Full wwPDB EM Validation Report ⓘ

Nov 2, 2022 – 02:51 AM EDT

PDB ID	:	5T9V
EMDB ID	:	EMD-8376
Title	:	Structure of rabbit RyR1 (Caffeine/ATP/Ca2+ dataset, class 1)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-09
Resolution	:	4.40 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:

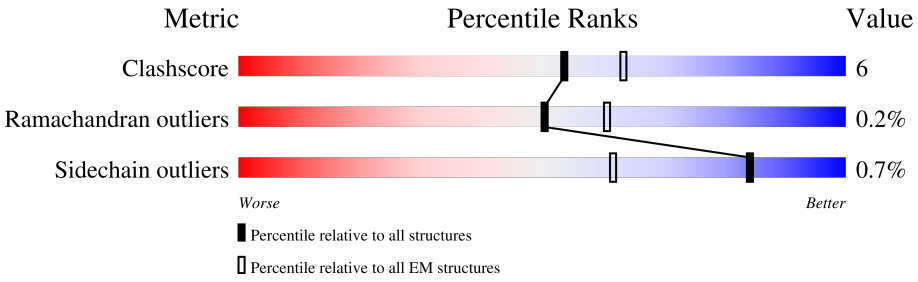
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.40 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	77% 81% 18% ·
1	F	108	77% 81% 18% ·
1	H	108	75% 81% 18% ·
1	J	108	75% 81% 19% ·
2	B	4416	66% 83% 12% 5%
2	E	4416	66% 83% 11% 5%
2	G	4416	65% 83% 11% 5%
2	I	4416	65% 83% 12% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 121456 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.

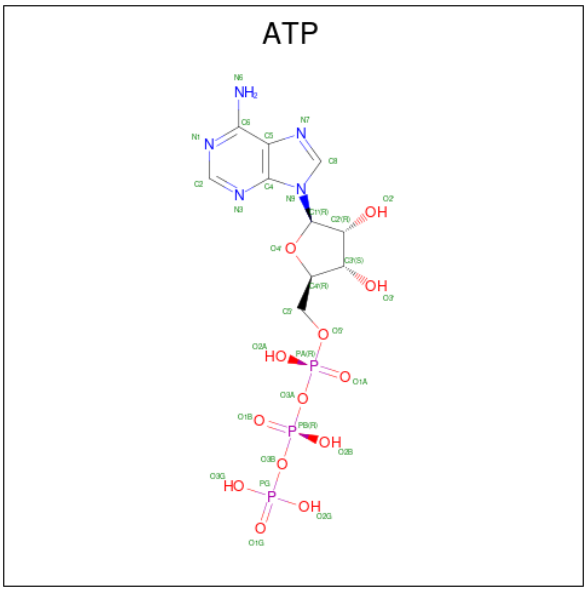
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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.

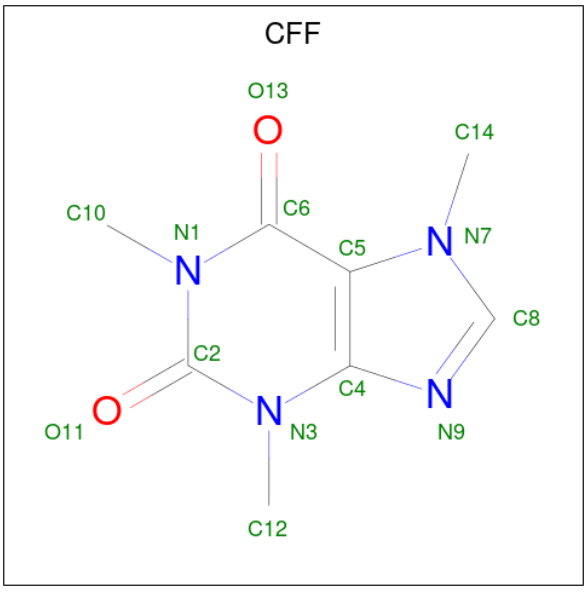
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

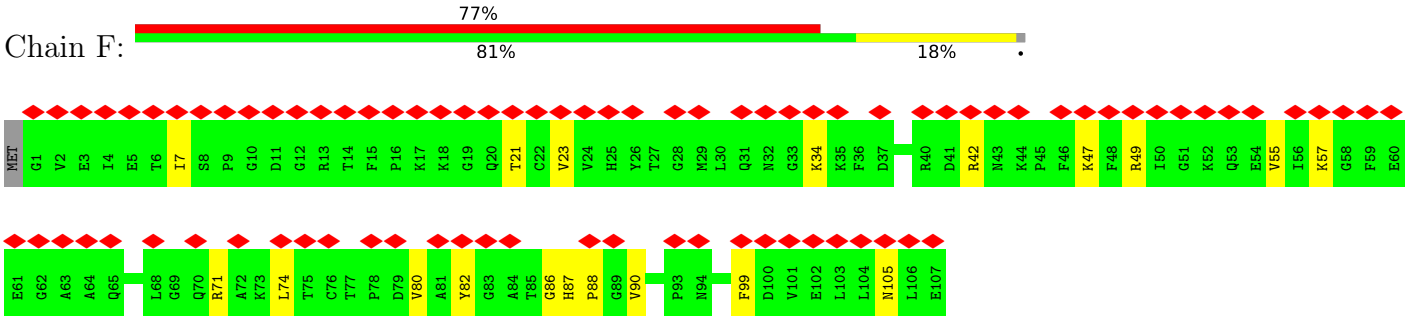
Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Ca	0
			1	1	
6	G	1	Total	Ca	0
			1	1	
6	I	1	Total	Ca	0
			1	1	
6	E	1	Total	Ca	0
			1	1	

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.

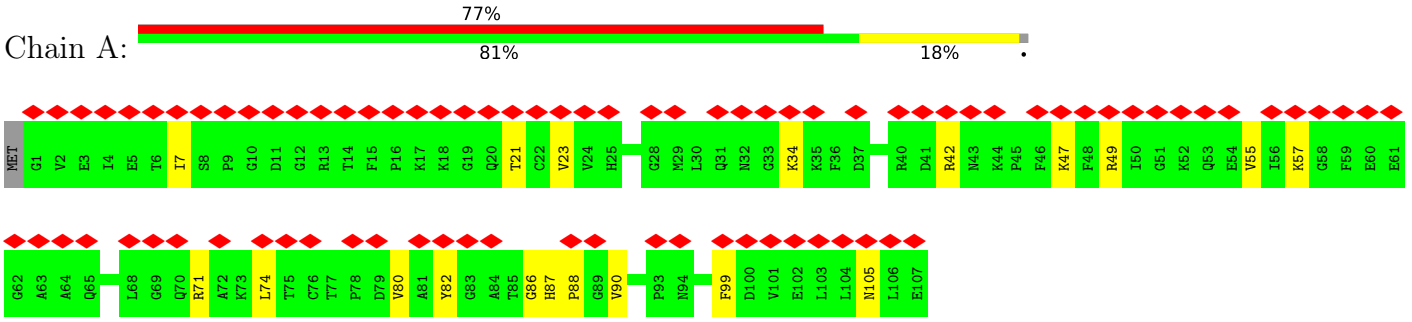
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



