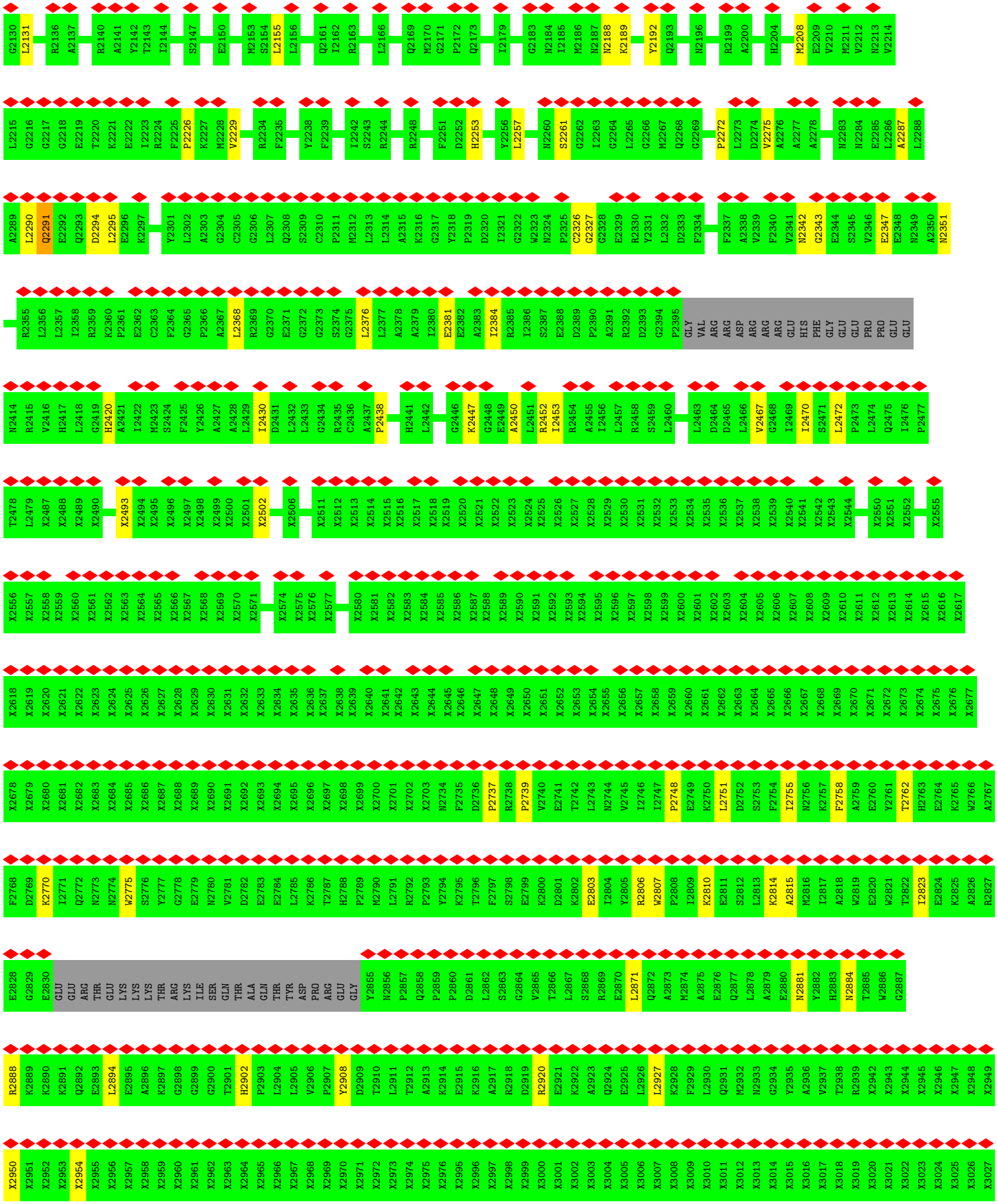
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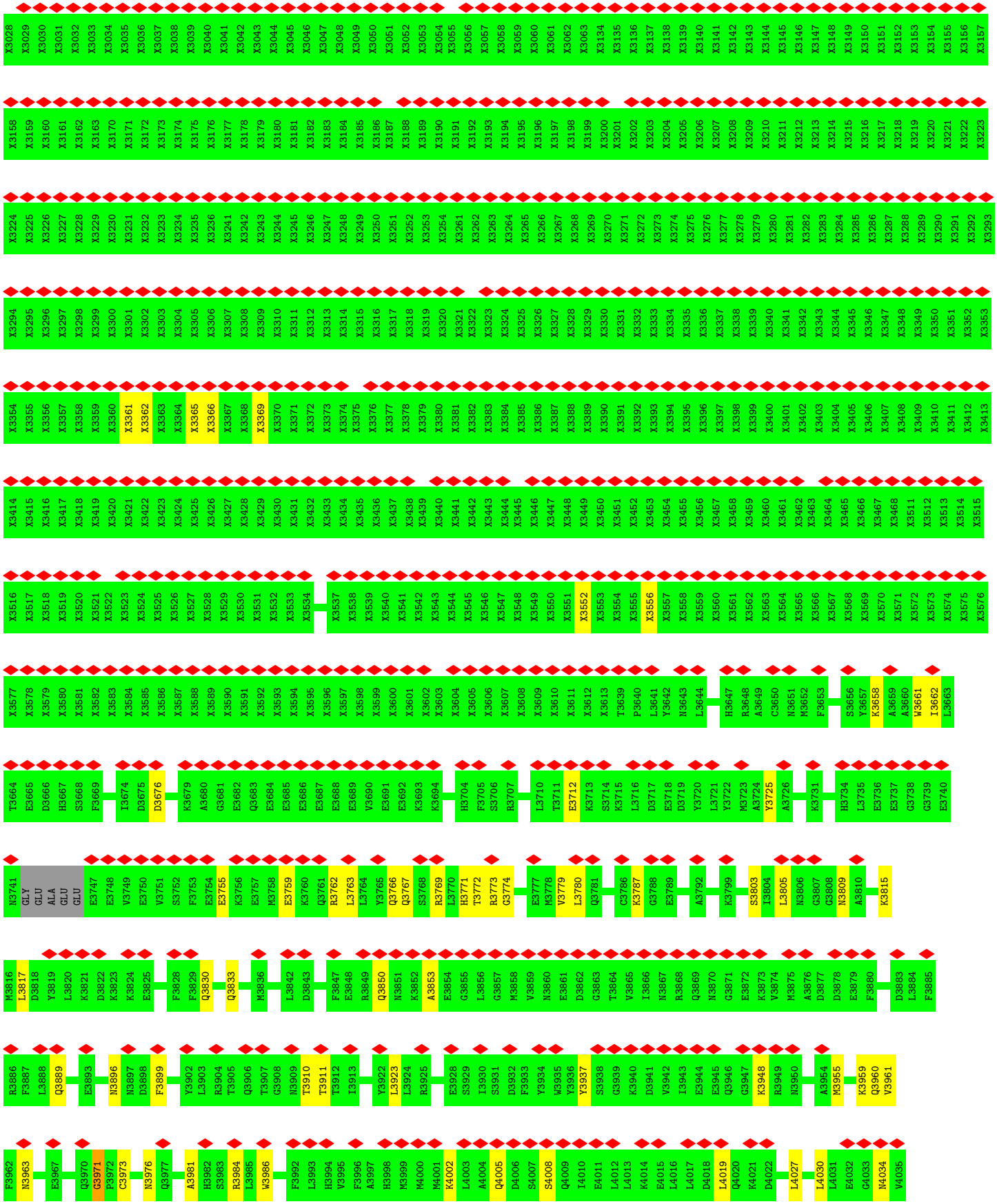
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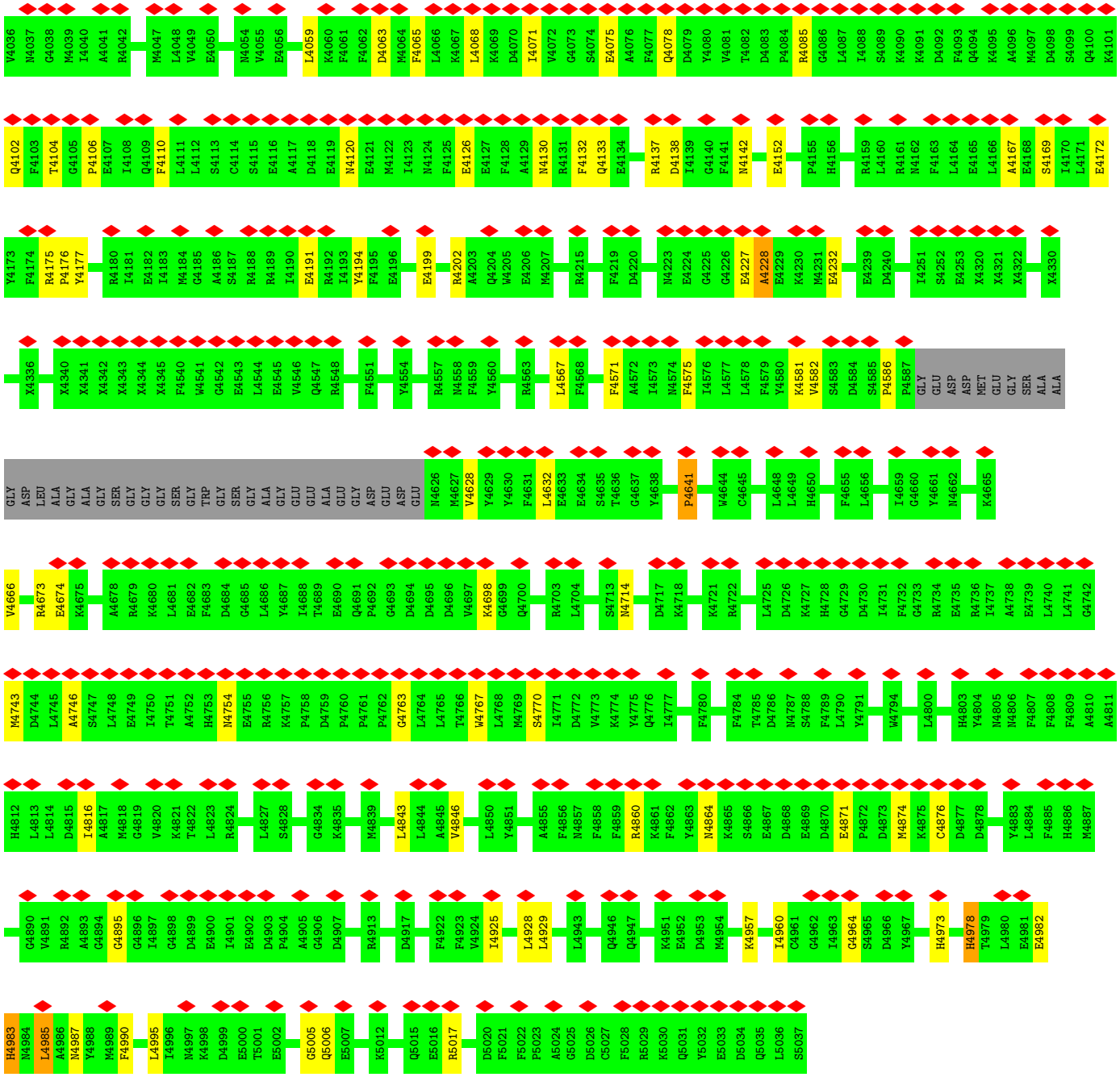

• Molecule 2: Ryanodine receptor 1

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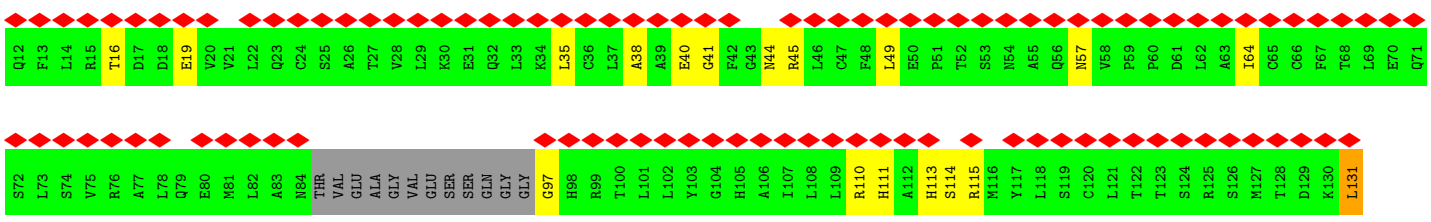