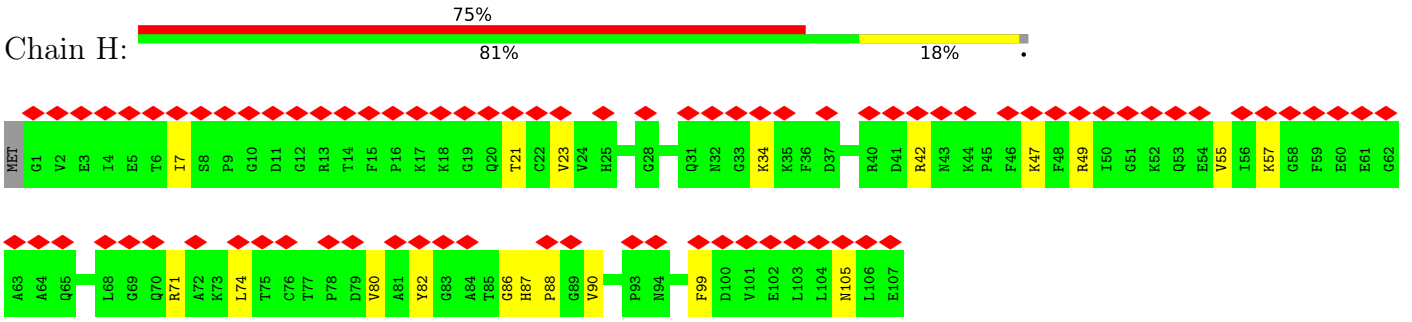
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



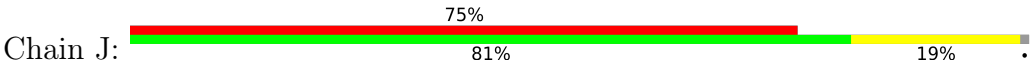
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

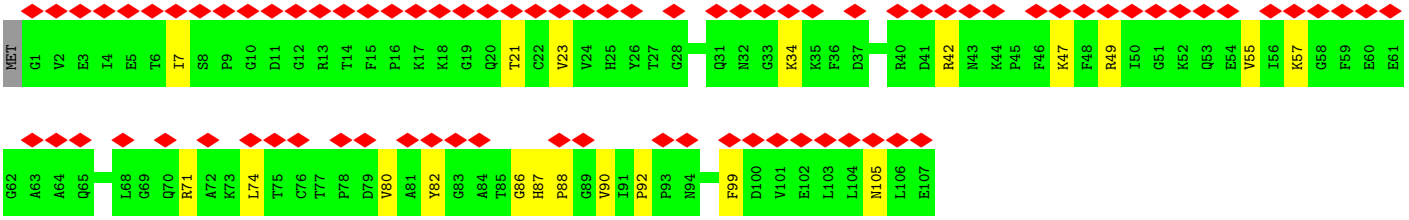
Chain H:



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

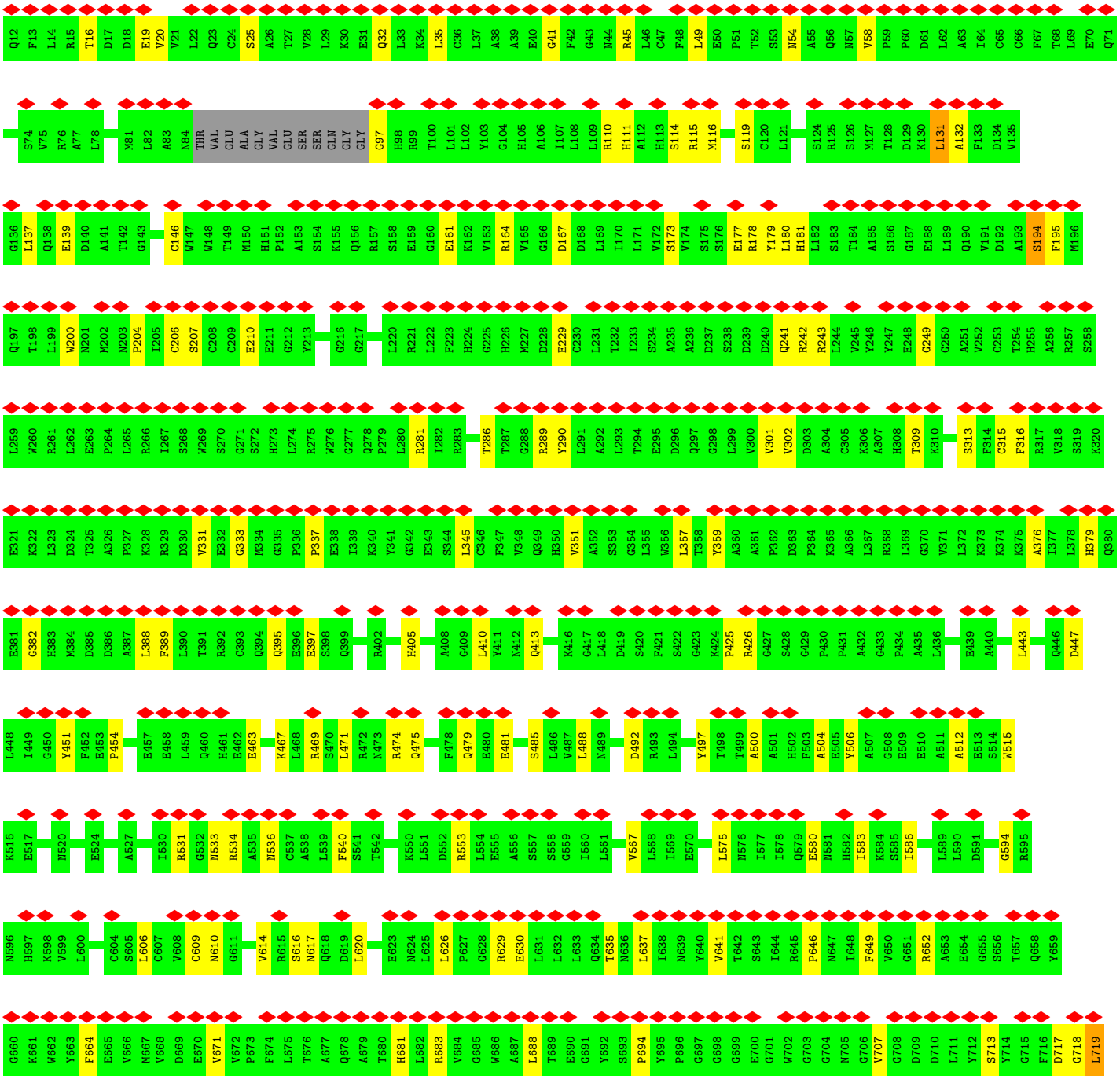
Chain J:

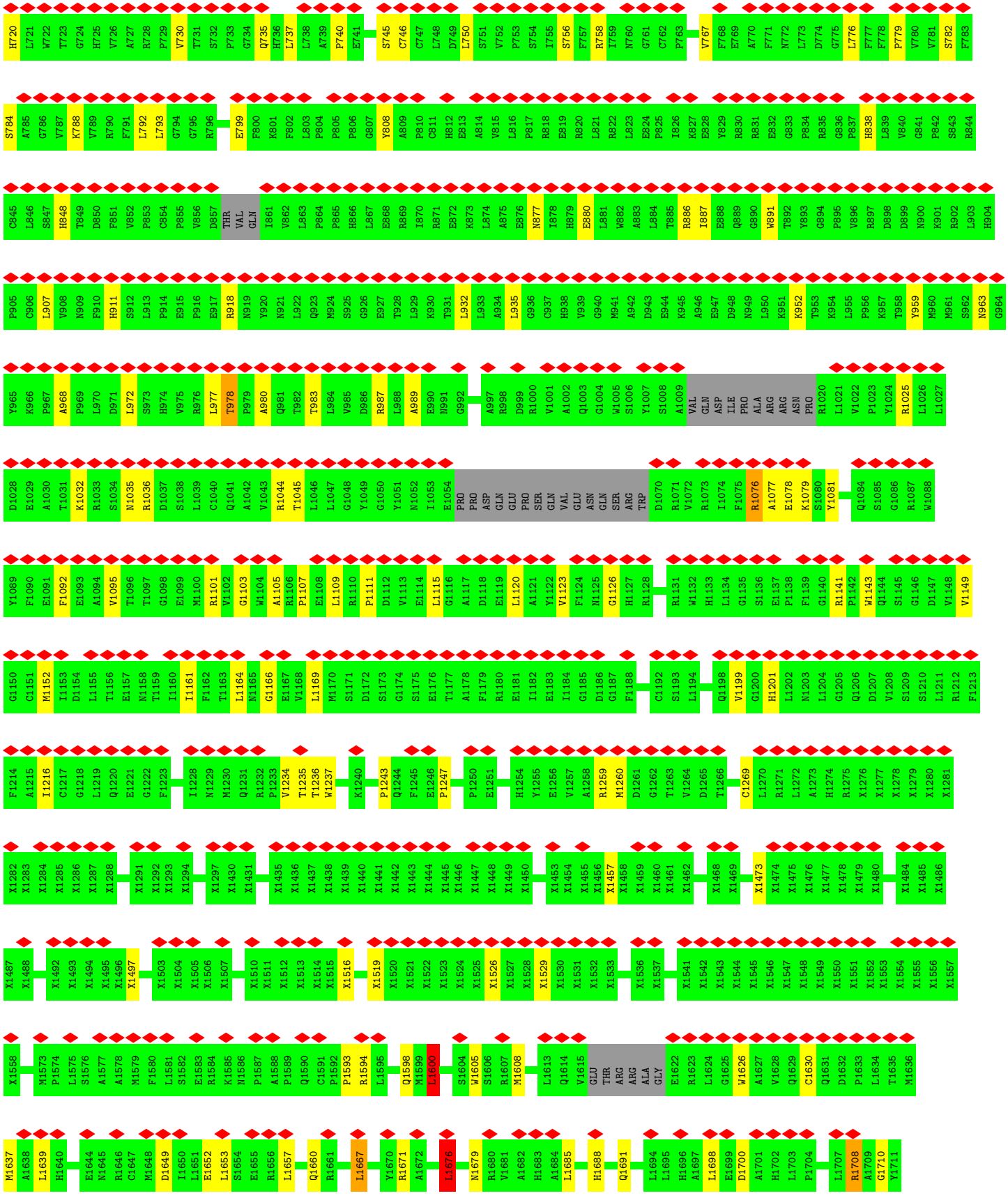




• Molecule 2: Ryanodine receptor 1

Chain B:

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S784 A785 G786 V787 K788 V789 R790 F791 L792 L793 G794 G795 R796 E799 F800 K801 F802 L803 P804 P805 H806 G807 Y808 A809 P810 C811 H812 E813 A814 V815 L816 P817 R818 E819 R820 L821 R822 L823 E824 P825 I826 K827 E828 Y829 R830 R831 E832 G833 P834 R835 G836 P837 H838 L839 V840 G841 P842 S843 R844
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G1150 C1151 M1152 I1153 D1154 L1155 T1156 E1157 N1158 T1159 I1160 I1161 F1162 T1163 L1164 N1165 G1166 E1167 V1168 L1169 M1170 S1171 D1172 S1173 G1174 S1175 E1176 T1177 A1178 F1179 R1180 E1181 I1182 E1183 I1184 G1185 D1186 G1187 F1188 C1192 S1193 L1194 Q1198 V1199 G1200 H1201 L1202 N1203 L1204 G1205 Q1206 D1207 V1208 S1209 S1210 L1211 R1212 F1213
F1214 A1215 I1216 C1217 G1218 L1219 Q1220 E1221 G1222 F1223 T1228 N1229 M1230 Q1231 R1232 P1233 V1234 T1235 T1236 W1237 K1240 P1243 Q1244 F1245 E1246 P1247 P1250 E1251 H1254 Y1255 E1256 V1257 A1258 R1259 M1260 D1261 G1262 T1263 V1264 D1265 T1266 C1269 L1270 R1271 L1272 A1273 H1274 R1275 X1276 X1277 X1278 X1279 X1280 X1281
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X1558 M1573 P1574 L1575 S1576 A1577 A1578 M1579 F1580 L1581 S1582 E1583 R1584 K1585 N1586 P1587 A1588 P1589 Q1590 C1591 P1592 P1593 R1594 L1595 Q1598 