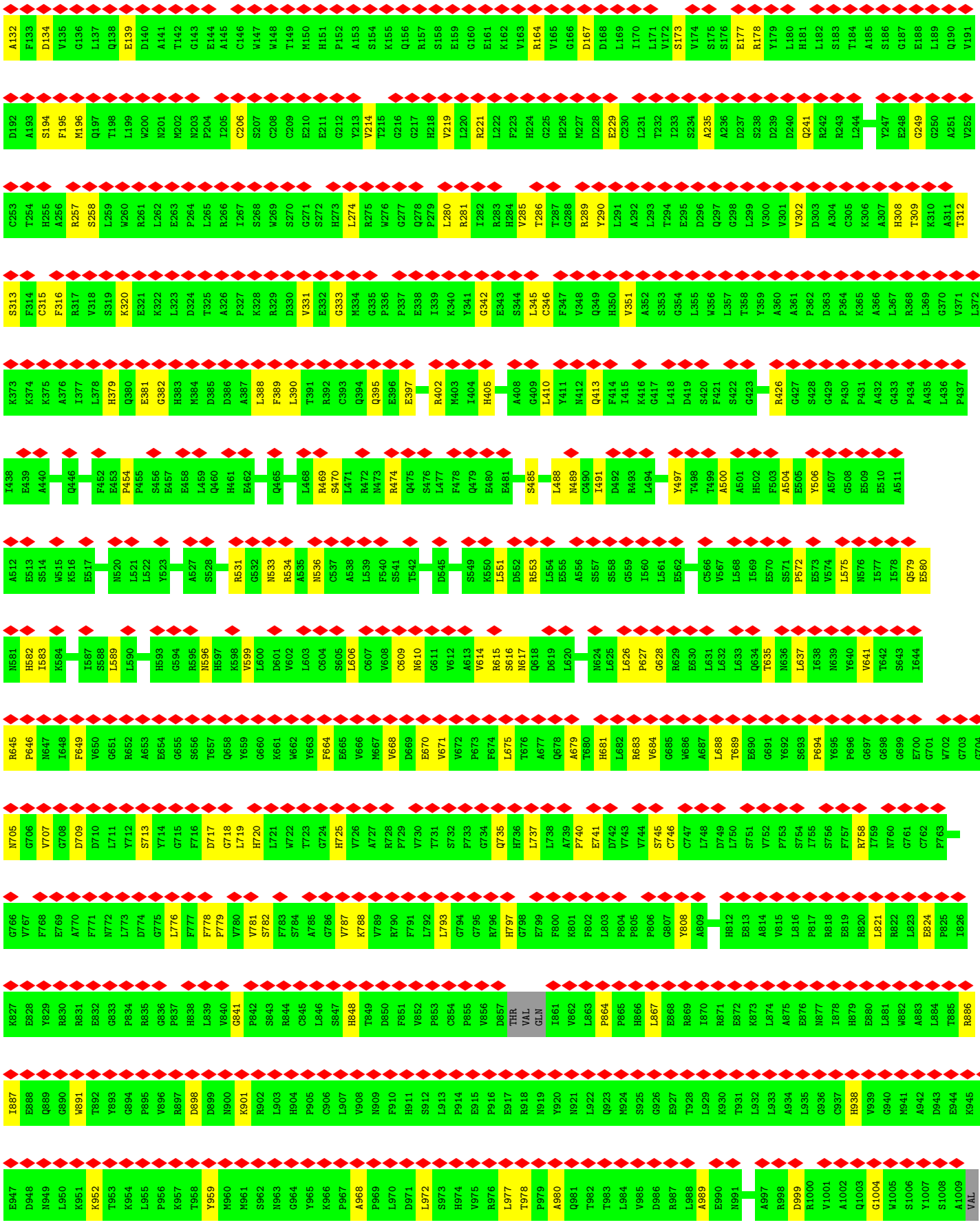
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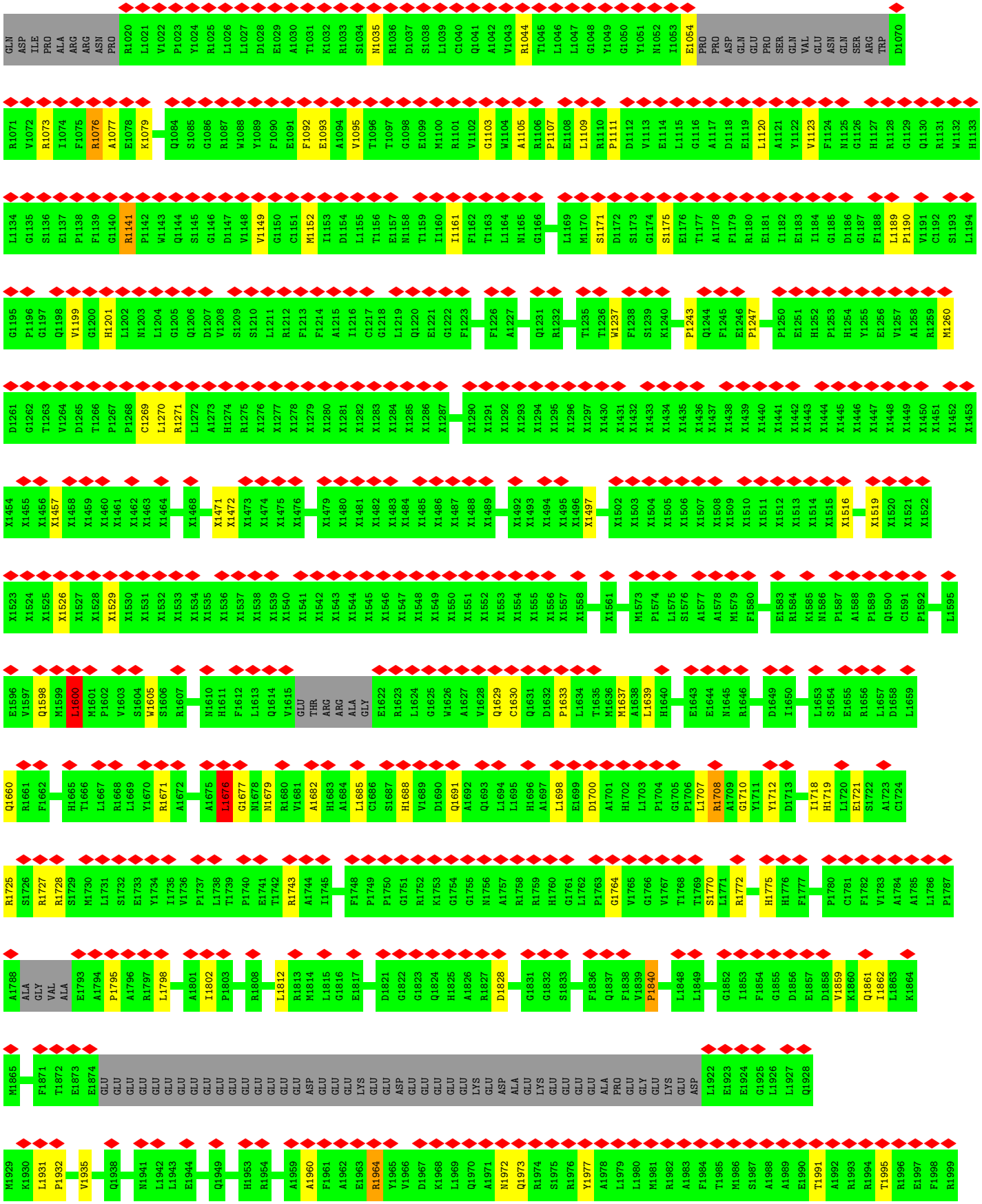
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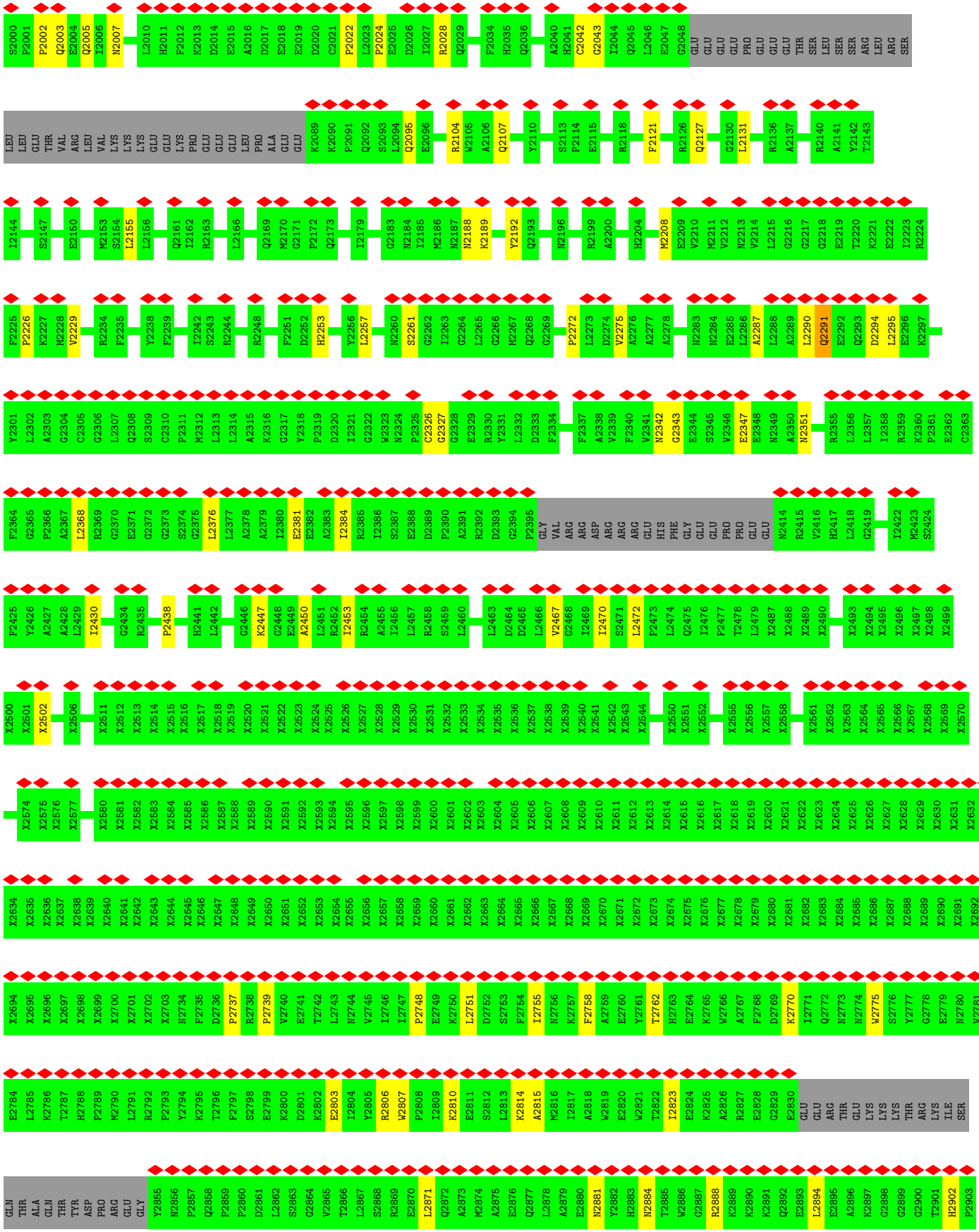
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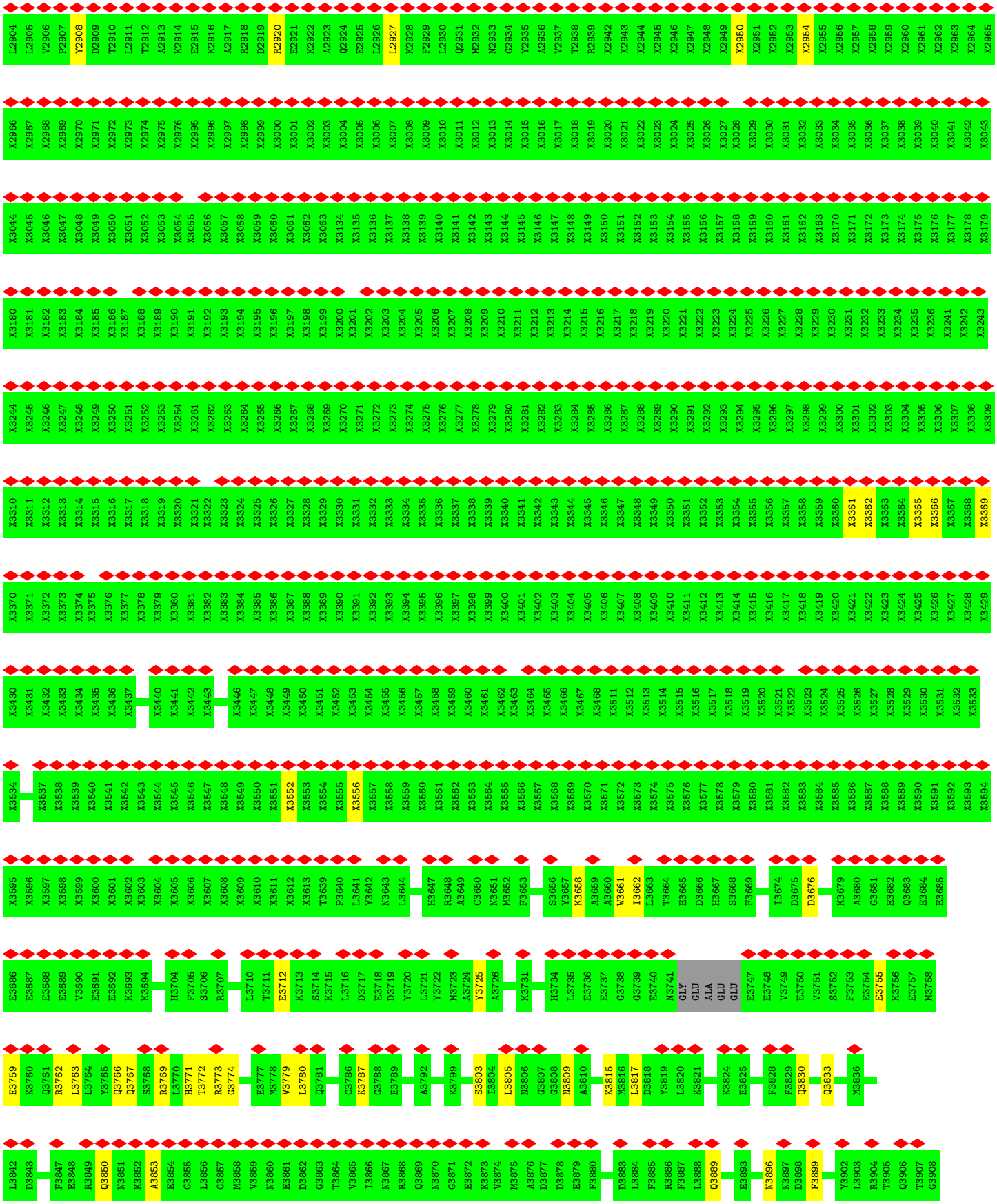
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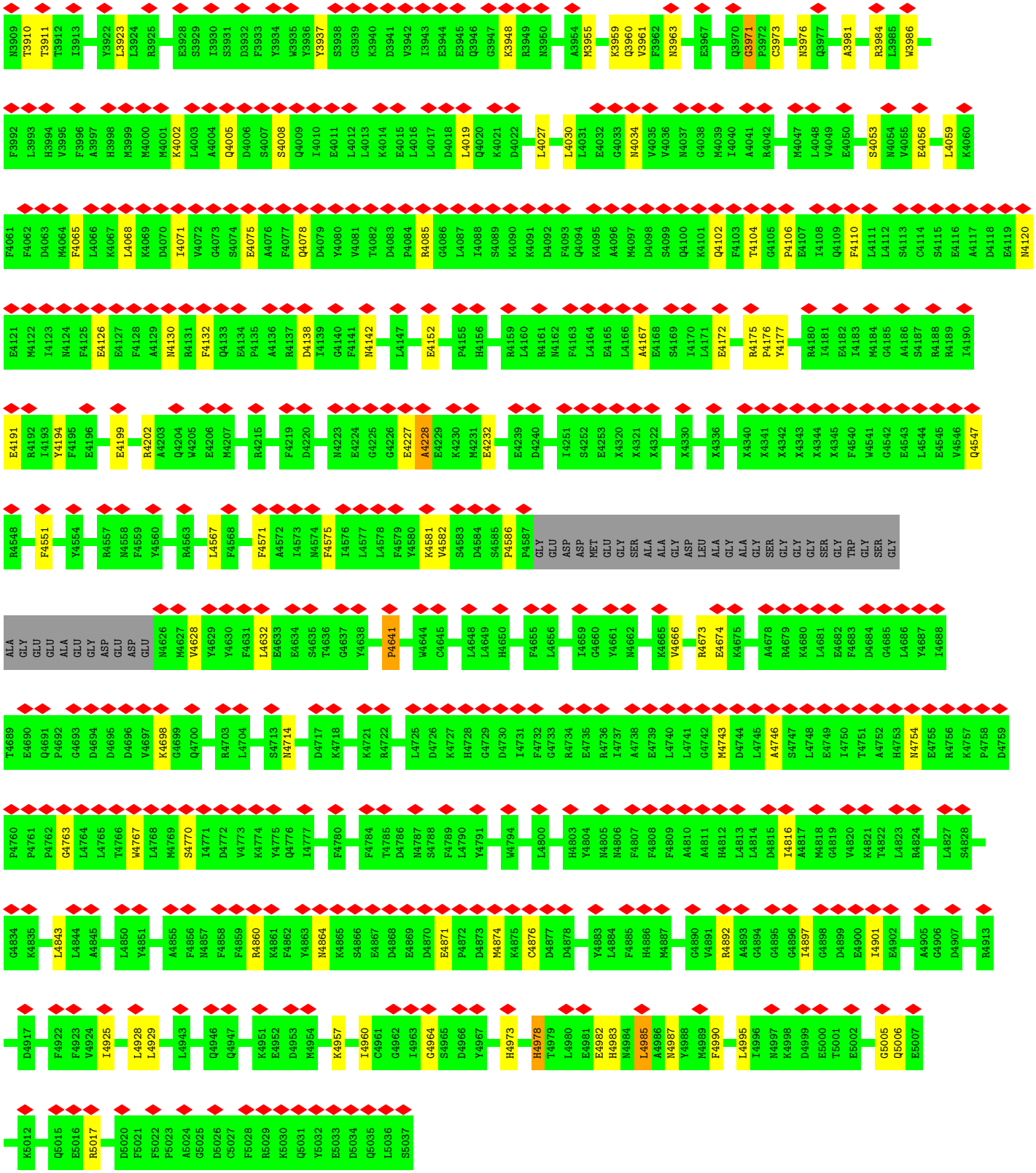
N3909 T3910 T3911 I3912 I3913 Y3922 L3923 L3924 R3925 E3928 S3929 I3930 S3931 D3932 F3933 Y3934 W3935 Y3936 Y3937 S3938 G3939 K3940 D3941 D3942 V3942 I3943 E3944 E3945 Q3946 G3947 K3948 R3949 N3950 A3954 M3955 K3959 Q3960 V3961 F3962 N3963 E3967 Q3970 G3971 P3972 C3973 N3976 Q3977 A3981 R3984 L3985 W3986
F3992 L3993 H3994 V3995 F3996 A3997 H3998 M3999 M4000 M4001 K4002 L4003 A4004 Q4005 D4006 S4007 S4008 Q4009 I4010 E4011 L4012 L4013 K4014 E4015 L4016 L4017 D4018 L4019 Q4020 K4021 D4022 L4027 L4030 L4031 E4032 G4033 N4034 V4035 V4036 N4037 G4038 M4039 I4040 A4041 R4042 M4047 L4048 V4049 E4050 S4053 N4054 V4055 E4056 L4059 K4060
F4061 F4062 D4063 M4064 F4065 L4066 K4067 L4068 K4069 D4070 I4071 V4072 G4073 S4074 E4075 A4076 F4077 Q4078 D4079 Y4080 V4081 T4082 D4083 P4084 R4085 G4086 L4087 I4088 S4089 K4090 K4091 D4092 F4093 Q4094 K4095 A4096 M4097 D4098 S4099 Q4100 K4101 Q4102 F4103 T4104 G4105 P4106 E4107 I4108 Q4109 F4110 L4111 L4112 S4113 C4114 S4115 E4116 A4117 D4118 E4119 N4120
E4121 M4122 I4123 N4124 F4125 E4126 E4127 F4128 A4129 N4130 R4131 F4132 Q4133 E4134 P4135 A4136 R4137 D4138 I4139 G4140 F4141 N4142 L4147 E4152 P4155 H4156 R4159 L4160 R4161 N4162 F4163 L4164 E4165 L4166 A4167 E4168 S4169 I4170 L4171 E4172 R4175 P4176 Y4177 R4180 I4181 E4182 I4183 M4184 G4185 A4186 S4187 R4188 R4189 I4190
E4191 R4192 I4193 Y4194 F4195 E4196 E4199 R4202 A4203 Q4204 W4205 E4206 M4207 R4215 F4219 D4220 N4223 E4224 G4225 G4226 E4227 A4228 E4229 K4230 M4231 E4232 E4239 D4240 I4251 S4252 E4253 X4320 X4321 X4322 X4330 X4336 X4340 X4341 X4342 X4343 X4344 X4345 F4540 W4541 G4542 E4543 L4544 E4545 V4546 Q4547
R4548 F4551 Y4554 R4557 N4558 F4559 Y4560 R4563 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 SER GLY GLY GLY SER GLY TRP GLY SER GLY
ALA GLY GLU GLU ALA GLU GLY ASP GLU GLU N4626 M4627 V4628 Y4629 Y4630 F4631 L4632 E4633 E4634 S4635 T4636 G4637 Y4638 P4641 W4644 C4645 L4648 L4649 H4650 F4655 L4656 I4659 G4660 Y4661 M4662 K4665 V4666 R4673 E4674 K4675 A4678 R4679 K4680 L4681 E4682 F4683 D4684 G4685 L4686 Y4687 I4688
T4689 E4690 Q4691 P4692 G4693 D4694 D4695 D4696 V4697 K4698 G4699 Q4700 R4703 L4704 S4713 N4714 D4717 K4718 K4721 R4722 L4725 D4726 K4727 H4728 G4729 D4730 I4731 F4732 G4733 R4734 E4735 R4736 I4737 A4738 E4739 L4740 L4741 G4742 M4743 D4744 L4745 A4746 S4747 L4748 E4749 I4750 T4751 A4752 H4753 N4754 E4755 R4756 K4757 P4758 D4759
P4760 P4761 P4762 G4763 L4764 L4765 T4766 W4767 L4768 M4769 S4770 I4771 D4772 V4773 K4774 Y4775 Q4776 I4777 F4780 F4784 T4785 D4786 N4787 S4788 F4789 L4790 Y4791 W4794 L4800 H4803 Y4804 N4805 N4806 F4807 F4808 F4809 A4810 A4811 H4812 L4813 L4814 D4815 I4816 A4817 M4818 G4819 V4820 K4821 T4822 L4823 R4824 L4827 S4828
G4834 K4835 L4843 L4844 A4845 L4850 Y4851 A4855 F4856 N4857 F4858 F4859 R4860 K4861 F4862 Y4863 N4864 K4865 S4866 E4867 D4868 E4869 D4870 E4871 P4872 D4873 M4874 K4875 C4876 D4877 D4878 Y4883 L4884 F4885 H4886 M4887 G4890 V4891 R4892 A4893 G4894 G4895 G4896 I4897 G4898 D4899 E4900 I4901 E4902 A4905 G4906 D4907 R4913
D4917 F4922 F4923 V4924 I4925 L4928 L4929 L4943 Q4946 Q4947 K4951 E4952 D4953 M4954 K4957 I4960 C4961 G4962 I4963 G4964 S4965 D4966 Y4967 H4973 H4978 T4979 L4980 E4981 E4982 H4983 N4984 L4985 A4986 N4987 Y4988 M4989 F4990 L4995 I4996 N4997 K4998 D4999 E5000 T5001 E5002 G5005 Q5006 E5007
K5012 Q5015 E5016 R5017 D5020 F5021 F5022 P5023 A5024 G5025 D5026 C5027 F5028 R5029 K5030 Q5031 Y5032 E5033 D5034 Q5035 L5036 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	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	0.058	Depositor
Minimum map value	-0.029	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	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

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	0.30	0/834	0.52	0/1123
1	F	0.30	0/834	0.52	0/1123
1	H	0.30	0/834	0.53	0/1123
1	J	0.30	0/834	0.52	0/1123
2	B	0.29	0/25428	0.54	6/34534 (0.0%)
2	E	0.30	0/25428	0.54	6/34534 (0.0%)
2	G	0.29	0/25428	0.54	6/34534 (0.0%)
2	I	0.30	0/25428	0.54	6/34534 (0.0%)
All	All	0.30	0/105048	0.54	24/142628 (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	16
2	E	0	16
2	G	0	16
2	I	0	16
All	All	0	64

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	131	LEU	CA-CB-CG	8.01	133.72	115.30
2	B	131	LEU	CA-CB-CG	8.00	133.69	115.30
2	E	131	LEU	CA-CB-CG	7.99	133.68	115.30
2	I	131	LEU	CA-CB-CG	7.99	133.66	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	4985	LEU	CA-CB-CG	7.25	131.97	115.30
2	I	4985	LEU	CA-CB-CG	7.25	131.97	115.30
2	E	4985	LEU	CA-CB-CG	7.25	131.96	115.30
2	G	4985	LEU	CA-CB-CG	7.24	131.95	115.30
2	B	1600	LEU	CA-CB-CG	6.59	130.46	115.30
2	I	1600	LEU	CA-CB-CG	6.59	130.46	115.30
2	E	1600	LEU	CA-CB-CG	6.59	130.45	115.30
2	G	1600	LEU	CA-CB-CG	6.58	130.42	115.30
2	E	1676	LEU	CA-CB-CG	6.56	130.38	115.30
2	I	1676	LEU	CA-CB-CG	6.55	130.38	115.30
2	B	1676	LEU	CA-CB-CG	6.55	130.37	115.30
2	G	1676	LEU	CA-CB-CG	6.55	130.36	115.30
2	E	977	LEU	CA-CB-CG	5.71	128.43	115.30
2	I	977	LEU	CA-CB-CG	5.70	128.41	115.30
2	G	977	LEU	CA-CB-CG	5.70	128.40	115.30
2	B	977	LEU	CA-CB-CG	5.69	128.39	115.30
2	I	688	LEU	CA-CB-CG	5.09	127.02	115.30
2	E	688	LEU	CA-CB-CG	5.08	126.99	115.30
2	B	688	LEU	CA-CB-CG	5.07	126.97	115.30
2	G	688	LEU	CA-CB-CG	5.07	126.97	115.30

There are no chirality outliers.

All (64) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	312	THR	Peptide
2	B	3971	GLY	Peptide
2	B	4228	ALA	Peptide
2	B	4641	PRO	Peptide
2	B	4666	VAL	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	E	1676	LEU	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	312	THR	Peptide
2	E	3971	GLY	Peptide
2	E	4228	ALA	Peptide
2	E	4641	PRO	Peptide
2	E	4666	VAL	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4228	ALA	Peptide
2	G	4641	PRO	Peptide
2	G	4666	VAL	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	312	THR	Peptide
2	I	3971	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	I	4228	ALA	Peptide
2	I	4641	PRO	Peptide
2	I	4666	VAL	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	16	0
1	F	818	0	824	18	0
1	H	818	0	824	15	0
1	J	818	0	824	14	0
2	B	29499	0	24746	268	0
2	E	29499	0	24746	273	0
2	G	29499	0	24746	261	0
2	I	29499	0	24746	262	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
All	All	121272	0	102280	1100	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 5.