M1599 L1600 S1604 W1605 S1606 R1607 M1608 L1613 Q1614 V1615 GLU THR ARG ARG ALA GLY E1622 R1623 L1624 G1625 W1626 A1627 V1628 Q1629 C1630 Q1631 D1632 P1633 L1634 T1635 M1636
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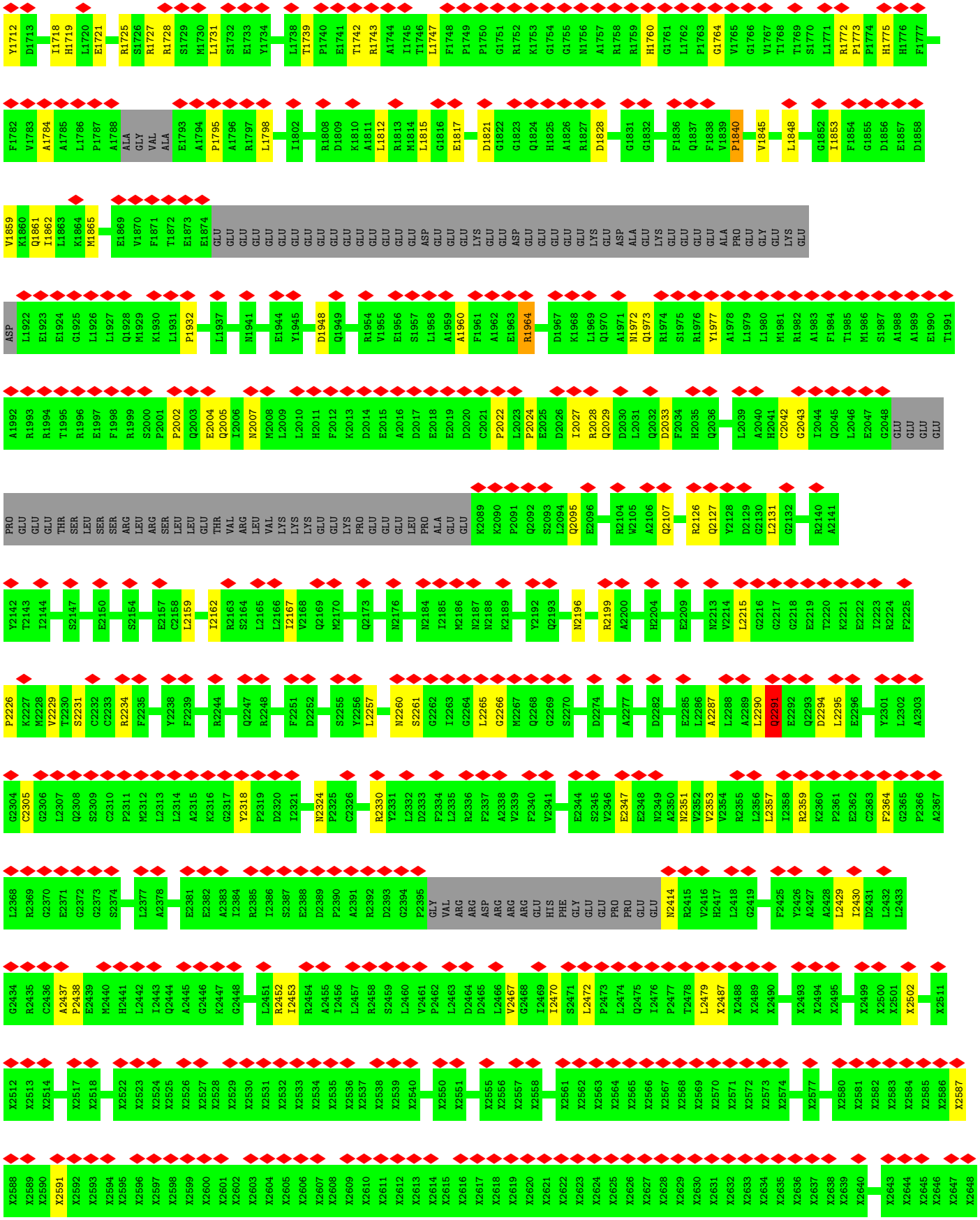
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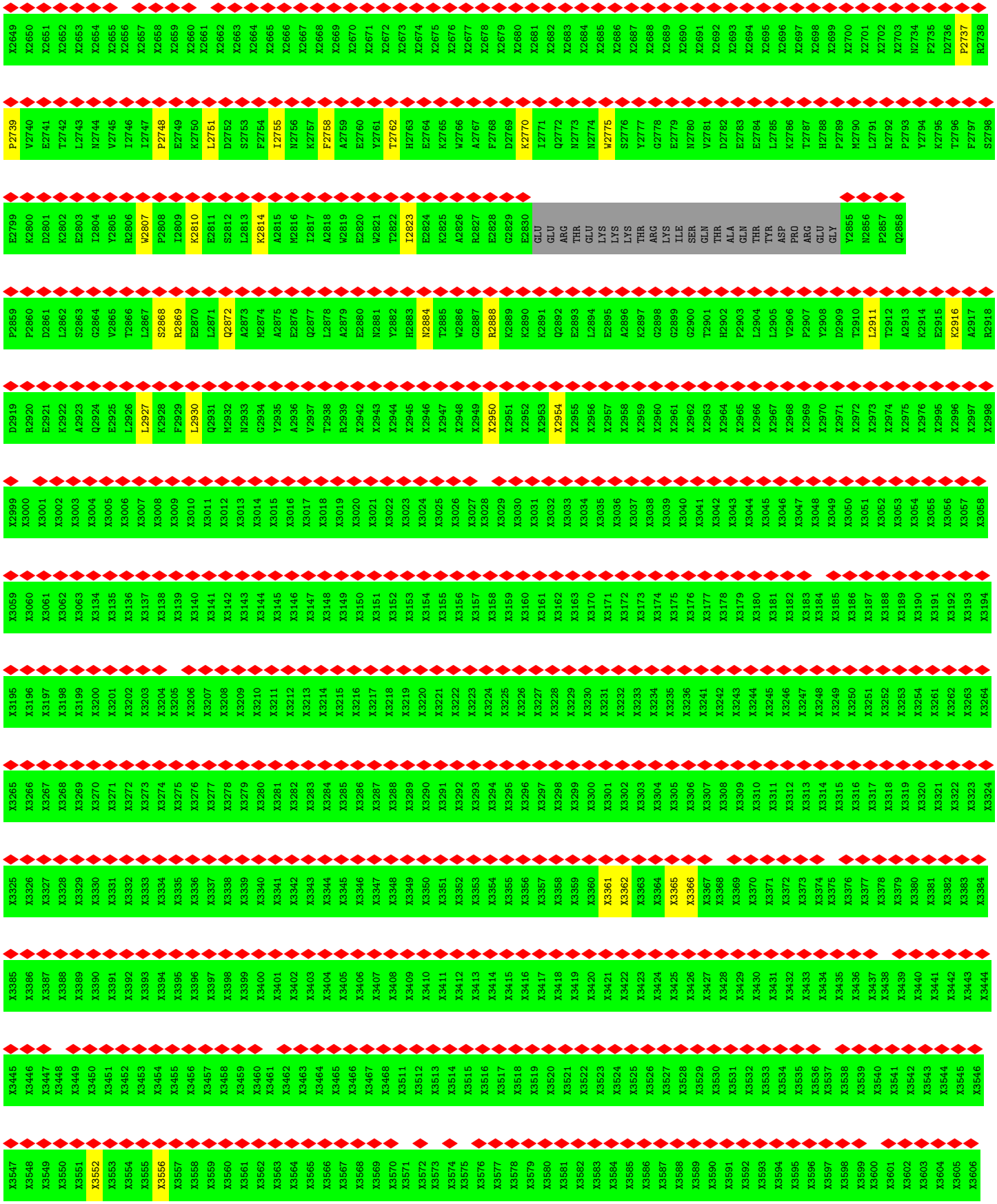
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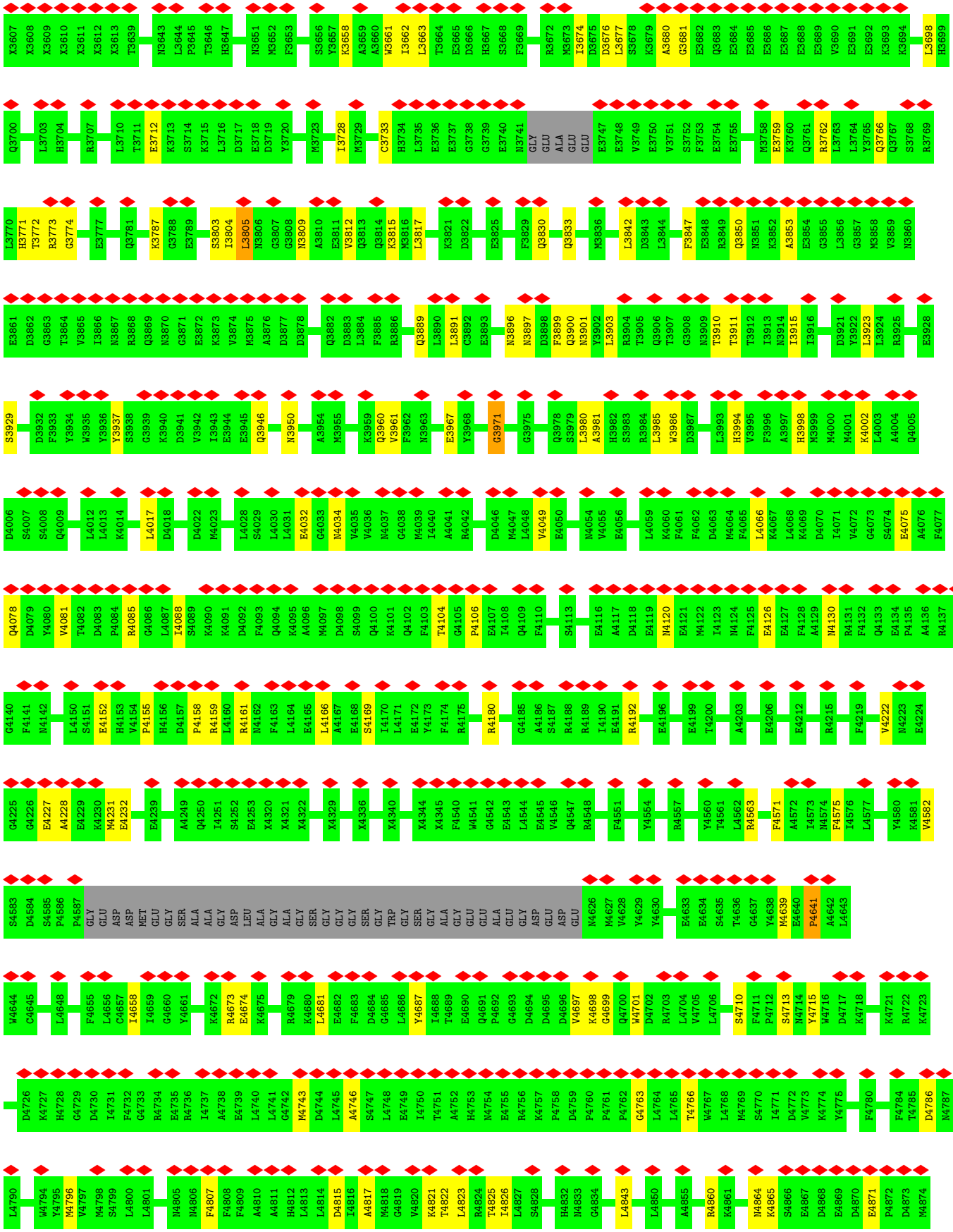
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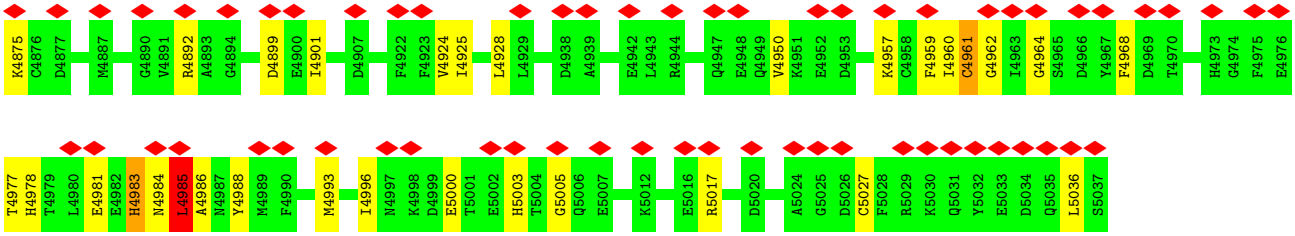
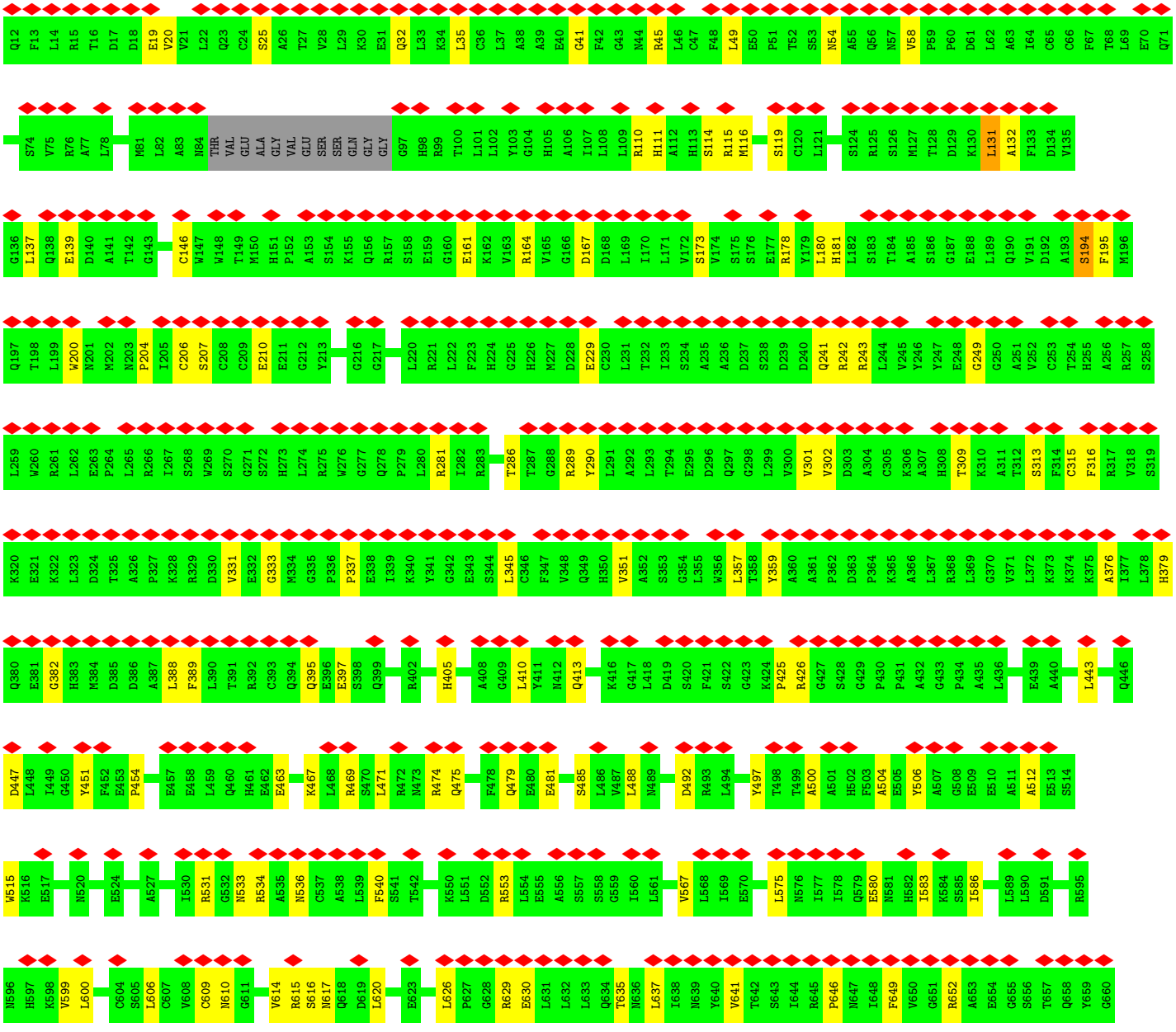
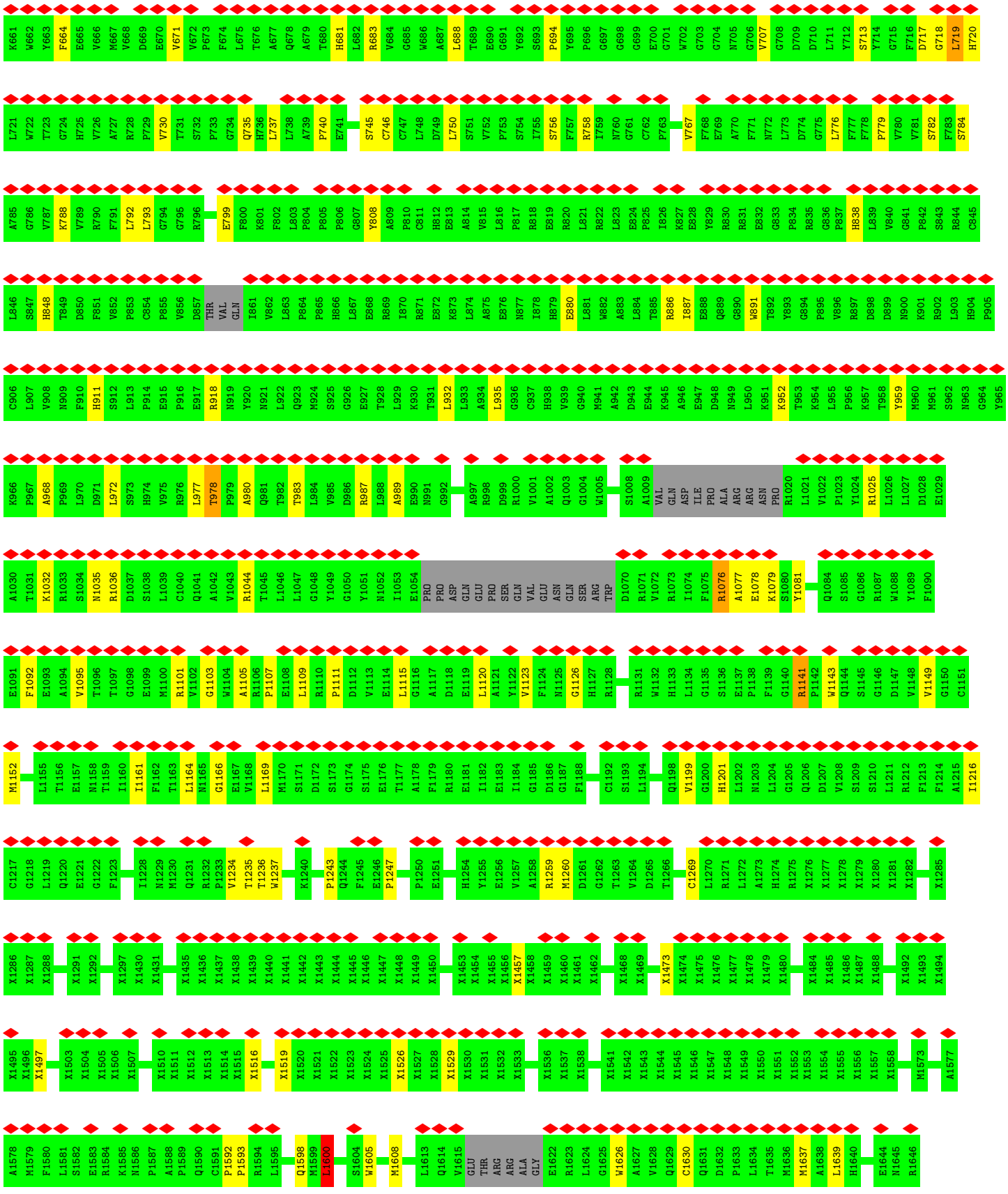


• Molecule 2: Ryanodine receptor 1

Chain G:

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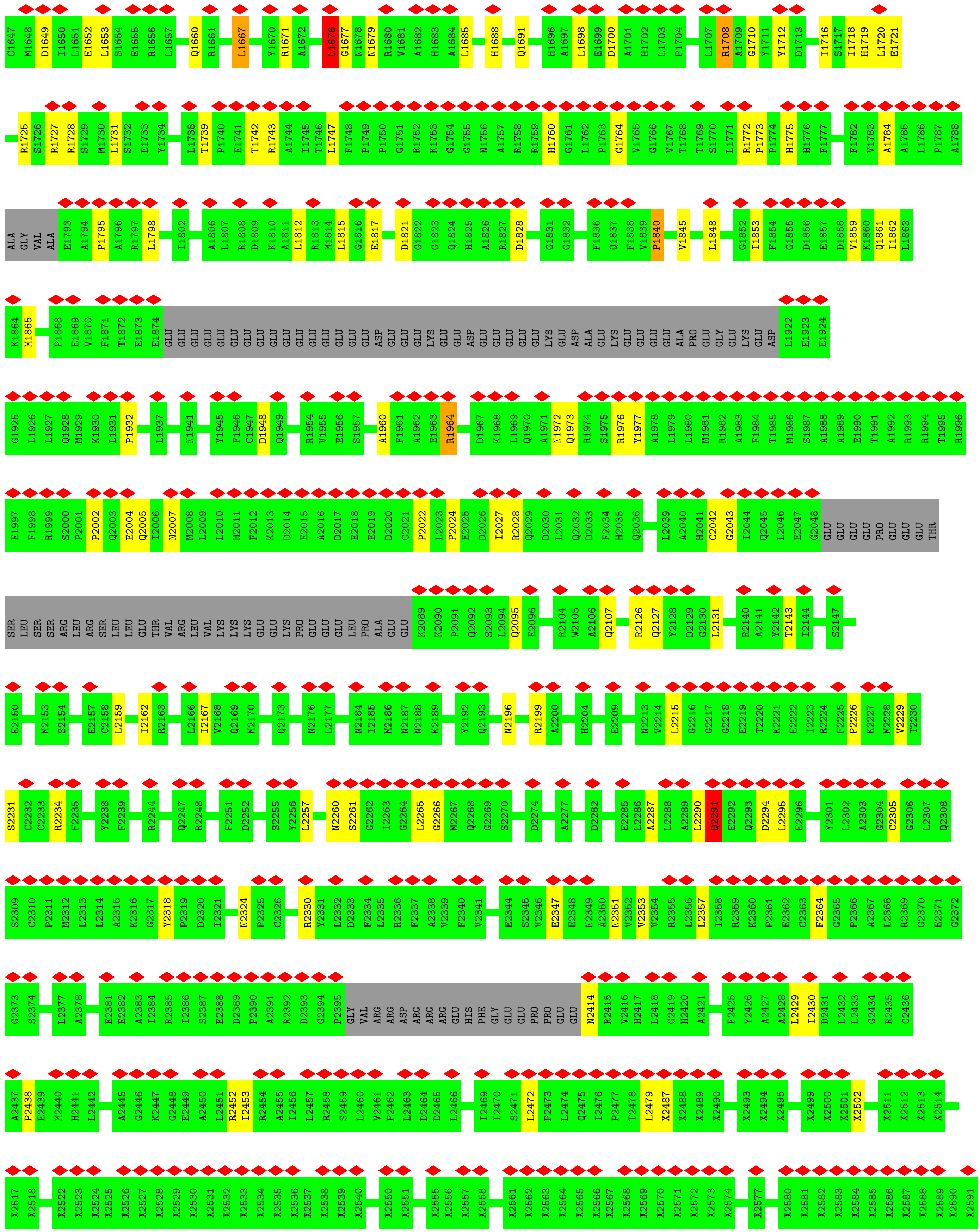
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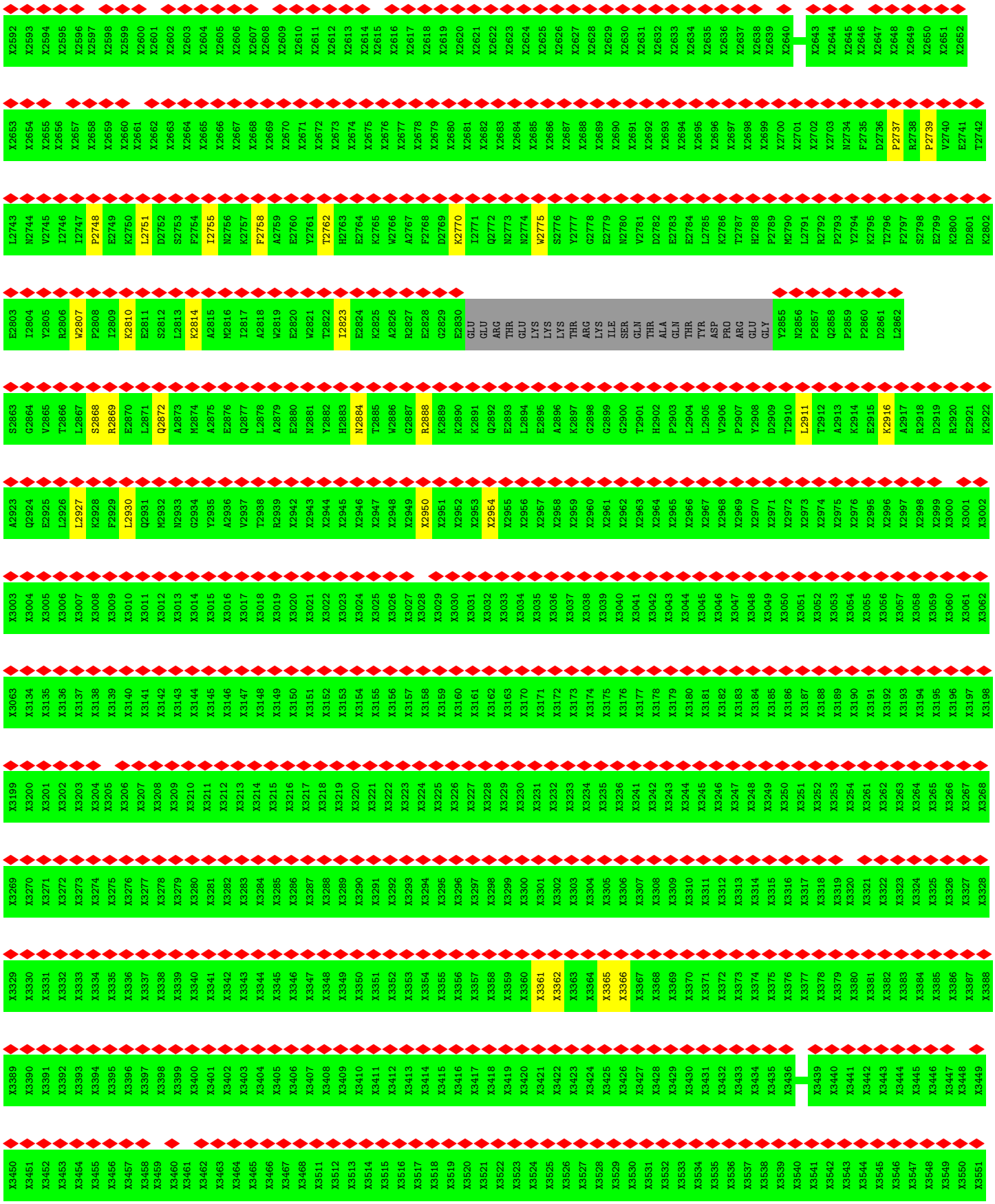
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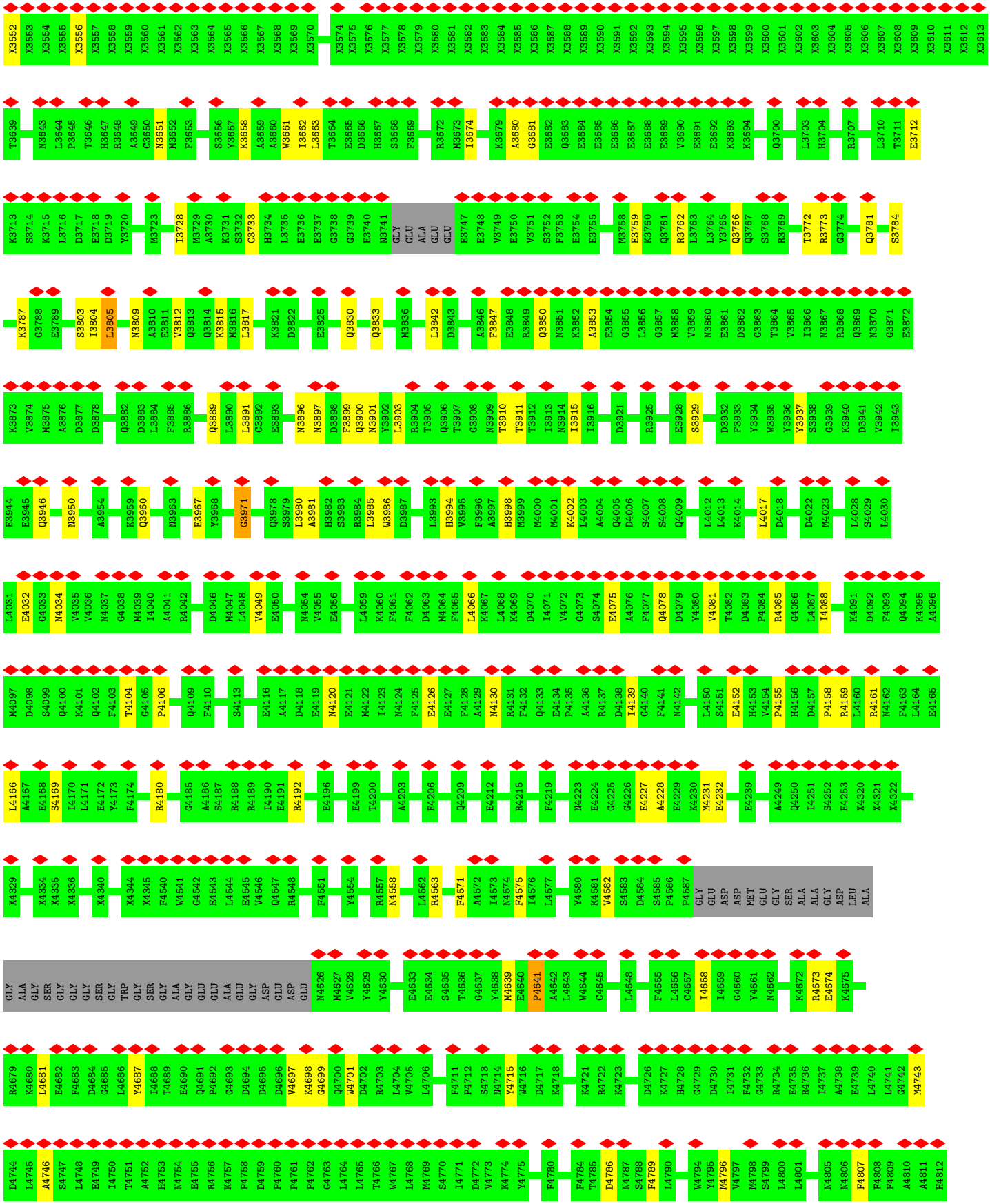
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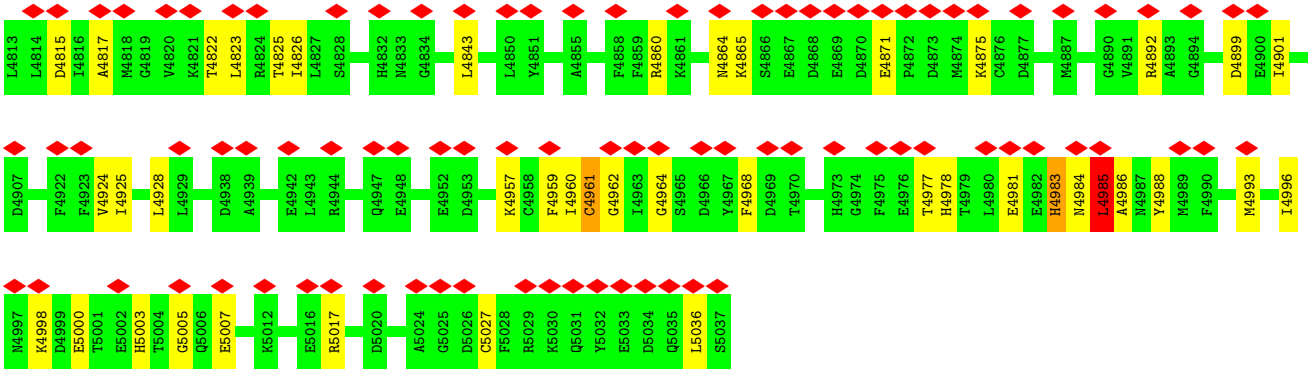
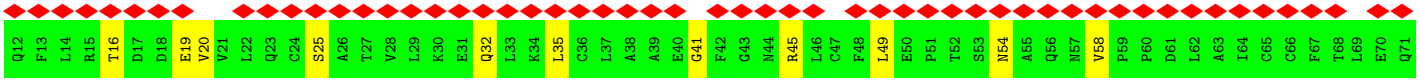
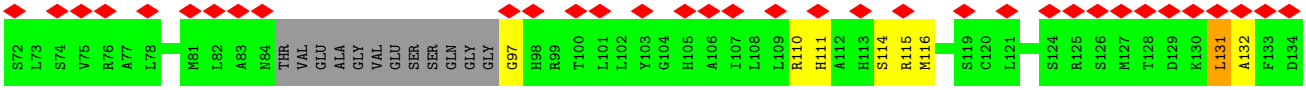
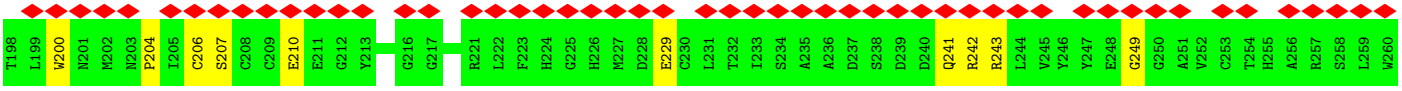