All (1100) 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:I:379:HIS:HD2	2:I:382:GLY:H	1.40	0.68
2:E:379:HIS:HD2	2:E:382:GLY:H	1.40	0.67
2:B:379:HIS:HD2	2:B:382:GLY:H	1.40	0.67
2:G:379:HIS:HD2	2:G:382:GLY:H	1.40	0.66
2:B:3773:ARG:HG3	2:B:3815:LYS:HZ3	1.61	0.65
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.61	0.65
2:I:3773:ARG:HG3	2:I:3815:LYS:HZ3	1.62	0.64
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.61	0.64
2:E:938:HIS:HB2	2:E:1054:GLU:HB2	1.79	0.64
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.61	0.64
2:I:938:HIS:HB2	2:I:1054:GLU:HB2	1.79	0.64
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.81	0.63
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.81	0.63
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.81	0.63
2:G:938:HIS:HB2	2:G:1054:GLU:HB2	1.79	0.62
2:B:938:HIS:HB2	2:B:1054:GLU:HB2	1.79	0.62
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.81	0.62
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.82	0.62
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.82	0.61
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.82	0.61
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.82	0.61
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.32	0.61
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.32	0.61
2:G:3773:ARG:HG3	2:G:3815:LYS:HZ3	1.65	0.61
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.33	0.61
2:E:331:VAL:HG12	2:E:333:GLY:H	1.65	0.61
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.82	0.61
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.32	0.61
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.82	0.61
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.83	0.61
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.83	0.61
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.82	0.61
2:G:3755:GLU:O	2:G:3762:ARG:NH2	2.34	0.61
2:I:3755:GLU:O	2:I:3762:ARG:NH2	2.34	0.61
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.83	0.61
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.83	0.60
2:B:3755:GLU:O	2:B:3762:ARG:NH2	2.34	0.60
2:B:331:VAL:HG12	2:B:333:GLY:H	1.65	0.60
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.83	0.60
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.82	0.60
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.83	0.60
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.82	0.60
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.83	0.60
2:E:3755:GLU:O	2:E:3762:ARG:NH2	2.34	0.60
2:G:331:VAL:HG12	2:G:333:GLY:H	1.65	0.60
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.35	0.60
2:I:683:ARG:NH1	2:I:707:VAL:O	2.34	0.60
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.35	0.60
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.82	0.60
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.35	0.60
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.83	0.59
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.84	0.59
2:I:331:VAL:HG12	2:I:333:GLY:H	1.66	0.59
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.83	0.59
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.82	0.59
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.83	0.59
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.83	0.59
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.83	0.59
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.82	0.59
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.85	0.59
2:E:683:ARG:NH1	2:E:707:VAL:O	2.34	0.59
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.36	0.59
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.85	0.58
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.85	0.58
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.86	0.58
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.35	0.58
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.84	0.58
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.86	0.58
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.36	0.58
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.86	0.58
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.85	0.58
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.37	0.58
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.86	0.58
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.37	0.58
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.37	0.57
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.86	0.57
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.37	0.57
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.85	0.57
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.37	0.57
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.37	0.57
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.37	0.57
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.36	0.57
2:I:4172:GLU:HA	2:I:4175:ARG:HE	1.69	0.57
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.87	0.57
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.36	0.57
2:E:132:ALA:HA	2:E:194:SER:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.37	0.57
2:G:614:VAL:HG22	2:G:616:SER:H	1.69	0.57
2:B:614:VAL:HG22	2:B:616:SER:H	1.69	0.56
2:I:614:VAL:HG22	2:I:616:SER:H	1.69	0.56
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.86	0.56
2:G:4172:GLU:HA	2:G:4175:ARG:HE	1.69	0.56
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.87	0.56
2:E:4172:GLU:HA	2:E:4175:ARG:HE	1.69	0.56
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.87	0.56
2:B:132:ALA:HA	2:B:194:SER:HB2	1.87	0.56
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.88	0.56
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.86	0.56
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.88	0.56
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.88	0.56
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.87	0.56
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.39	0.56
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.39	0.56
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.39	0.56
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.86	0.56
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.39	0.56
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.87	0.56
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.39	0.56
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.39	0.56
2:G:132:ALA:HA	2:G:194:SER:HB2	1.87	0.56
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.88	0.56
1:A:5:GLU:HB2	1:A:73:LYS:HB3	1.88	0.56
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.87	0.56
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.87	0.56
2:I:132:ALA:HA	2:I:194:SER:HB2	1.87	0.56
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.88	0.56
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.87	0.56
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.88	0.56
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.88	0.56
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.88	0.56
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.88	0.56
2:G:1271:ARG:HA	2:G:1471:UNK:HA	1.88	0.56
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.88	0.56
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.87	0.55
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.88	0.55
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.88	0.55
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.89	0.55
2:I:1271:ARG:HA	2:I:1471:UNK:HA	1.88	0.55
2:E:1271:ARG:HA	2:E:1471:UNK:HA	1.88	0.55
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.39	0.55
2:G:2347:GLU:O	2:G:2351:ASN:N	2.39	0.55
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.89	0.55
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.89	0.55
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.39	0.55
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.40	0.55
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.39	0.55
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.87	0.55
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.88	0.55
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.38	0.55
2:B:683:ARG:NH1	2:B:707:VAL:O	2.34	0.55
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.89	0.55
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.89	0.55
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.39	0.55
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.89	0.55
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.72	0.55
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.88	0.55
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.89	0.55
1:F:5:GLU:HB2	1:F:73:LYS:HB3	1.88	0.55
2:E:614:VAL:HG22	2:E:616:SER:H	1.69	0.55
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.40	0.55
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.39	0.55
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.89	0.55
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.39	0.55
2:B:4172:GLU:HA	2:B:4175:ARG:HE	1.69	0.55
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.88	0.55
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.40	0.55
2:I:241:GLN:O	2:I:289:ARG:NH1	2.37	0.55
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.89	0.55
2:B:1271:ARG:HA	2:B:1471:UNK:HA	1.88	0.55
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.72	0.55
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.40	0.55
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.40	0.55
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.88	0.55
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.89	0.55
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.89	0.55
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.72	0.55
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:164:ARG:N	2:I:167:ASP:OD2	2.41	0.54
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.89	0.54
2:G:683:ARG:NH1	2:G:707:VAL:O	2.33	0.54
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.72	0.54
1:H:5:GLU:HB2	1:H:73:LYS:HB3	1.88	0.54
1:J:5:GLU:HB2	1:J:73:LYS:HB3	1.88	0.54
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.89	0.54
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.89	0.54
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.40	0.54
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.89	0.54
2:E:4763:GLY:H	2:E:4767:TRP:HE1	1.56	0.54
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.41	0.54
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.88	0.54
2:B:4978:HIS:HA	2:B:4982:GLU:HB2	1.90	0.54
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.41	0.54
2:B:4763:GLY:H	2:B:4767:TRP:HE1	1.56	0.54
2:E:609:CYS:SG	2:E:610:ASN:N	2.80	0.54
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.89	0.54
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.89	0.54
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.72	0.54
2:G:4763:GLY:H	2:G:4767:TRP:HE1	1.56	0.54
2:I:4978:HIS:HA	2:I:4982:GLU:HB2	1.90	0.54
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.40	0.54
2:G:164:ARG:N	2:G:167:ASP:OD2	2.41	0.54
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.88	0.54
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.90	0.54
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.73	0.54
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.90	0.54
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.90	0.53
2:E:4978:HIS:HA	2:E:4982:GLU:HB2	1.90	0.53
2:G:241:GLN:O	2:G:289:ARG:NH1	2.37	0.53
2:G:609:CYS:SG	2:G:610:ASN:N	2.80	0.53
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.73	0.53
2:B:609:CYS:SG	2:B:610:ASN:N	2.80	0.53
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.91	0.53
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.41	0.53
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.74	0.53
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.41	0.53
2:I:2347:GLU:O	2:I:2351:ASN:N	2.39	0.53
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.73	0.53
2:I:609:CYS:SG	2:I:610:ASN:N	2.80	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.74	0.53
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.73	0.53
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.90	0.53
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.73	0.53
2:I:4763:GLY:H	2:I:4767:TRP:HE1	1.56	0.53
2:E:164:ARG:N	2:E:167:ASP:OD2	2.41	0.53
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.74	0.53
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.90	0.53
2:E:978:THR:HB	2:E:980:ALA:H	1.74	0.53
2:G:3973:CYS:SG	2:G:3976:ASN:ND2	2.82	0.53
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.73	0.53
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.41	0.53
2:B:3973:CYS:SG	2:B:3976:ASN:ND2	2.82	0.53
2:E:2347:GLU:O	2:E:2351:ASN:N	2.39	0.53
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.73	0.53
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.91	0.53
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.73	0.53
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.42	0.53
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.91	0.53
2:B:978:THR:HB	2:B:980:ALA:H	1.74	0.53
2:I:3973:CYS:SG	2:I:3976:ASN:ND2	2.82	0.53
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.74	0.53
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	1.91	0.53
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.41	0.53
2:B:164:ARG:N	2:B:167:ASP:OD2	2.41	0.52
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.40	0.52
2:G:290:TYR:O	2:G:302:VAL:N	2.43	0.52
2:G:4978:HIS:HA	2:G:4982:GLU:HB2	1.90	0.52
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.74	0.52
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.74	0.52
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.74	0.52
2:G:645:ARG:N	2:G:824:GLU:O	2.40	0.52
2:B:2347:GLU:O	2:B:2351:ASN:N	2.39	0.52
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.91	0.52
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.75	0.52
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.73	0.52
2:G:978:THR:HB	2:G:980:ALA:H	1.74	0.52
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	1.91	0.52
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.42	0.52
2:E:470:SER:O	2:E:474:ARG:NE	2.39	0.52
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.92	0.52
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.92	0.52
2:E:290:TYR:O	2:E:302:VAL:N	2.42	0.52
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.92	0.52
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.75	0.52
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.41	0.52
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.43	0.52
2:I:290:TYR:O	2:I:302:VAL:N	2.42	0.52
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.74	0.52
2:E:1660:GLN:HG3	2:E:1707:LEU:HD13	1.92	0.52
2:E:3973:CYS:SG	2:E:3976:ASN:ND2	2.82	0.52
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.43	0.52
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.91	0.52
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.43	0.52
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.43	0.52
2:I:978:THR:HB	2:I:980:ALA:H	1.74	0.52
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.42	0.52
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.91	0.52
2:B:1660:GLN:HG3	2:B:1707:LEU:HD13	1.92	0.52
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.74	0.52
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.74	0.52
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.91	0.51
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.92	0.51
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	1.91	0.51
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.44	0.51
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.93	0.51
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.92	0.51
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.93	0.51
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.43	0.51
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.43	0.51
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.91	0.51
2:B:290:TYR:O	2:B:302:VAL:N	2.43	0.51
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.93	0.51
2:B:3984:ARG:HH22	2:I:161:GLU:HG2	1.74	0.51
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.43	0.51
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.43	0.51
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.93	0.51
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.75	0.51
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.43	0.51
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.92	0.51
2:I:645:ARG:N	2:I:824:GLU:O	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:345:LEU:HD23	2:E:389:PHE:HB3	1.93	0.51
2:G:345:LEU:HD23	2:G:389:PHE:HB3	1.93	0.51
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.75	0.51
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.92	0.51
2:B:241:GLN:O	2:B:289:ARG:NH1	2.37	0.51
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.39	0.51
2:B:3948:LYS:NZ	2:B:4008:SER:O	2.44	0.51
2:I:315:CYS:SG	2:I:316:PHE:N	2.84	0.51
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.92	0.51
2:G:1660:GLN:HG3	2:G:1707:LEU:HD13	1.92	0.51
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.91	0.51
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.93	0.51
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.41	0.51
2:I:2452:ARG:HH12	2:G:177:GLU:HG3	1.76	0.51
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.93	0.51
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.93	0.51
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.43	0.51
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.93	0.51
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.75	0.51
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.44	0.51
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.75	0.51
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.93	0.51
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.43	0.51
2:G:4567:LEU:HA	2:G:4816:ILE:HD12	1.93	0.51
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.92	0.50
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.43	0.50
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.39	0.50
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.92	0.50
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.93	0.50
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.93	0.50
2:B:1516:UNK:N	2:B:1529:UNK:O	2.45	0.50
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.75	0.50
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.92	0.50
2:G:470:SER:O	2:G:474:ARG:NE	2.40	0.50
2:G:1516:UNK:N	2:G:1529:UNK:O	2.45	0.50
2:G:2095:GLN:NE2	2:G:2127:GLN:O	2.42	0.50
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.92	0.50
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.94	0.50
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.93	0.50
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.75	0.50
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:CYS:SG	2:B:316:PHE:N	2.84	0.50
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.92	0.50
2:E:315:CYS:SG	2:E:316:PHE:N	2.84	0.50
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.93	0.50
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.93	0.50
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.92	0.50
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	1.91	0.50
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.92	0.50
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.94	0.50
2:I:345:LEU:HD23	2:I:389:PHE:HB3	1.93	0.50
2:I:572:PRO:HA	2:I:575:LEU:HD13	1.94	0.50
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.92	0.50
2:E:4065:PHE:HB3	2:E:4132:PHE:CE2	2.47	0.50
2:E:4176:PRO:O	2:E:4202:ARG:NH1	2.45	0.50
2:E:4567:LEU:HA	2:E:4816:ILE:HD12	1.93	0.50
2:G:864:PRO:HD2	2:G:867:LEU:HD12	1.94	0.50
2:B:572:PRO:HA	2:B:575:LEU:HD13	1.94	0.50
2:B:4176:PRO:O	2:B:4202:ARG:NH1	2.45	0.50
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.93	0.50
2:G:315:CYS:SG	2:G:316:PHE:N	2.84	0.50
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.93	0.50
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.92	0.50
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.44	0.50
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.94	0.50
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.93	0.50
2:E:1516:UNK:N	2:E:1529:UNK:O	2.45	0.50
2:E:3948:LYS:NZ	2:E:4008:SER:O	2.44	0.50
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.93	0.50
2:G:4065:PHE:HB3	2:G:4132:PHE:CE2	2.47	0.50
2:G:4176:PRO:O	2:G:4202:ARG:NH1	2.45	0.50
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.94	0.50
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.93	0.50
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.93	0.50
2:B:4065:PHE:HB3	2:B:4132:PHE:CE2	2.47	0.50
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.92	0.50
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.94	0.50
2:B:4567:LEU:HA	2:B:4816:ILE:HD12	1.93	0.50
2:I:1660:GLN:HG3	2:I:1707:LEU:HD13	1.92	0.50
2:I:2871:LEU:HD22	2:I:2927:LEU:HD22	1.94	0.50
2:E:572:PRO:HA	2:E:575:LEU:HD13	1.94	0.50
2:E:3773:ARG:HG3	2:E:3815:LYS:HZ3	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.93	0.50
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.93	0.50
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.44	0.50
2:B:470:SER:O	2:B:474:ARG:NE	2.40	0.49
2:B:2871:LEU:HD22	2:B:2927:LEU:HD22	1.94	0.49
2:I:3762:ARG:H	2:I:4754:ASN:HA	1.77	0.49
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.77	0.49
2:I:4176:PRO:O	2:I:4202:ARG:NH1	2.45	0.49
2:I:4567:LEU:HA	2:I:4816:ILE:HD12	1.93	0.49
2:E:173:SER:HB3	2:E:178:ARG:H	1.77	0.49
2:E:241:GLN:O	2:E:289:ARG:NH1	2.37	0.49
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.43	0.49
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.93	0.49
1:J:26:TYR:OH	1:J:42:ARG:NH2	2.45	0.49
2:B:3762:ARG:H	2:B:4754:ASN:HA	1.77	0.49
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.77	0.49
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.46	0.49
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.92	0.49
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.46	0.49
1:A:82:TYR:O	1:A:86:GLY:N	2.43	0.49
2:B:345:LEU:HD23	2:B:389:PHE:HB3	1.93	0.49
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.44	0.49
2:I:1516:UNK:N	2:I:1529:UNK:O	2.45	0.49
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.92	0.49
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.94	0.49
2:G:2871:LEU:HD22	2:G:2927:LEU:HD22	1.94	0.49
2:B:309:THR:O	2:B:313:SER:OG	2.31	0.49
2:B:864:PRO:HD2	2:B:867:LEU:HD12	1.94	0.49
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.46	0.49
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.94	0.49
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.94	0.49
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.94	0.49
2:I:3948:LYS:NZ	2:I:4008:SER:O	2.44	0.49
2:E:2871:LEU:HD22	2:E:2927:LEU:HD22	1.94	0.49
2:G:309:THR:O	2:G:313:SER:OG	2.31	0.49
2:G:572:PRO:HA	2:G:575:LEU:HD13	1.94	0.49
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.94	0.49
2:G:4767:TRP:HE3	2:G:4770:SER:HB2	1.78	0.49
2:B:286:THR:HA	2:B:405:HIS:HB2	1.95	0.49
2:I:286:THR:HA	2:I:405:HIS:HB2	1.95	0.49
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.95	0.49
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.94	0.49
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.44	0.49
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.46	0.49
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.93	0.49
2:B:645:ARG:N	2:B:824:GLU:O	2.40	0.49
2:B:999:ASP:O	2:B:1004:GLY:N	2.46	0.49
2:B:4767:TRP:HE3	2:B:4770:SER:HB2	1.78	0.49
2:I:864:PRO:HD2	2:I:867:LEU:HD12	1.94	0.49
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.94	0.49
2:E:999:ASP:O	2:E:1004:GLY:N	2.46	0.49
1:F:26:TYR:OH	1:F:42:ARG:NH2	2.45	0.49
1:A:26:TYR:OH	1:A:42:ARG:NH2	2.45	0.49
2:I:309:THR:O	2:I:313:SER:OG	2.31	0.49
2:I:4767:TRP:HE3	2:I:4770:SER:HB2	1.78	0.49
2:E:3762:ARG:H	2:E:4754:ASN:HA	1.77	0.49
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.93	0.49
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.78	0.49
1:H:6:THR:HA	1:H:72:ALA:HA	1.94	0.49
1:H:26:TYR:OH	1:H:42:ARG:NH2	2.45	0.49
2:B:173:SER:HB3	2:B:178:ARG:H	1.77	0.49
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.95	0.49
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.46	0.49
2:I:134:ASP:OD1	2:I:134:ASP:N	2.46	0.49
2:I:999:ASP:O	2:I:1004:GLY:N	2.46	0.49
2:E:286:THR:HA	2:E:405:HIS:HB2	1.95	0.49
2:E:309:THR:O	2:E:313:SER:OG	2.31	0.49
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.46	0.49
2:E:4767:TRP:HE3	2:E:4770:SER:HB2	1.78	0.49
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.93	0.49
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.93	0.49
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.94	0.49
2:G:286:THR:HA	2:G:405:HIS:HB2	1.95	0.49
2:G:2121:PHE:O	2:G:3725:TYR:OH	2.30	0.49
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.46	0.49
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.94	0.49
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.94	0.49
2:I:16:THR:OG1	2:I:97:GLY:O	2.31	0.49
2:I:173:SER:HB3	2:I:178:ARG:H	1.77	0.49
2:I:2368:LEU:HD13	2:I:2376:LEU:HD23	1.95	0.49
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4065:PHE:HB3	2:I:4132:PHE:CE2	2.47	0.49
2:G:999:ASP:O	2:G:1004:GLY:N	2.46	0.49
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.77	0.49
2:G:3948:LYS:NZ	2:G:4008:SER:O	2.44	0.49
1:A:6:THR:HA	1:A:72:ALA:HA	1.94	0.48
2:I:4138:ASP:O	2:I:4142:ASN:ND2	2.46	0.48
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.78	0.48
2:E:606:LEU:O	2:E:617:ASN:ND2	2.46	0.48
2:E:3767:GLN:NE2	2:E:3803:SER:O	2.46	0.48
1:F:6:THR:HA	1:F:72:ALA:HA	1.94	0.48
2:B:2095:GLN:NE2	2:B:2127:GLN:O	2.42	0.48
2:I:3767:GLN:NE2	2:I:3803:SER:O	2.46	0.48
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.46	0.48
2:E:4987:ASN:HA	2:E:4990:PHE:HD2	1.78	0.48
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.96	0.48
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.96	0.48
2:B:641:VAL:HG11	2:B:681:HIS:HD1	1.79	0.48
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.47	0.48
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.96	0.48
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.47	0.48
2:I:4987:ASN:HA	2:I:4990:PHE:HD2	1.78	0.48
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.85	0.48
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.46	0.48
2:G:4138:ASP:O	2:G:4142:ASN:ND2	2.47	0.48
2:B:2368:LEU:HD13	2:B:2376:LEU:HD23	1.95	0.48
2:B:4071:ILE:HD11	2:B:4102:GLN:HE21	1.79	0.48
2:E:641:VAL:HG11	2:E:681:HIS:HD1	1.79	0.48
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.95	0.48
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.94	0.48
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.95	0.48
2:G:1270:LEU:O	2:G:1472:UNK:N	2.47	0.48
2:G:3762:ARG:H	2:G:4754:ASN:HA	1.77	0.48
2:I:641:VAL:HG11	2:I:681:HIS:HD1	1.79	0.48
2:I:1270:LEU:O	2:I:1472:UNK:N	2.47	0.48
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.46	0.48
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.39	0.48
2:E:1270:LEU:O	2:E:1472:UNK:N	2.47	0.48
2:E:4138:ASP:O	2:E:4142:ASN:ND2	2.47	0.48
2:G:2368:LEU:HD13	2:G:2376:LEU:HD23	1.95	0.48
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.96	0.48
2:I:606:LEU:O	2:I:617:ASN:ND2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.96	0.48
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.47	0.48
2:E:4071:ILE:HD11	2:E:4102:GLN:HE21	1.79	0.48
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.94	0.48
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.78	0.48
2:B:606:LEU:O	2:B:617:ASN:ND2	2.46	0.48
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.96	0.48
2:B:1991:THR:O	2:B:1995:THR:OG1	2.32	0.48
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.96	0.48
2:I:1991:THR:O	2:I:1995:THR:OG1	2.32	0.48
2:E:2368:LEU:HD13	2:E:2376:LEU:HD23	1.95	0.48
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.39	0.48
2:G:606:LEU:O	2:G:617:ASN:ND2	2.46	0.48
1:J:6:THR:HA	1:J:72:ALA:HA	1.94	0.48
2:B:280:LEU:HD21	2:B:316:PHE:HE2	1.78	0.48
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.43	0.48
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.96	0.48
2:I:2121:PHE:O	2:I:3725:TYR:OH	2.30	0.48
2:G:16:THR:OG1	2:G:97:GLY:O	2.31	0.48
2:G:4987:ASN:HA	2:G:4990:PHE:HD2	1.78	0.48
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.95	0.48
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.96	0.48
2:E:4059:LEU:HD13	2:E:4167:ALA:HB2	1.96	0.48
2:G:4071:ILE:HD11	2:G:4102:GLN:HE21	1.79	0.48
1:F:82:TYR:O	1:F:86:GLY:N	2.43	0.48
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.96	0.48
2:B:1270:LEU:O	2:B:1472:UNK:N	2.47	0.48
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.46	0.48
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.96	0.48
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.96	0.48
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.96	0.48
2:G:134:ASP:OD1	2:G:134:ASP:N	2.46	0.48
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	1.96	0.47
2:I:280:LEU:HD21	2:I:316:PHE:HE2	1.78	0.47
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.96	0.47
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	1.96	0.47
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.77	0.47
2:G:173:SER:HB3	2:G:178:ARG:H	1.77	0.47
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.96	0.47
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	1.96	0.47
1:J:82:TYR:O	1:J:86:GLY:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:ASP:OD1	2:B:134:ASP:N	2.46	0.47
2:B:3767:GLN:NE2	2:B:3803:SER:O	2.46	0.47
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	1.96	0.47
2:I:1077:ALA:HB3	2:I:1189:LEU:HD11	1.96	0.47
2:I:4071:ILE:HD11	2:I:4102:GLN:HE21	1.79	0.47
2:G:1171:SER:HG	2:G:1175:SER:H	1.59	0.47
2:G:1247:PRO:HA	2:G:1598:GLN:HA	1.96	0.47
2:G:1991:THR:O	2:G:1995:THR:OG1	2.32	0.47
2:B:16:THR:OG1	2:B:97:GLY:O	2.31	0.47
2:B:4138:ASP:O	2:B:4142:ASN:ND2	2.46	0.47
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.33	0.47
2:B:4957:LYS:HG2	2:B:4964:GLY:HA2	1.97	0.47
2:B:4987:ASN:HA	2:B:4990:PHE:HD2	1.78	0.47
2:I:485:SER:O	2:I:489:ASN:N	2.43	0.47
2:I:579:GLN:H	2:I:582:HIS:HD2	1.63	0.47
2:E:134:ASP:N	2:E:134:ASP:OD1	2.46	0.47
2:E:1077:ALA:HB3	2:E:1189:LEU:HD11	1.97	0.47
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.47	0.47
2:B:4059:LEU:HD13	2:B:4167:ALA:HB2	1.96	0.47
2:I:470:SER:O	2:I:474:ARG:NE	2.39	0.47
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.96	0.47
2:I:1457:UNK:N	2:I:1497:UNK:O	2.47	0.47
2:I:4059:LEU:HD13	2:I:4167:ALA:HB2	1.96	0.47
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.96	0.47
2:E:1991:THR:O	2:E:1995:THR:OG1	2.32	0.47
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.95	0.47
2:G:1457:UNK:N	2:G:1497:UNK:O	2.47	0.47
2:G:4571:PHE:O	2:G:4575:PHE:N	2.48	0.47
2:B:1077:ALA:HB3	2:B:1189:LEU:HD11	1.96	0.47
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.88	0.47
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.48	0.47
2:E:280:LEU:HD21	2:E:316:PHE:HE2	1.78	0.47
2:E:2095:GLN:NE2	2:E:2127:GLN:O	2.42	0.47
2:G:485:SER:O	2:G:489:ASN:N	2.43	0.47
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.88	0.47
2:I:4571:PHE:O	2:I:4575:PHE:N	2.48	0.47
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.96	0.47
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.80	0.47
2:G:3767:GLN:NE2	2:G:3803:SER:O	2.46	0.47
2:B:454:PRO:HG2	2:B:531:ARG:HH12	1.80	0.47
2:B:1457:UNK:N	2:B:1497:UNK:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.96	0.47
2:I:4228:ALA:O	2:I:4232:GLU:N	2.48	0.47
2:I:4957:LYS:HG2	2:I:4964:GLY:HA2	1.97	0.47
2:E:454:PRO:HG2	2:E:531:ARG:HH12	1.80	0.47
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	1.97	0.47
2:E:4571:PHE:O	2:E:4575:PHE:N	2.48	0.47
2:G:280:LEU:HD21	2:G:316:PHE:HE2	1.78	0.47
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.80	0.47
2:G:1077:ALA:HB3	2:G:1189:LEU:HD11	1.97	0.47
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.96	0.47
2:B:342:GLY:N	2:B:390:LEU:O	2.48	0.47
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.96	0.47
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.96	0.47
2:E:1247:PRO:HA	2:E:1598:GLN:HA	1.96	0.47
2:E:2121:PHE:O	2:E:3725:TYR:OH	2.30	0.47
2:G:641:VAL:HG11	2:G:681:HIS:HD1	1.79	0.47
2:B:1247:PRO:HA	2:B:1598:GLN:HA	1.96	0.47
2:B:4892:ARG:NH2	2:I:4895:GLY:O	2.39	0.47
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.80	0.47
2:E:16:THR:OG1	2:E:97:GLY:O	2.31	0.47
2:E:670:GLU:HG3	2:E:787:VAL:HG13	1.97	0.47
2:G:579:GLN:H	2:G:582:HIS:HD2	1.63	0.47
1:A:11:ASP:OD1	1:A:67:SER:OG	2.30	0.47
2:B:579:GLN:H	2:B:582:HIS:HD2	1.63	0.47
2:B:670:GLU:HG3	2:B:787:VAL:HG13	1.97	0.47
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.88	0.47
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.96	0.47
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.96	0.47
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.80	0.46
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.85	0.46
2:G:342:GLY:N	2:G:390:LEU:O	2.48	0.46
2:G:1243:PRO:HB2	2:G:1600:LEU:HD22	1.97	0.46
2:G:4228:ALA:O	2:G:4232:GLU:N	2.48	0.46
2:E:161:GLU:HG2	2:G:3984:ARG:HH22	1.80	0.46
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.88	0.46
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.97	0.46
2:B:1694:LEU:O	2:B:1712:TYR:OH	2.25	0.46
2:B:2208:MET:SD	2:B:2253:HIS:ND1	2.85	0.46
2:E:1457:UNK:N	2:E:1497:UNK:O	2.47	0.46
2:E:2208:MET:SD	2:E:2253:HIS:ND1	2.85	0.46
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4191:GLU:OE1	2:B:5006:GLN:NE2	2.48	0.46
2:B:4571:PHE:O	2:B:4575:PHE:N	2.48	0.46
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.98	0.46
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.80	0.46
2:E:579:GLN:H	2:E:582:HIS:HD2	1.63	0.46
2:E:4191:GLU:OE1	2:E:5006:GLN:NE2	2.48	0.46
2:E:4957:LYS:HG2	2:E:4964:GLY:HA2	1.97	0.46
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.80	0.46
2:B:221:ARG:NE	2:B:258:SER:OG	2.43	0.46
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.46	0.46
2:I:1247:PRO:HA	2:I:1598:GLN:HA	1.96	0.46
2:I:3771:HIS:O	2:I:3774:GLY:N	2.45	0.46
2:I:4925:ILE:HA	2:I:4929:LEU:HD23	1.98	0.46
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.48	0.46
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.98	0.46
2:B:4228:ALA:O	2:B:4232:GLU:N	2.48	0.46
2:E:649:PHE:HB3	2:E:776:LEU:HD13	1.98	0.46
2:E:4227:GLU:OE2	2:G:4973:HIS:ND1	2.49	0.46
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.80	0.46
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.85	0.46
2:B:1972:ASN:HD21	2:B:2024:PRO:HB3	1.81	0.46
2:B:2810:LYS:O	2:B:2814:LYS:N	2.45	0.46
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.97	0.46
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.33	0.46
2:E:342:GLY:N	2:E:390:LEU:O	2.48	0.46
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.98	0.46
2:E:1972:ASN:HD21	2:E:2024:PRO:HB3	1.81	0.46
2:G:4059:LEU:HD13	2:G:4167:ALA:HB2	1.96	0.46
2:B:649:PHE:HB3	2:B:776:LEU:HD13	1.98	0.46
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.80	0.46
2:E:221:ARG:NE	2:E:258:SER:OG	2.44	0.46
2:E:3759:GLU:OE1	2:E:3762:ARG:NH2	2.43	0.46
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.98	0.46
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.96	0.46
2:G:689:THR:H	2:G:778:PHE:HE2	1.64	0.46
2:G:4957:LYS:HG2	2:G:4964:GLY:HA2	1.97	0.46
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.48	0.46
2:I:1972:ASN:HD21	2:I:2024:PRO:HB3	1.81	0.46
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.48	0.46
2:G:4191:GLU:OE1	2:G:5006:GLN:NE2	2.48	0.46
1:F:34:LYS:HD3	2:E:629:ARG:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.80	0.46
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	1.97	0.46
2:I:4191:GLU:OE1	2:I:5006:GLN:NE2	2.48	0.46
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.46	0.46
2:G:3759:GLU:OE1	2:G:3762:ARG:NH2	2.43	0.46
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.82	0.45
2:B:4005:GLN:HE21	2:B:4110:PHE:HE1	1.64	0.45
2:I:346:CYS:N	2:I:388:LEU:O	2.49	0.45
2:I:4581:LYS:HD2	2:I:4632:LEU:HD22	1.98	0.45
2:E:485:SER:O	2:E:489:ASN:N	2.43	0.45
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.98	0.45
2:G:395:GLN:HG3	2:G:397:GLU:H	1.81	0.45
2:G:3959:LYS:O	2:G:3963:ASN:ND2	2.49	0.45
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.46	0.45
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.99	0.45
2:I:2208:MET:SD	2:I:2253:HIS:ND1	2.85	0.45
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.98	0.45
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.98	0.45
2:E:395:GLN:HG3	2:E:397:GLU:H	1.81	0.45
2:E:4005:GLN:HE21	2:E:4110:PHE:HE1	1.64	0.45
2:G:346:CYS:N	2:G:388:LEU:O	2.49	0.45
2:G:4005:GLN:HE21	2:G:4110:PHE:HE1	1.64	0.45
2:G:4925:ILE:HA	2:G:4929:LEU:HD23	1.98	0.45
2:I:670:GLU:HG3	2:I:787:VAL:HG13	1.97	0.45
2:I:689:THR:H	2:I:778:PHE:HE2	1.64	0.45
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.30	0.45
2:E:379:HIS:CD2	2:E:381:GLU:H	2.35	0.45
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.80	0.45
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.52	0.45
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.81	0.45
2:E:2272:PRO:HA	2:E:2275:VAL:HG12	1.99	0.45
2:E:3365:UNK:O	2:E:3369:UNK:N	2.50	0.45
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.81	0.45
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	1.99	0.45
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.98	0.45
1:H:82:TYR:O	1:H:86:GLY:N	2.43	0.45
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	1.99	0.45
2:B:3959:LYS:O	2:B:3963:ASN:ND2	2.49	0.45
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	1.99	0.45
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.98	0.45
2:E:689:THR:H	2:E:778:PHE:HE2	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.33	0.45
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.98	0.45
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.99	0.45
2:B:346:CYS:N	2:B:388:LEU:O	2.49	0.45
2:B:379:HIS:CD2	2:B:381:GLU:H	2.35	0.45
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.98	0.45
2:E:3959:LYS:O	2:E:3963:ASN:ND2	2.49	0.45
2:G:649:PHE:HB3	2:G:776:LEU:HD13	1.98	0.45
2:G:670:GLU:HG3	2:G:787:VAL:HG13	1.97	0.45
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.99	0.45
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.99	0.45
2:B:4581:LYS:HD2	2:B:4632:LEU:HD22	1.98	0.45
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.98	0.45
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.97	0.45
2:E:346:CYS:N	2:E:388:LEU:O	2.49	0.45
2:G:379:HIS:CD2	2:G:381:GLU:H	2.35	0.45
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.99	0.45
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.98	0.45
2:B:4925:ILE:HA	2:B:4929:LEU:HD23	1.98	0.45
2:I:342:GLY:N	2:I:390:LEU:O	2.48	0.45
2:I:649:PHE:HB3	2:I:776:LEU:HD13	1.98	0.45
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.98	0.45
2:G:2272:PRO:HA	2:G:2275:VAL:HG12	1.99	0.45
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.82	0.45
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.81	0.45
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.52	0.45
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	1.99	0.45
2:E:2908:TYR:OH	2:E:2920:ARG:NE	2.48	0.45
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.98	0.45
2:G:4075:GLU:HA	2:G:4078:GLN:HB2	1.99	0.45
2:B:41:GLY:O	2:B:45:ARG:NH1	2.50	0.45
2:B:395:GLN:HG3	2:B:397:GLU:H	1.81	0.45
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	1.97	0.45
2:B:2272:PRO:HA	2:B:2275:VAL:HG12	1.99	0.45
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	1.99	0.45
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.81	0.45
2:E:2810:LYS:O	2:E:2814:LYS:N	2.45	0.45
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	1.99	0.45
2:E:4581:LYS:HD2	2:E:4632:LEU:HD22	1.98	0.45
2:G:41:GLY:O	2:G:45:ARG:NH1	2.50	0.45
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.99	0.45
2:G:3771:HIS:O	2:G:3774:GLY:N	2.45	0.45
2:B:177:GLU:HG3	2:E:2452:ARG:HH12	1.81	0.44
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.52	0.44
2:B:3365:UNK:O	2:B:3369:UNK:N	2.50	0.44
2:I:395:GLN:HG3	2:I:397:GLU:H	1.81	0.44
2:E:4228:ALA:O	2:E:4232:GLU:N	2.48	0.44
2:G:1972:ASN:HD21	2:G:2024:PRO:HB3	1.81	0.44
2:G:3759:GLU:HG3	2:G:3763:LEU:HD22	1.99	0.44
2:G:4581:LYS:HD2	2:G:4632:LEU:HD22	1.98	0.44
2:B:689:THR:H	2:B:778:PHE:HE2	1.64	0.44
2:B:3981:ALA:HA	2:B:3986:TRP:HE1	1.83	0.44
2:I:4075:GLU:HA	2:I:4078:GLN:HB2	1.99	0.44
2:E:645:ARG:N	2:E:824:GLU:O	2.40	0.44
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.82	0.44
2:B:243:ARG:NH1	2:B:301:VAL:O	2.44	0.44
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.85	0.44
2:B:2381:GLU:HA	2:B:2384:ILE:HD12	2.00	0.44
2:B:4075:GLU:HA	2:B:4078:GLN:HB2	1.99	0.44
2:I:379:HIS:CD2	2:I:381:GLU:H	2.35	0.44
2:I:3365:UNK:O	2:I:3369:UNK:N	2.50	0.44
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.53	0.44
2:E:3766:GLN:HG3	2:E:3769:ARG:HH12	1.83	0.44
2:I:793:LEU:HD22	2:I:821:LEU:HD13	2.00	0.44
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.53	0.44
2:I:4005:GLN:HE21	2:I:4110:PHE:HE1	1.64	0.44
2:E:41:GLY:O	2:E:45:ARG:NH1	2.50	0.44
2:E:4925:ILE:HA	2:E:4929:LEU:HD23	1.98	0.44
2:G:3766:GLN:HG3	2:G:3769:ARG:HH12	1.83	0.44
2:I:3759:GLU:HG3	2:I:3763:LEU:HD22	1.99	0.44
2:I:3959:LYS:O	2:I:3963:ASN:ND2	2.49	0.44
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.98	0.44
2:G:2810:LYS:O	2:G:2814:LYS:N	2.45	0.44
2:G:3365:UNK:O	2:G:3369:UNK:N	2.50	0.44
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.98	0.44
2:B:2121:PHE:O	2:B:3725:TYR:OH	2.30	0.44
2:E:3552:UNK:O	2:E:3556:UNK:N	2.51	0.44
2:E:3981:ALA:HA	2:E:3986:TRP:HE1	1.82	0.44
2:B:793:LEU:HD22	2:B:821:LEU:HD13	2.00	0.44
2:B:3552:UNK:O	2:B:3556:UNK:N	2.51	0.44
2:B:3766:GLN:HG3	2:B:3769:ARG:HH12	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.99	0.44
2:E:4895:GLY:O	2:G:4892:ARG:NH2	2.43	0.44
2:G:111:HIS:CD2	2:G:114:SER:H	2.36	0.44
2:G:3552:UNK:O	2:G:3556:UNK:N	2.51	0.44
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.82	0.44
2:B:214:VAL:HG12	2:B:274:LEU:HD12	2.00	0.44
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.98	0.44
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.99	0.44
2:I:2272:PRO:HA	2:I:2275:VAL:HG12	1.99	0.44
2:I:2950:UNK:O	2:I:2954:UNK:N	2.51	0.44
2:I:3981:ALA:HA	2:I:3986:TRP:HE1	1.83	0.44
2:E:793:LEU:HD12	2:E:797:HIS:HB2	2.00	0.44
2:E:4075:GLU:HA	2:E:4078:GLN:HB2	1.99	0.44
2:B:668:VAL:O	2:B:741:GLU:N	2.49	0.44
2:B:2950:UNK:O	2:B:2954:UNK:N	2.51	0.44
2:E:2381:GLU:HA	2:E:2384:ILE:HD12	2.00	0.44
2:E:2815:ALA:HB3	2:E:2881:ASN:HD21	1.83	0.44
2:G:2381:GLU:HA	2:G:2384:ILE:HD12	2.00	0.44
2:G:2950:UNK:O	2:G:2954:UNK:N	2.51	0.44
2:B:111:HIS:CD2	2:B:114:SER:H	2.36	0.43
2:B:793:LEU:HD12	2:B:797:HIS:HB2	2.00	0.43
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.53	0.43
2:I:3552:UNK:O	2:I:3556:UNK:N	2.51	0.43
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	1.99	0.43
2:G:214:VAL:HG12	2:G:274:LEU:HD12	2.00	0.43
2:B:2815:ALA:HB3	2:B:2881:ASN:HD21	1.83	0.43
2:I:111:HIS:CD2	2:I:114:SER:H	2.36	0.43
2:E:626:LEU:HG	2:E:628:GLY:H	1.83	0.43
2:E:1936:LYS:O	2:E:1940:CYS:N	2.47	0.43
2:E:2758:PHE:O	2:E:2762:THR:N	2.52	0.43
2:B:626:LEU:HG	2:B:628:GLY:H	1.83	0.43
2:E:2950:UNK:O	2:E:2954:UNK:N	2.51	0.43
2:G:793:LEU:HD12	2:G:797:HIS:HB2	2.00	0.43
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.84	0.43
2:I:1105:ALA:N	2:I:1189:LEU:O	2.51	0.43
2:I:3766:GLN:HG3	2:I:3769:ARG:HH12	1.83	0.43
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.46	0.43
2:E:3362:UNK:O	2:E:3366:UNK:N	2.52	0.43
2:G:3362:UNK:O	2:G:3366:UNK:N	2.52	0.43
2:G:4065:PHE:HD1	2:G:4068:LEU:HD22	1.83	0.43
1:A:55:VAL:HA	2:B:1784:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:709:ASP:HB3	2:B:725:HIS:CE1	2.54	0.43
2:B:898:ASP:HB3	2:B:901:LYS:HB2	2.00	0.43
2:B:2758:PHE:O	2:B:2762:THR:N	2.52	0.43
2:I:214:VAL:HG12	2:I:274:LEU:HD12	2.00	0.43
2:I:2467:VAL:HA	2:I:2470:ILE:HD12	2.01	0.43
2:I:4065:PHE:HD1	2:I:4068:LEU:HD22	1.83	0.43
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.84	0.43
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.53	0.43
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	1.99	0.43
1:A:21:THR:HA	1:A:49:ARG:HA	2.01	0.43
2:I:313:SER:HB3	2:I:351:VAL:HB	2.01	0.43
2:I:4864:ASN:HA	2:I:4874:MET:HG2	2.01	0.43
2:E:111:HIS:CD2	2:E:114:SER:H	2.36	0.43
2:E:668:VAL:O	2:E:741:GLU:N	2.49	0.43
2:E:1105:ALA:N	2:E:1189:LEU:O	2.51	0.43
2:G:793:LEU:HD22	2:G:821:LEU:HD13	2.00	0.43
2:G:2467:VAL:HA	2:G:2470:ILE:HD12	2.01	0.43
2:B:4586:PRO:HA	2:B:4628:VAL:HG11	2.01	0.43
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	2.01	0.43
2:I:2381:GLU:HA	2:I:2384:ILE:HD12	2.00	0.43
2:E:709:ASP:HB3	2:E:725:HIS:CE1	2.54	0.43
2:E:1141:ARG:H	2:E:1141:ARG:HD2	1.84	0.43
2:E:4864:ASN:HA	2:E:4874:MET:HG2	2.01	0.43
2:G:709:ASP:HB3	2:G:725:HIS:CE1	2.54	0.43
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	2.01	0.43
2:G:2815:ALA:HB3	2:G:2881:ASN:HD21	1.83	0.43
2:G:4586:PRO:HA	2:G:4628:VAL:HG11	2.01	0.43
2:B:1679:ASN:HA	2:B:1682:ALA:HB3	2.01	0.43
2:I:41:GLY:O	2:I:45:ARG:NH1	2.50	0.43
2:I:709:ASP:HB3	2:I:725:HIS:CE1	2.54	0.43
2:I:793:LEU:HD12	2:I:797:HIS:HB2	2.00	0.43
2:I:1679:ASN:HA	2:I:1682:ALA:HB3	2.01	0.43
2:I:3362:UNK:O	2:I:3366:UNK:N	2.52	0.43
2:I:3971:GLY:H	2:I:5005:GLY:HA3	1.84	0.43
2:I:4586:PRO:HA	2:I:4628:VAL:HG11	2.01	0.43
2:E:3759:GLU:HG3	2:E:3763:LEU:HD22	1.99	0.43
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.33	0.43
2:G:3971:GLY:H	2:G:5005:GLY:HA3	1.84	0.43
2:B:2257:LEU:O	2:B:2261:SER:N	2.52	0.43
2:B:3771:HIS:O	2:B:3774:GLY:N	2.45	0.43
2:B:3971:GLY:H	2:B:5005:GLY:HA3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4864:ASN:HA	2:B:4874:MET:HG2	2.01	0.43
2:B:4973:HIS:ND1	2:I:4227:GLU:OE2	2.51	0.43
2:E:793:LEU:HD22	2:E:821:LEU:HD13	2.00	0.43
1:F:21:THR:HA	1:F:49:ARG:HA	2.01	0.43
1:J:7:ILE:HB	1:J:71:ARG:HB3	2.01	0.43
2:B:500:ALA:HB1	2:B:504:ALA:HB2	2.01	0.43
2:B:3759:GLU:HG3	2:B:3763:LEU:HD22	1.99	0.43
2:B:4065:PHE:HD1	2:B:4068:LEU:HD22	1.83	0.43
2:I:2815:ALA:HB3	2:I:2881:ASN:HD21	1.83	0.43
2:E:898:ASP:HB3	2:E:901:LYS:HB2	2.00	0.43
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.84	0.43
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.84	0.43
2:G:2257:LEU:O	2:G:2261:SER:N	2.52	0.43
2:I:596:ASN:HB3	2:I:599:VAL:HG22	2.01	0.42
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	2.01	0.42
2:E:214:VAL:HG12	2:E:274:LEU:HD12	2.00	0.42
2:E:313:SER:HB3	2:E:351:VAL:HB	2.01	0.42
2:E:615:ARG:NH2	2:E:1677:GLY:O	2.52	0.42
2:E:4586:PRO:HA	2:E:4628:VAL:HG11	2.01	0.42
2:G:2894:LEU:HD11	2:G:2902:HIS:HB2	2.01	0.42
2:G:3361:UNK:O	2:G:3365:UNK:N	2.52	0.42
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.38	0.42
1:A:7:ILE:HB	1:A:71:ARG:HB3	2.01	0.42
1:J:21:THR:HA	1:J:49:ARG:HA	2.01	0.42
2:B:1105:ALA:N	2:B:1189:LEU:O	2.51	0.42
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.84	0.42
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.84	0.42
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	2.02	0.42
2:E:500:ALA:HB1	2:E:504:ALA:HB2	2.01	0.42
2:E:2257:LEU:O	2:E:2261:SER:N	2.52	0.42
2:G:3981:ALA:HA	2:G:3986:TRP:HE1	1.83	0.42
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.84	0.42
2:I:626:LEU:HG	2:I:628:GLY:H	1.83	0.42
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	2.02	0.42
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	2.01	0.42
2:G:313:SER:HB3	2:G:351:VAL:HB	2.01	0.42
2:G:898:ASP:HB3	2:G:901:LYS:HB2	2.00	0.42
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	2.01	0.42
2:G:1679:ASN:HA	2:G:1682:ALA:HB3	2.01	0.42
2:G:4864:ASN:HA	2:G:4874:MET:HG2	2.01	0.42
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	2.01	0.42
2:I:1859:VAL:HA	2:I:1862:ILE:HG12	2.01	0.42
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.84	0.42
2:E:596:ASN:HB3	2:E:599:VAL:HG22	2.01	0.42
2:E:2467:VAL:HA	2:E:2470:ILE:HD12	2.01	0.42
2:E:4065:PHE:HD1	2:E:4068:LEU:HD22	1.83	0.42
2:G:626:LEU:HG	2:G:628:GLY:H	1.83	0.42
2:B:2467:VAL:HA	2:B:2470:ILE:HD12	2.01	0.42
2:I:221:ARG:NE	2:I:258:SER:OG	2.43	0.42
2:I:2257:LEU:O	2:I:2261:SER:N	2.52	0.42
2:I:2447:LYS:HG3	2:I:2450:ALA:H	1.84	0.42
2:I:3759:GLU:OE1	2:I:3762:ARG:NH2	2.43	0.42
2:G:2447:LYS:HG3	2:G:2450:ALA:H	1.84	0.42
1:J:92:PRO:HD3	2:I:627:PRO:HB2	2.00	0.42
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.84	0.42
2:B:1770:SER:OG	2:B:1772:ARG:NE	2.53	0.42
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	2.02	0.42
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	2.02	0.42
2:B:3362:UNK:O	2:B:3366:UNK:N	2.52	0.42
2:I:898:ASP:HB3	2:I:901:LYS:HB2	2.00	0.42
2:I:2894:LEU:HD11	2:I:2902:HIS:HB2	2.02	0.42
2:I:3361:UNK:O	2:I:3365:UNK:N	2.52	0.42
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.01	0.42
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	2.02	0.42
2:E:3923:LEU:HD13	2:E:3961:VAL:HG11	2.02	0.42
2:E:3971:GLY:H	2:E:5005:GLY:HA3	1.84	0.42
2:E:4063:ASP:OD1	2:E:4169:SER:OG	2.30	0.42
2:G:668:VAL:O	2:G:741:GLU:N	2.49	0.42
2:G:1141:ARG:H	2:G:1141:ARG:HD2	1.84	0.42
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	2.02	0.42
2:B:1171:SER:OG	2:B:1175:SER:N	2.45	0.42
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	2.02	0.42
2:I:320:LYS:NZ	2:I:381:GLU:O	2.36	0.42
2:E:788:LYS:HG2	2:E:1629:GLN:HA	2.01	0.42
2:G:221:ARG:NE	2:G:258:SER:OG	2.43	0.42
2:G:2908:TYR:OH	2:G:2920:ARG:NE	2.48	0.42
2:G:3923:LEU:HD13	2:G:3961:VAL:HG11	2.02	0.42
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	2.02	0.42
2:B:2447:LYS:HG3	2:B:2450:ALA:H	1.84	0.42
2:B:3361:UNK:O	2:B:3365:UNK:N	2.52	0.42
2:E:2447:LYS:HG3	2:E:2450:ALA:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3361:UNK:O	2:E:3365:UNK:N	2.52	0.42
2:G:195:PHE:HB3	2:G:196:MET:HG2	2.02	0.42
2:G:1093:GLU:OE1	2:G:1201:HIS:NE2	2.50	0.42
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	2.02	0.42
2:B:313:SER:HB3	2:B:351:VAL:HB	2.01	0.42
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	2.02	0.42
2:I:1770:SER:OG	2:I:1772:ARG:NE	2.53	0.42
2:I:4177:TYR:CE1	2:I:4199:GLU:HB3	2.55	0.42
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	2.02	0.42
1:H:21:THR:HA	1:H:49:ARG:HA	2.01	0.42
2:I:788:LYS:HG2	2:I:1629:GLN:HA	2.02	0.42
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.85	0.42
2:E:1663:HIS:O	2:E:1667:LEU:N	2.52	0.42
2:E:3771:HIS:O	2:E:3774:GLY:N	2.45	0.42
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.85	0.42
2:G:615:ARG:NH2	2:G:1677:GLY:O	2.52	0.42
2:G:788:LYS:HG2	2:G:1629:GLN:HA	2.01	0.42
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.84	0.42
1:F:71:ARG:HH22	2:E:679:ALA:HB2	1.85	0.41
1:H:7:ILE:HB	1:H:71:ARG:HB3	2.01	0.41
2:I:195:PHE:HB3	2:I:196:MET:HG2	2.02	0.41
2:I:776:LEU:HG	2:I:848:HIS:HA	2.02	0.41
2:I:2758:PHE:O	2:I:2762:THR:N	2.52	0.41
2:I:4027:LEU:HA	2:I:4030:LEU:HD12	2.02	0.41
2:E:2894:LEU:HD11	2:E:2902:HIS:HB2	2.02	0.41
2:G:1105:ALA:N	2:G:1189:LEU:O	2.51	0.41
1:F:55:VAL:HA	2:E:1784:ALA:HA	2.02	0.41
2:B:3759:GLU:OE1	2:B:3762:ARG:NH2	2.43	0.41
2:I:615:ARG:NH2	2:I:1677:GLY:O	2.52	0.41
2:I:684:VAL:HA	2:I:781:VAL:HA	2.02	0.41
2:I:2810:LYS:HE2	2:I:2814:LYS:HE3	2.03	0.41
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	2.01	0.41
2:G:776:LEU:HG	2:G:848:HIS:HA	2.02	0.41
2:G:1770:SER:OG	2:G:1772:ARG:NE	2.53	0.41
2:B:161:GLU:HG2	2:E:3984:ARG:HH22	1.85	0.41
2:B:2908:TYR:OH	2:B:2920:ARG:NE	2.48	0.41
2:B:4177:TYR:CE1	2:B:4199:GLU:HB3	2.55	0.41
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	2.01	0.41
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.02	0.41
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.85	0.41
2:I:914:PRO:O	2:I:918:ARG:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3923:LEU:HD13	2:I:3961:VAL:HG11	2.02	0.41
2:E:914:PRO:O	2:E:918:ARG:N	2.49	0.41
2:E:1770:SER:OG	2:E:1772:ARG:NE	2.53	0.41
2:G:2810:LYS:HE2	2:G:2814:LYS:HE3	2.03	0.41
2:G:4547:GLN:O	2:G:4551:PHE:N	2.49	0.41
1:F:87:HIS:HA	1:F:88:PRO:HD3	1.93	0.41
2:B:596:ASN:HB3	2:B:599:VAL:HG22	2.01	0.41
2:B:788:LYS:HG2	2:B:1629:GLN:HA	2.01	0.41
2:B:1936:LYS:O	2:B:1940:CYS:N	2.47	0.41
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.85	0.41
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	2.02	0.41
2:E:195:PHE:HB3	2:E:196:MET:HG2	2.02	0.41
2:E:4843:LEU:HD22	2:E:4928:LEU:HD11	2.03	0.41
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	2.02	0.41
2:G:500:ALA:HB1	2:G:504:ALA:HB2	2.01	0.41
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	2.02	0.41
2:G:2208:MET:SD	2:G:2253:HIS:ND1	2.85	0.41
2:G:4177:TYR:CE1	2:G:4199:GLU:HB3	2.55	0.41
2:G:4843:LEU:HD22	2:G:4928:LEU:HD11	2.03	0.41
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.93	0.41
2:B:1859:VAL:HA	2:B:1862:ILE:HG12	2.01	0.41
2:B:2894:LEU:HD11	2:B:2902:HIS:HB2	2.02	0.41
2:B:4897:ILE:HG12	2:B:4901:ILE:HD13	2.02	0.41
2:E:745:SER:N	2:E:758:ARG:O	2.43	0.41
2:E:2034:PHE:O	2:E:2038:LEU:N	2.54	0.41
2:E:4027:LEU:HA	2:E:4030:LEU:HD12	2.02	0.41
2:G:2758:PHE:O	2:G:2762:THR:N	2.52	0.41
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.02	0.41
2:E:1973:GLN:O	2:E:1977:TYR:N	2.54	0.41
2:G:596:ASN:HB3	2:G:599:VAL:HG22	2.01	0.41
2:B:2810:LYS:HE2	2:B:2814:LYS:HE3	2.03	0.41
2:I:347:PHE:HE1	2:I:386:ASP:HB2	1.86	0.41
2:I:500:ALA:HB1	2:I:504:ALA:HB2	2.01	0.41
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	2.02	0.41
2:E:235:ALA:HA	2:E:257:ARG:HD3	2.02	0.41
2:E:2810:LYS:HE2	2:E:2814:LYS:HE3	2.03	0.41
2:G:1859:VAL:HA	2:G:1862:ILE:HG12	2.01	0.41
1:F:7:ILE:HB	1:F:71:ARG:HB3	2.01	0.41
1:H:71:ARG:HH22	2:G:679:ALA:HB2	1.86	0.41
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.78	0.41
2:B:2874:MET:O	2:B:2878:LEU:N	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	2.02	0.41
2:I:2908:TYR:OH	2:I:2920:ARG:NE	2.48	0.41
2:I:4897:ILE:HG12	2:I:4901:ILE:HD13	2.02	0.41
2:E:70:GLU:HG3	2:E:117:TYR:HE1	1.86	0.41
2:E:864:PRO:HA	2:E:865:PRO:HD3	1.94	0.41
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	2.02	0.41
2:E:4133:GLN:HE22	2:E:4137:ARG:HG3	1.86	0.41
2:E:4177:TYR:CE1	2:E:4199:GLU:HB3	2.55	0.41
2:G:235:ALA:HA	2:G:257:ARG:HD3	2.02	0.41
2:G:1973:GLN:O	2:G:1977:TYR:N	2.54	0.41
2:G:4027:LEU:HA	2:G:4030:LEU:HD12	2.02	0.41
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	2.02	0.41
2:G:4897:ILE:HG12	2:G:4901:ILE:HD13	2.02	0.41
2:B:195:PHE:HB3	2:B:196:MET:HG2	2.02	0.41
2:B:4133:GLN:HE22	2:B:4137:ARG:HG3	1.86	0.41
2:I:70:GLU:HG3	2:I:117:TYR:HE1	1.86	0.41
2:I:235:ALA:HA	2:I:257:ARG:HD3	2.02	0.41
2:I:2095:GLN:NE2	2:I:2127:GLN:O	2.42	0.41
2:I:4133:GLN:HE22	2:I:4137:ARG:HG3	1.86	0.41
2:B:70:GLU:HG3	2:B:117:TYR:HE1	1.86	0.40
2:B:206:CYS:SG	2:B:207:SER:N	2.94	0.40
2:B:615:ARG:NH2	2:B:1677:GLY:O	2.52	0.40
2:B:1639:LEU:N	2:B:1648:MET:O	2.54	0.40
2:B:4227:GLU:OE2	2:E:4973:HIS:ND1	2.55	0.40
2:I:206:CYS:SG	2:I:207:SER:N	2.94	0.40
2:I:4843:LEU:HA	2:I:4846:VAL:HG12	2.03	0.40
2:E:206:CYS:SG	2:E:207:SER:N	2.94	0.40
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.02	0.40
2:G:4053:SER:HA	2:G:4056:GLU:HB2	2.03	0.40
1:H:57:LYS:HB2	1:H:80:VAL:HB	2.04	0.40
2:B:3733:CYS:HB2	2:B:3803:SER:HB3	2.04	0.40
2:E:776:LEU:HG	2:E:848:HIS:HA	2.02	0.40
2:G:684:VAL:HA	2:G:781:VAL:HA	2.03	0.40
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.39	0.40
1:J:87:HIS:HA	1:J:88:PRO:HD3	1.93	0.40
2:B:38:ALA:HB1	2:B:64:ILE:HG13	2.04	0.40
2:B:347:PHE:HE1	2:B:386:ASP:HB2	1.86	0.40
2:B:583:ILE:H	2:B:583:ILE:HG13	1.69	0.40
2:B:870:ILE:HD11	2:B:1049:TYR:CG	2.57	0.40
2:B:4843:LEU:HD22	2:B:4928:LEU:HD11	2.03	0.40
2:I:1739:THR:H	2:I:1742:THR:HB	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2034:PHE:O	2:I:2038:LEU:N	2.54	0.40
2:E:113:HIS:CE1	2:E:402:ARG:HB3	2.57	0.40
2:E:870:ILE:HD11	2:E:1049:TYR:CG	2.57	0.40
2:E:1093:GLU:OE1	2:E:1201:HIS:NE2	2.50	0.40
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.39	0.40
2:E:4843:LEU:HA	2:E:4846:VAL:HG12	2.03	0.40
2:G:113:HIS:CE1	2:G:402:ARG:HB3	2.57	0.40
1:F:57:LYS:HB2	1:F:80:VAL:HB	2.04	0.40
2:B:684:VAL:HA	2:B:781:VAL:HA	2.03	0.40
2:B:776:LEU:HG	2:B:848:HIS:HA	2.02	0.40
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.39	0.40
2:B:4547:GLN:O	2:B:4551:PHE:N	2.49	0.40
2:I:243:ARG:NH1	2:I:301:VAL:O	2.44	0.40
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.02	0.40
2:I:3733:CYS:HB2	2:I:3803:SER:HB3	2.04	0.40
2:E:347:PHE:HE1	2:E:386:ASP:HB2	1.86	0.40
2:E:684:VAL:HA	2:E:781:VAL:HA	2.03	0.40
2:E:4982:GLU:HB3	2:E:4983:HIS:H	1.77	0.40
2:G:38:ALA:HB1	2:G:64:ILE:HG13	2.04	0.40
2:B:485:SER:O	2:B:489:ASN:N	2.43	0.40
2:B:4885:PHE:HE2	2:B:4901:ILE:HD11	1.87	0.40
2:I:38:ALA:HB1	2:I:64:ILE:HG13	2.04	0.40
2:I:1171:SER:OG	2:I:1175:SER:N	2.45	0.40
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.39	0.40
2:I:1973:GLN:O	2:I:1977:TYR:N	2.54	0.40
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.53	0.40
2:G:320:LYS:NZ	2:G:381:GLU:O	2.36	0.40
2:G:1189:LEU:HD12	2:G:1190:PRO:HD2	2.04	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%)	92 (88%)	13 (12%)	0	100	100
1	F	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
1	H	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
1	J	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
2	B	3235/4416 (73%)	2888 (89%)	343 (11%)	4 (0%)	51	85
2	E	3235/4416 (73%)	2888 (89%)	343 (11%)	4 (0%)	51	85
2	G	3235/4416 (73%)	2887 (89%)	344 (11%)	4 (0%)	51	85
2	I	3235/4416 (73%)	2888 (89%)	343 (11%)	4 (0%)	51	85
All	All	13360/18096 (74%)	11919 (89%)	1425 (11%)	16 (0%)	54	85

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	I	1708	ARG
2	E	1708	ARG
2	G	1708	ARG
2	B	1932	PRO
2	I	1932	PRO
2	E	1932	PRO
2	G	1932	PRO
2	B	1840	PRO
2	B	4641	PRO
2	I	1840	PRO
2	I	4641	PRO
2	E	1840	PRO
2	E	4641	PRO
2	G	1840	PRO
2	G	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	2493/3022 (82%)	2477 (99%)	16 (1%)	86 92
2	E	2493/3022 (82%)	2477 (99%)	16 (1%)	86 92
2	G	2493/3022 (82%)	2477 (99%)	16 (1%)	86 92
2	I	2493/3022 (82%)	2477 (99%)	16 (1%)	86 92
All	All	10324/12444 (83%)	10260 (99%)	64 (1%)	86 92

All (64) 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	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	3787	LYS
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4978	HIS
2	B	4983	HIS
2	B	4995	LEU
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3787	LYS
2	I	3896	ASN
2	I	4034	ASN

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Mol	Chain	Res	Type
2	I	4085	ARG
2	I	4120	ASN
2	I	4978	HIS
2	I	4983	HIS
2	I	4995	LEU
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3787	LYS
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4978	HIS
2	E	4983	HIS
2	E	4995	LEU
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	3787	LYS
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4978	HIS
2	G	4983	HIS
2	G	4995	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (152) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS

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Mol	Chain	Res	Type
1	A	87	HIS
1	H	87	HIS
1	J	87	HIS
2	B	57	ASN
2	B	111	HIS
2	B	113	HIS
2	B	151	HIS
2	B	273	HIS
2	B	379	HIS
2	B	412	ASN
2	B	413	GLN
2	B	479	GLN
2	B	582	HIS
2	B	949	ASN
2	B	1598	GLN
2	B	1679	ASN
2	B	1688	HIS
2	B	1691	GLN
2	B	1719	HIS
2	B	1760	HIS
2	B	1775	HIS
2	B	1972	ASN
2	B	2005	GLN
2	B	2127	GLN
2	B	3767	GLN
2	B	3781	GLN
2	B	3809	ASN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	3963	ASN
2	B	3976	ASN
2	B	4034	ASN
2	B	4102	GLN
2	B	4120	ASN
2	B	4130	ASN
2	B	4133	GLN
2	B	4142	ASN
2	I	57	ASN
2	I	111	HIS

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Mol	Chain	Res	Type
2	I	113	HIS
2	I	151	HIS
2	I	273	HIS
2	I	379	HIS
2	I	412	ASN
2	I	413	GLN
2	I	582	HIS
2	I	949	ASN
2	I	1598	GLN
2	I	1679	ASN
2	I	1688	HIS
2	I	1691	GLN
2	I	1719	HIS
2	I	1760	HIS
2	I	1775	HIS
2	I	1972	ASN
2	I	2005	GLN
2	I	2127	GLN
2	I	3700	GLN
2	I	3767	GLN
2	I	3781	GLN
2	I	3809	ASN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3963	ASN
2	I	3976	ASN
2	I	4034	ASN
2	I	4102	GLN
2	I	4120	ASN
2	I	4130	ASN
2	I	4133	GLN
2	I	4142	ASN
2	E	57	ASN
2	E	111	HIS
2	E	113	HIS
2	E	151	HIS
2	E	273	HIS
2	E	379	HIS
2	E	412	ASN

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Mol	Chain	Res	Type
2	E	413	GLN
2	E	479	GLN
2	E	582	HIS
2	E	949	ASN
2	E	1598	GLN
2	E	1679	ASN
2	E	1688	HIS
2	E	1691	GLN
2	E	1719	HIS
2	E	1760	HIS
2	E	1775	HIS
2	E	1972	ASN
2	E	2005	GLN
2	E	2127	GLN
2	E	3767	GLN
2	E	3781	GLN
2	E	3809	ASN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3963	ASN
2	E	3976	ASN
2	E	4034	ASN
2	E	4102	GLN
2	E	4120	ASN
2	E	4130	ASN
2	E	4133	GLN
2	E	4142	ASN
2	G	57	ASN
2	G	111	HIS
2	G	113	HIS
2	G	151	HIS
2	G	273	HIS
2	G	379	HIS
2	G	412	ASN
2	G	413	GLN
2	G	582	HIS
2	G	949	ASN
2	G	1598	GLN
2	G	1679	ASN

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Mol	Chain	Res	Type
2	G	1688	HIS
2	G	1691	GLN
2	G	1719	HIS
2	G	1760	HIS
2	G	1775	HIS
2	G	1972	ASN
2	G	2005	GLN
2	G	2127	GLN
2	G	3767	GLN
2	G	3781	GLN
2	G	3809	ASN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3963	ASN
2	G	3976	ASN
2	G	4034	ASN
2	G	4054	ASN
2	G	4102	GLN
2	G	4120	ASN
2	G	4130	ASN
2	G	4133	GLN
2	G	4142	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	I	14
2	E	14
2	G	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.36
1	I	4345:UNK	C	4540:PHE	N	73.36
1	E	4345:UNK	C	4540:PHE	N	73.36
1	G	4345:UNK	C	4540:PHE	N	73.36
1	B	3613:UNK	C	3639:THR	N	46.46
1	I	3613:UNK	C	3639:THR	N	46.46
1	E	3613:UNK	C	3639:THR	N	46.46
1	G	3613:UNK	C	3639:THR	N	46.46
1	B	4253:GLU	C	4320:UNK	N	27.46
1	I	4253:GLU	C	4320:UNK	N	27.46
1	E	4253:GLU	C	4320:UNK	N	27.46
1	G	4253:GLU	C	4320:UNK	N	27.46
1	B	3163:UNK	C	3170:UNK	N	15.87

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	3163:UNK	C	3170:UNK	N	15.87
1	E	3163:UNK	C	3170:UNK	N	15.87
1	G	3163:UNK	C	3170:UNK	N	15.87
1	B	3063:UNK	C	3134:UNK	N	14.92
1	I	3063:UNK	C	3134:UNK	N	14.92
1	E	3063:UNK	C	3134:UNK	N	14.92
1	G	3063:UNK	C	3134:UNK	N	14.92
1	B	3468:UNK	C	3511:UNK	N	14.79
1	I	3468:UNK	C	3511:UNK	N	14.79
1	E	3468:UNK	C	3511:UNK	N	14.79
1	G	3468:UNK	C	3511:UNK	N	14.79
1	B	2703:UNK	C	2734:ASN	N	13.42
1	I	2703:UNK	C	2734:ASN	N	13.42
1	E	2703:UNK	C	2734:ASN	N	13.42
1	G	2703:UNK	C	2734:ASN	N	13.42
1	B	3236:UNK	C	3241:UNK	N	13.13
1	I	3236:UNK	C	3241:UNK	N	13.13
1	E	3236:UNK	C	3241:UNK	N	13.13
1	G	3236:UNK	C	3241:UNK	N	13.13
1	B	1564:UNK	C	1573:MET	N	12.39
1	I	1564:UNK	C	1573:MET	N	12.39
1	E	1564:UNK	C	1573:MET	N	12.39
1	G	1564:UNK	C	1573:MET	N	12.39
1	B	2976:UNK	C	2995:UNK	N	12.28
1	I	2976:UNK	C	2995:UNK	N	12.28
1	E	2976:UNK	C	2995:UNK	N	12.28
1	G	2976:UNK	C	2995:UNK	N	12.28
1	B	3254:UNK	C	3261:UNK	N	8.43
1	I	3254:UNK	C	3261:UNK	N	8.43
1	E	3254:UNK	C	3261:UNK	N	8.43
1	G	3254:UNK	C	3261:UNK	N	8.43
1	B	1297:UNK	C	1430:UNK	N	6.02
1	I	1297:UNK	C	1430:UNK	N	6.02
1	E	1297:UNK	C	1430:UNK	N	6.02
1	G	1297:UNK	C	1430:UNK	N	6.02
1	B	2939:ARG	C	2942:UNK	N	3.58
1	I	2939:ARG	C	2942:UNK	N	3.58
1	E	2939:ARG	C	2942:UNK	N	3.58
1	G	2939:ARG	C	2942:UNK	N	3.58
1	B	2479:LEU	C	2487:UNK	N	3.25
1	I	2479:LEU	C	2487:UNK	N	3.25
1	E	2479:LEU	C	2487:UNK	N	3.25

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	2479:LEU	C	2487:UNK	N	3.25

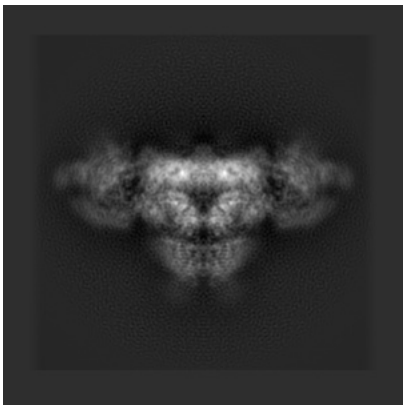
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8392. These allow visual inspection of the internal detail of the map and identification of artifacts.

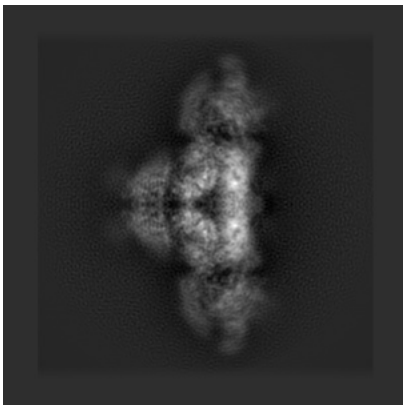
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

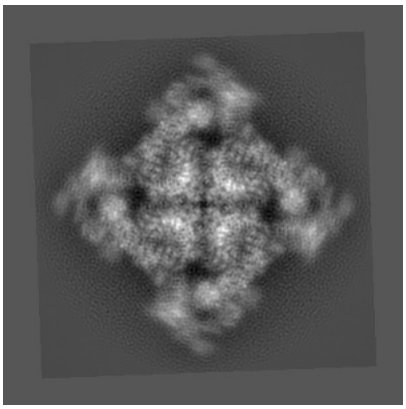
6.1.1 Primary map



X

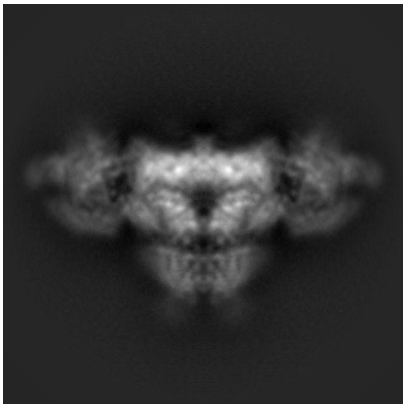


Y

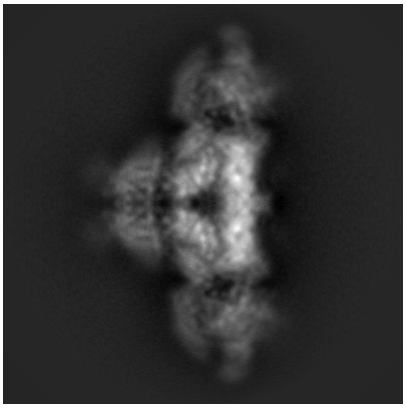


Z

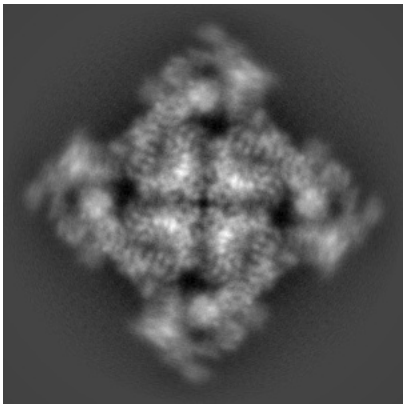
6.1.2 Raw map



X



Y



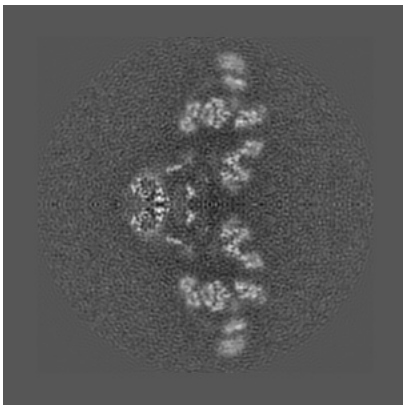
Z

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

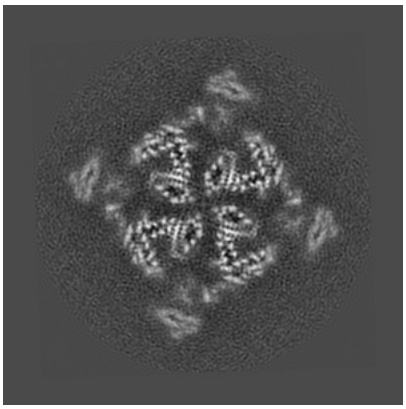
6.2 Central slices (i)

6.2.1 Primary map

X Index: 200

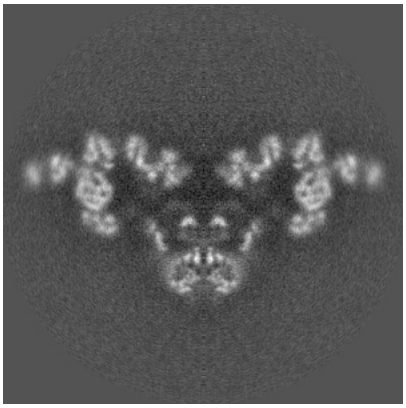


Y Index: 200

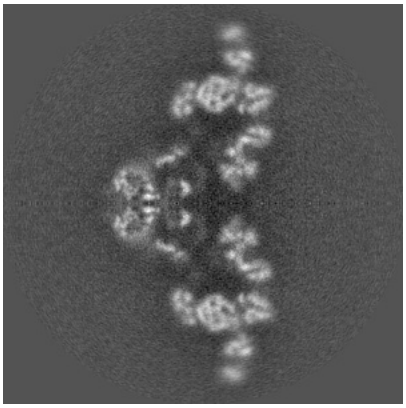


Z Index: 200

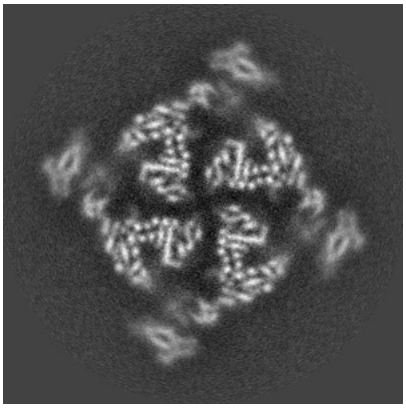
6.2.2 Raw map



X Index: 168



Y Index: 168

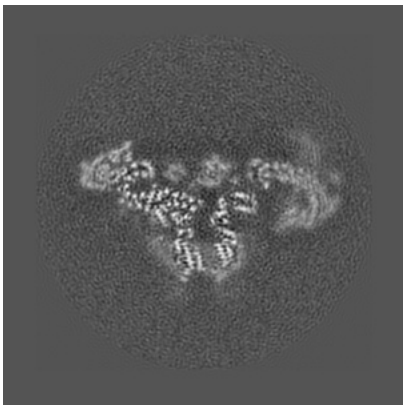


Z Index: 168

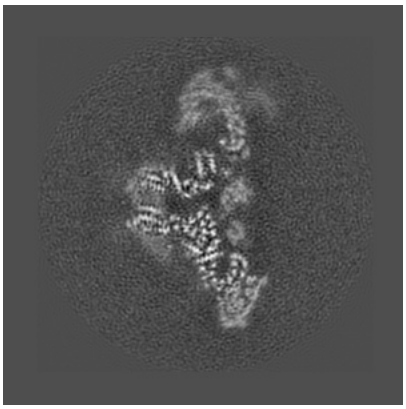
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

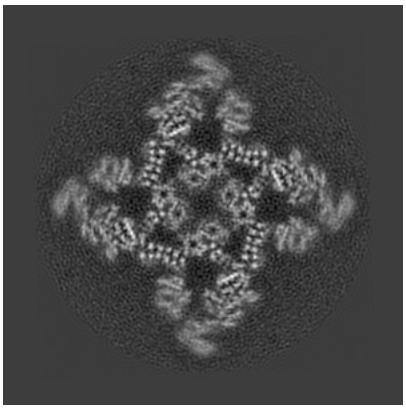
6.3.1 Primary map



X Index: 224

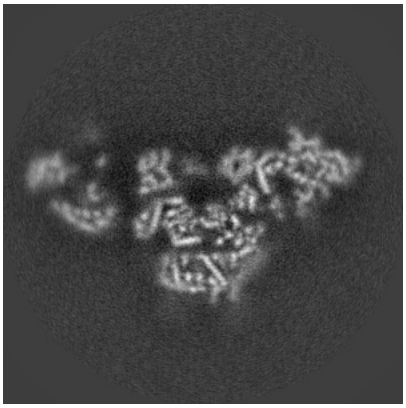


Y Index: 177

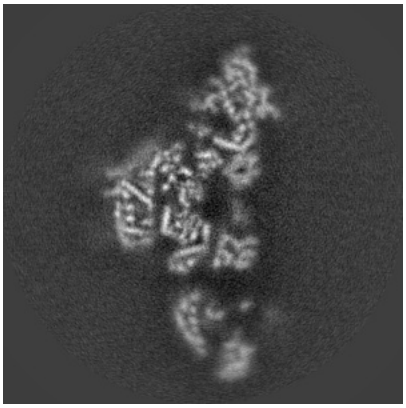


Z Index: 227

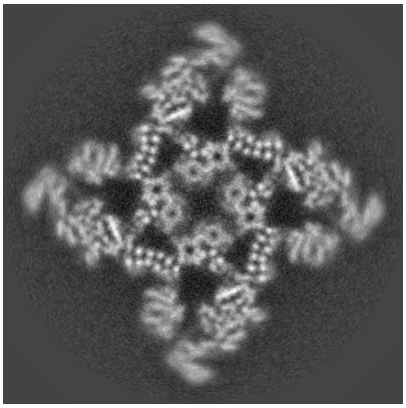
6.3.2 Raw map



X Index: 154



Y Index: 182



Z Index: 192

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

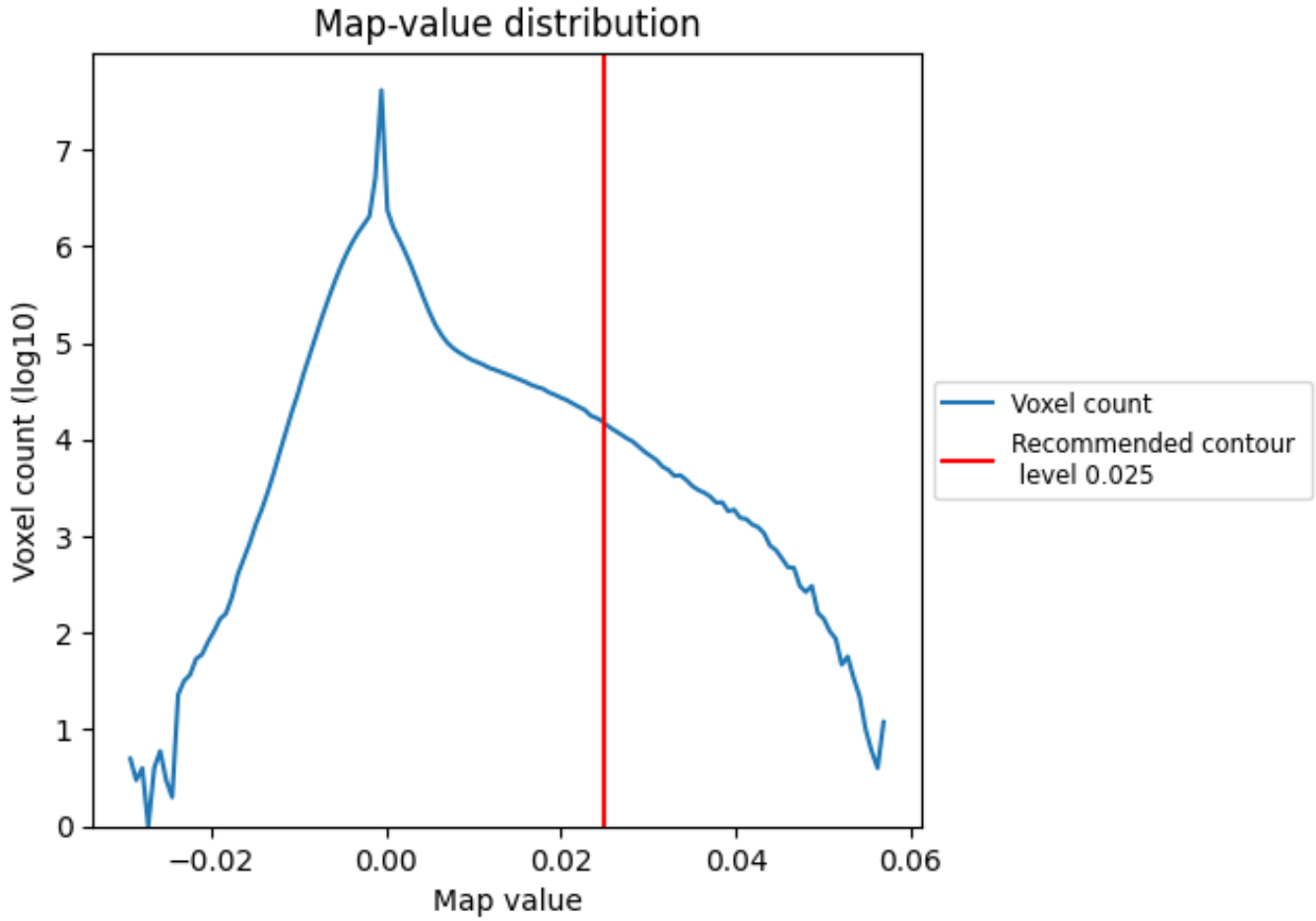
6.5 Mask visualisation (i)

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

7 Map analysis

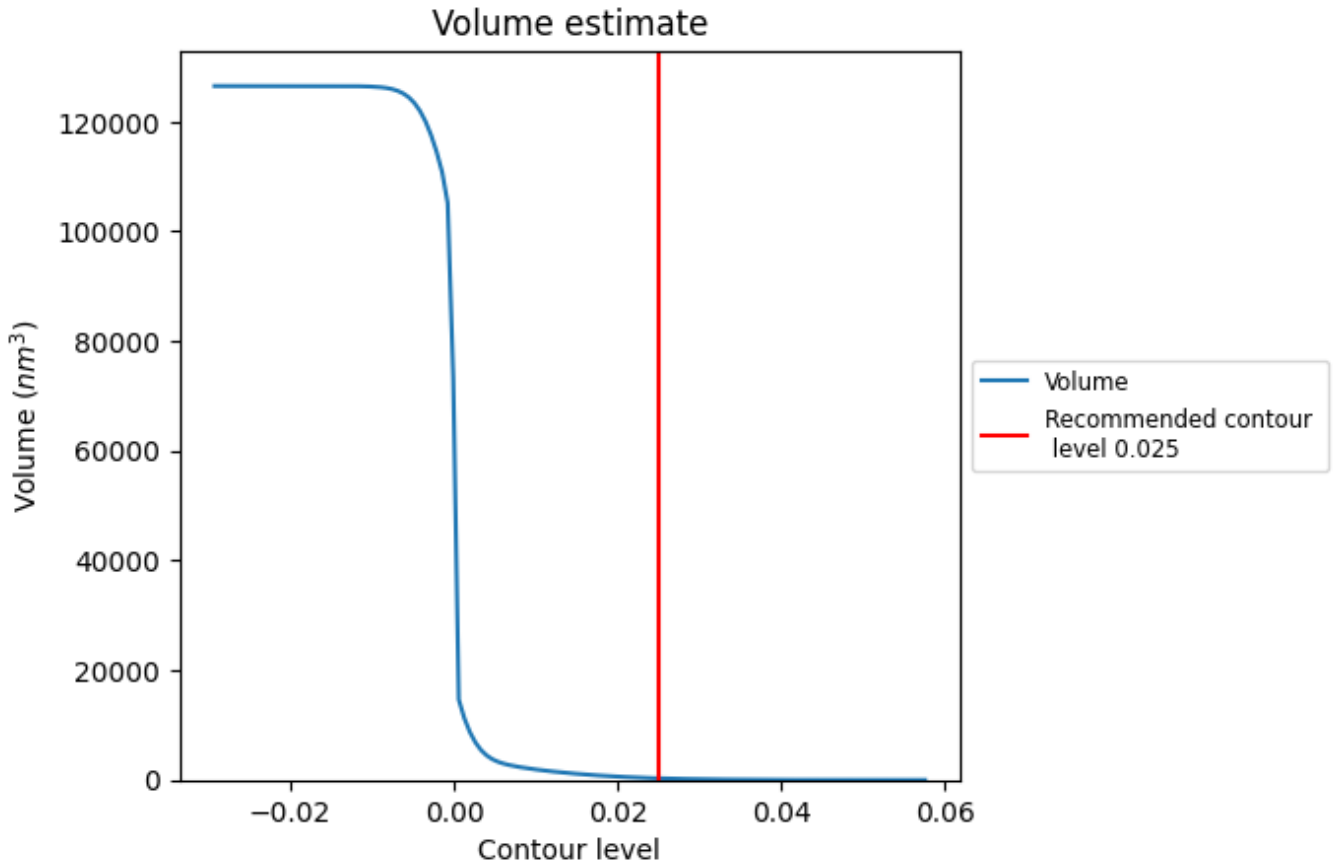
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

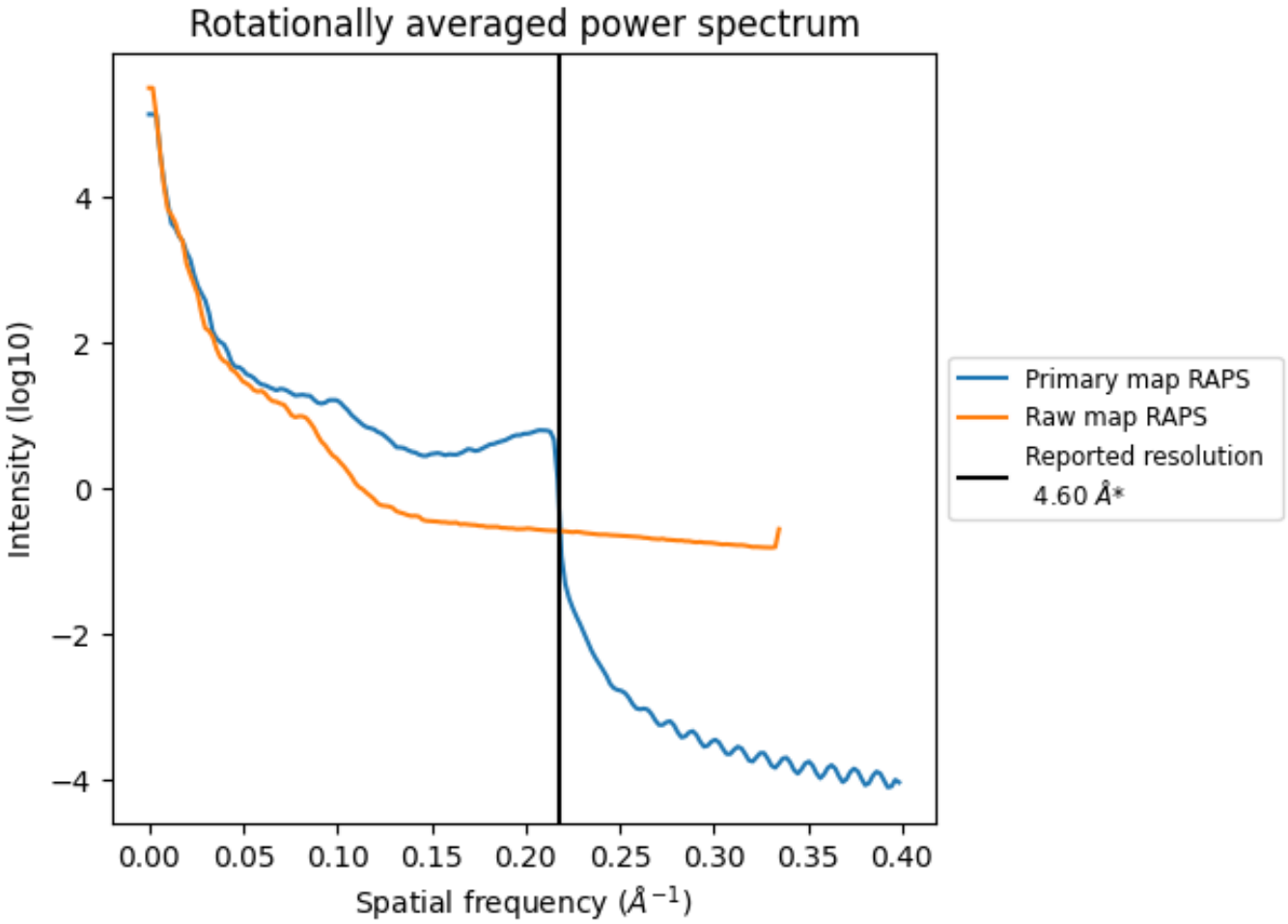
7.2 Volume estimate



The volume at the recommended contour level is 298 nm^3; this corresponds to an approximate mass of 269 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)

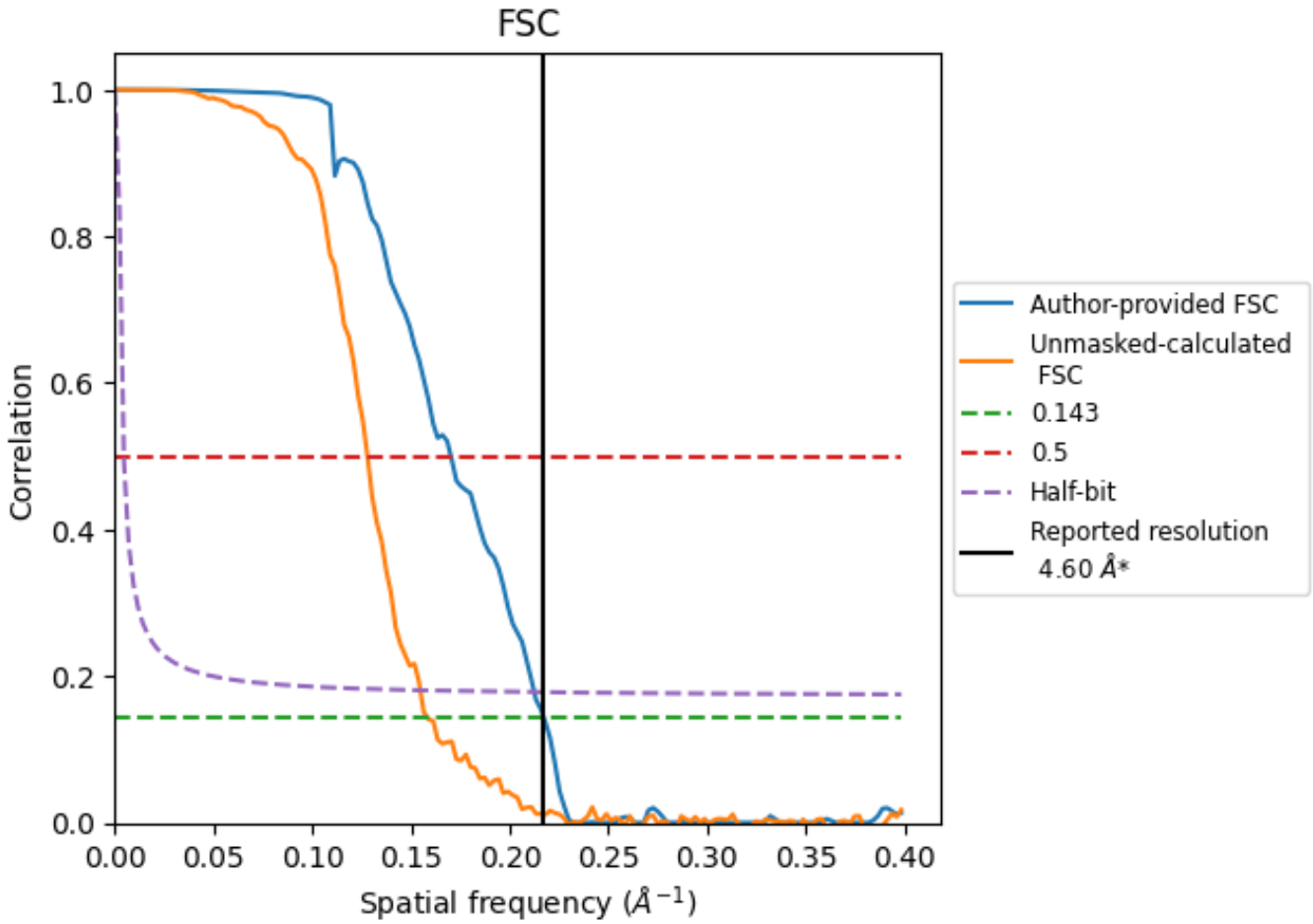


*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

8.2 Resolution estimates (i)

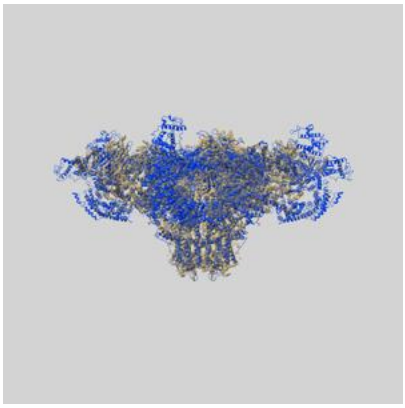
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.60	5.87	4.71
Unmasked-calculated*	6.31	7.81	6.46

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.31 differs from the reported value 4.6 by more than 10 %

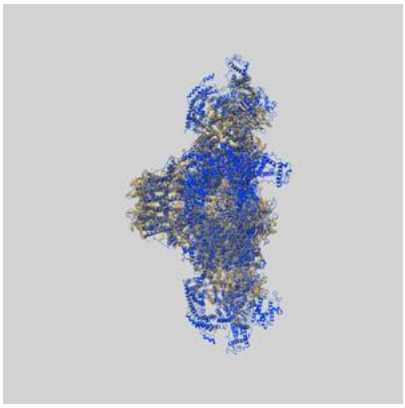
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8392 and PDB model 5TB1. Per-residue inclusion information can be found in section 3 on page 4.

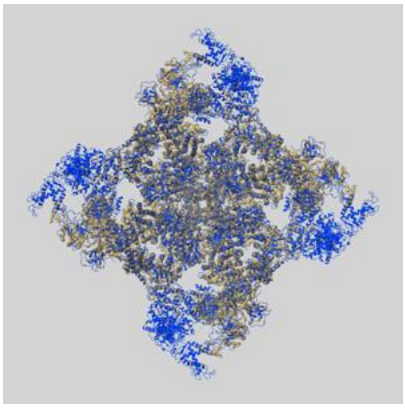
9.1 Map-model overlay



X



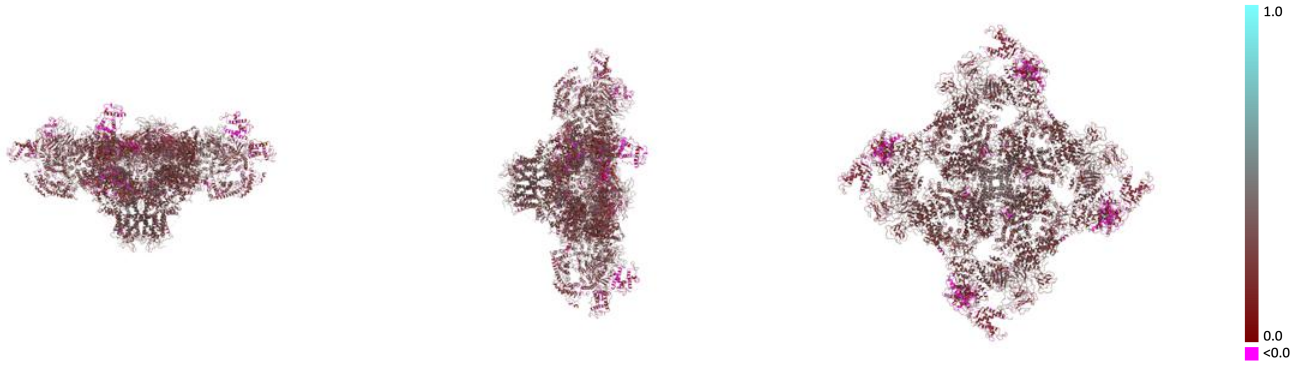
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

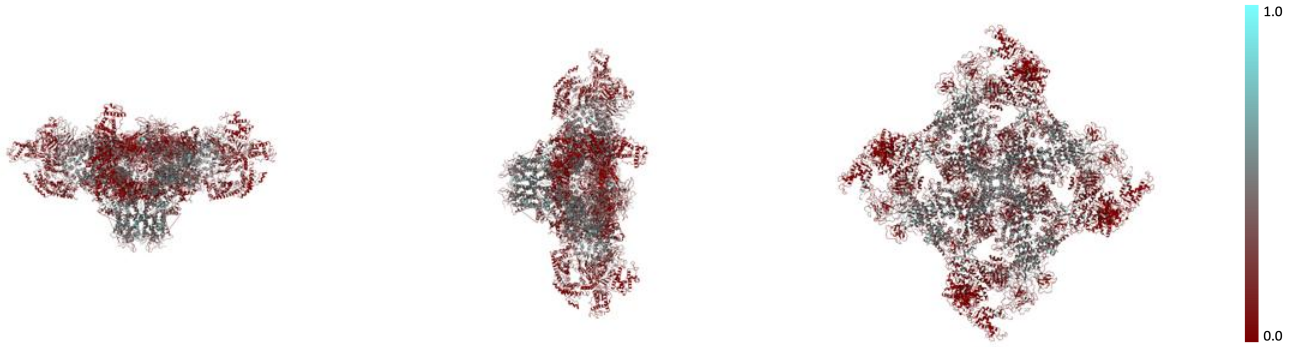
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

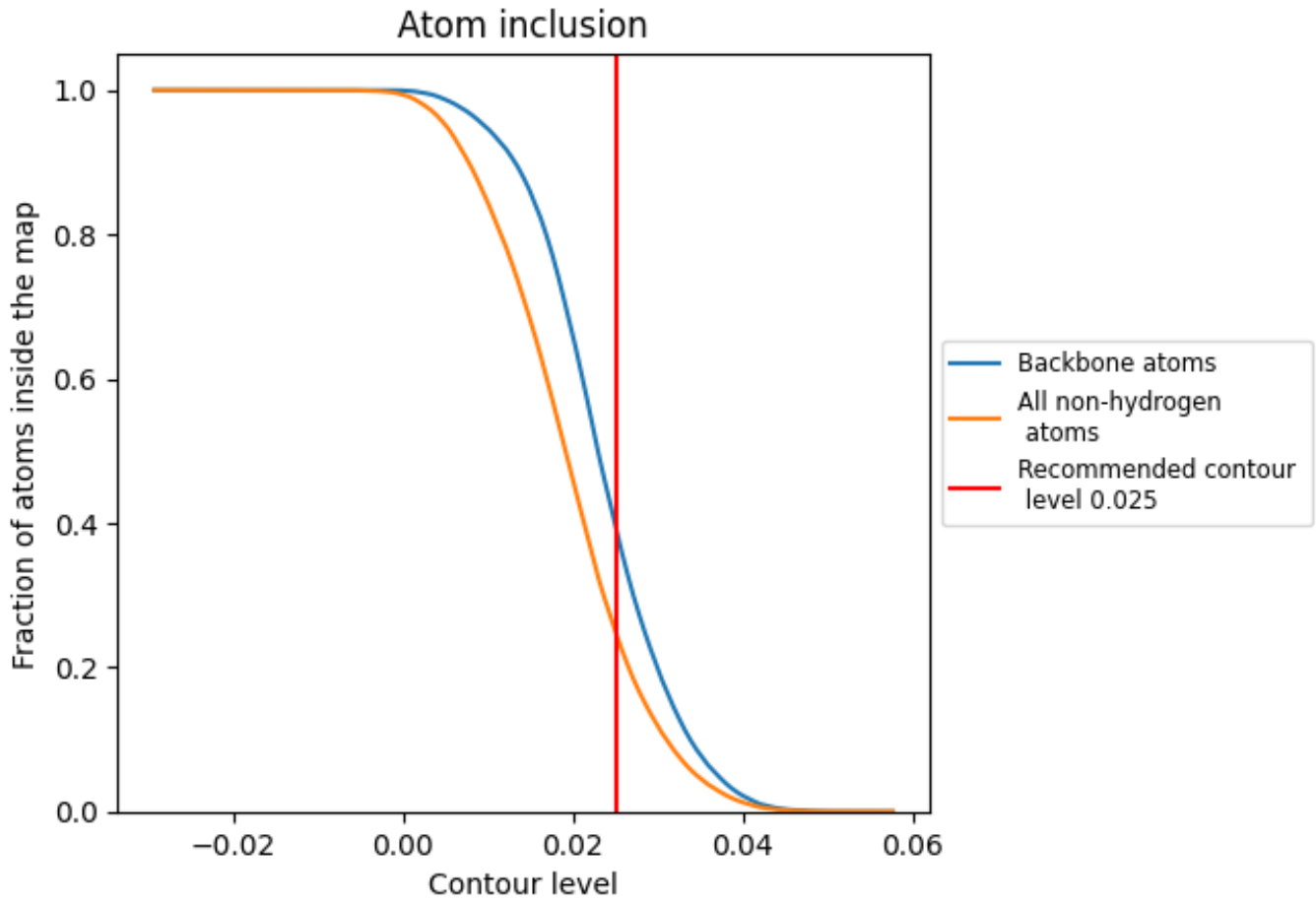
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 40% of all backbone atoms, 25% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2492	0.2600
A	0.1886	0.2650
B	0.2509	0.2600
E	0.2505	0.2600
F	0.1836	0.2700
G	0.2513	0.2600
H	0.1886	0.2670
I	0.2512	0.2590
J	0.1886	0.2640