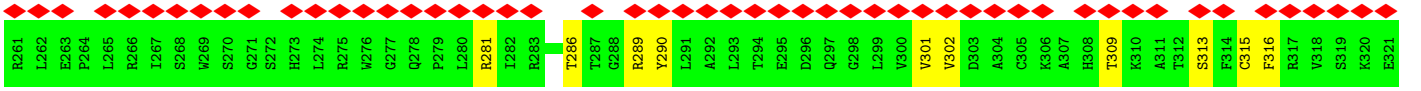
• Molecule 2: Ryanodine receptor 1

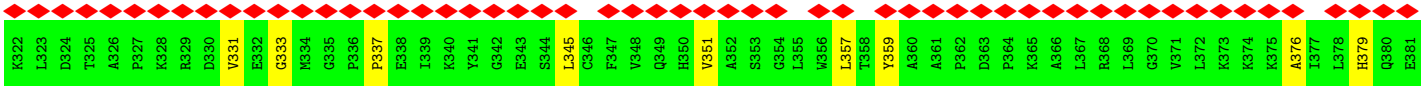
Chain I:

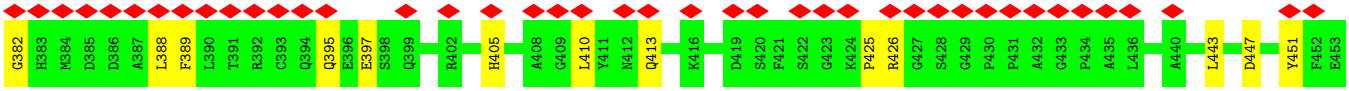


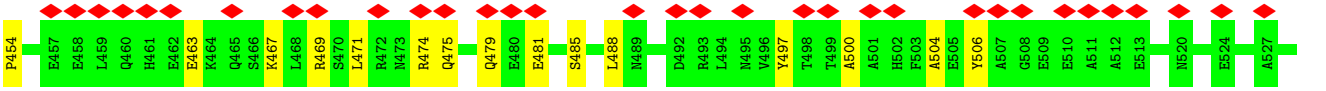


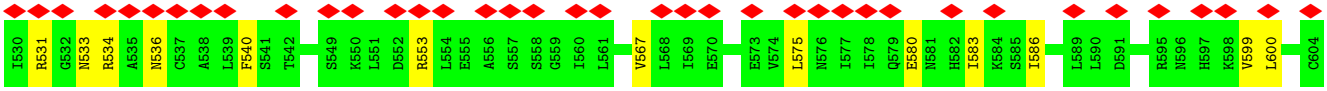


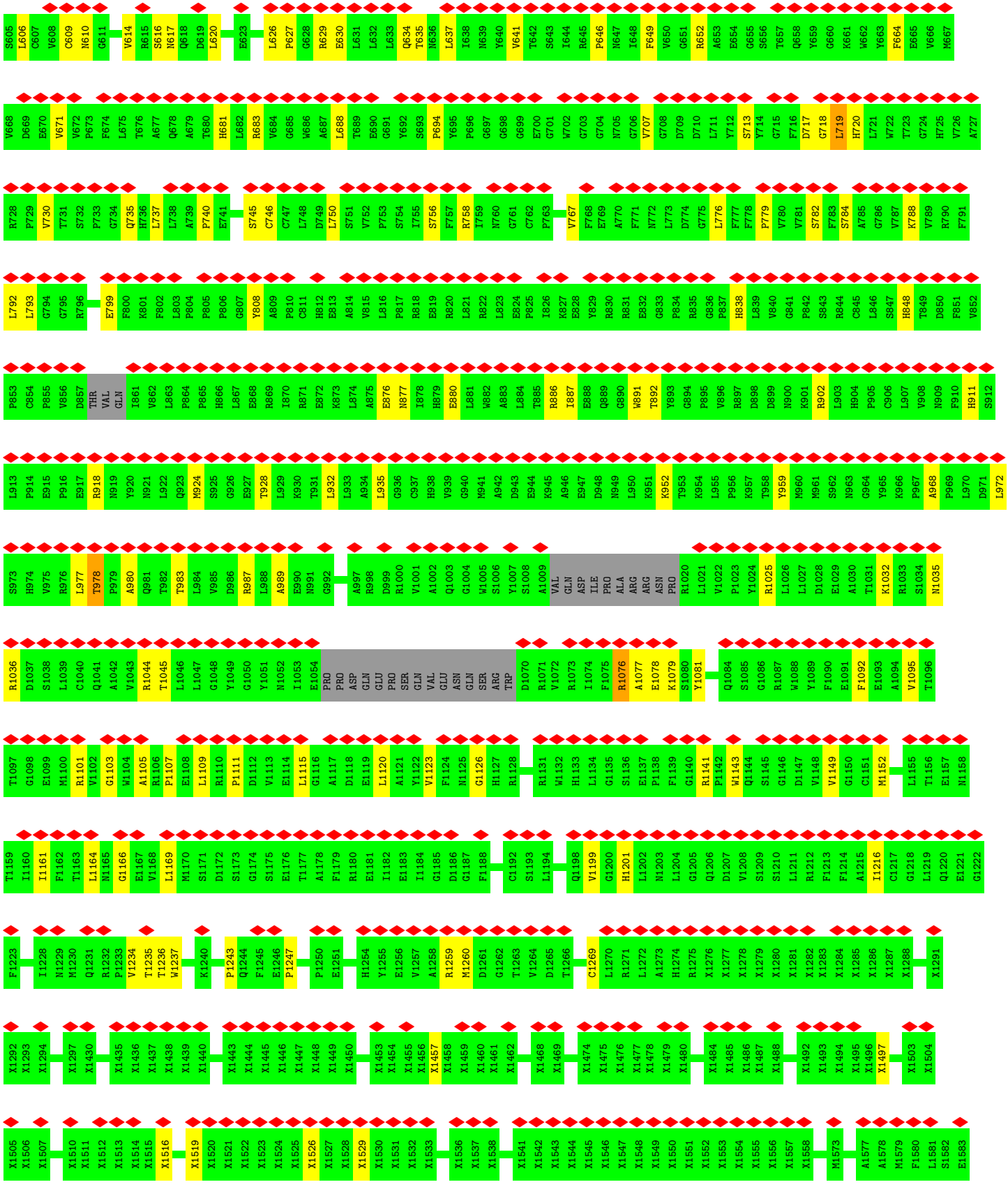








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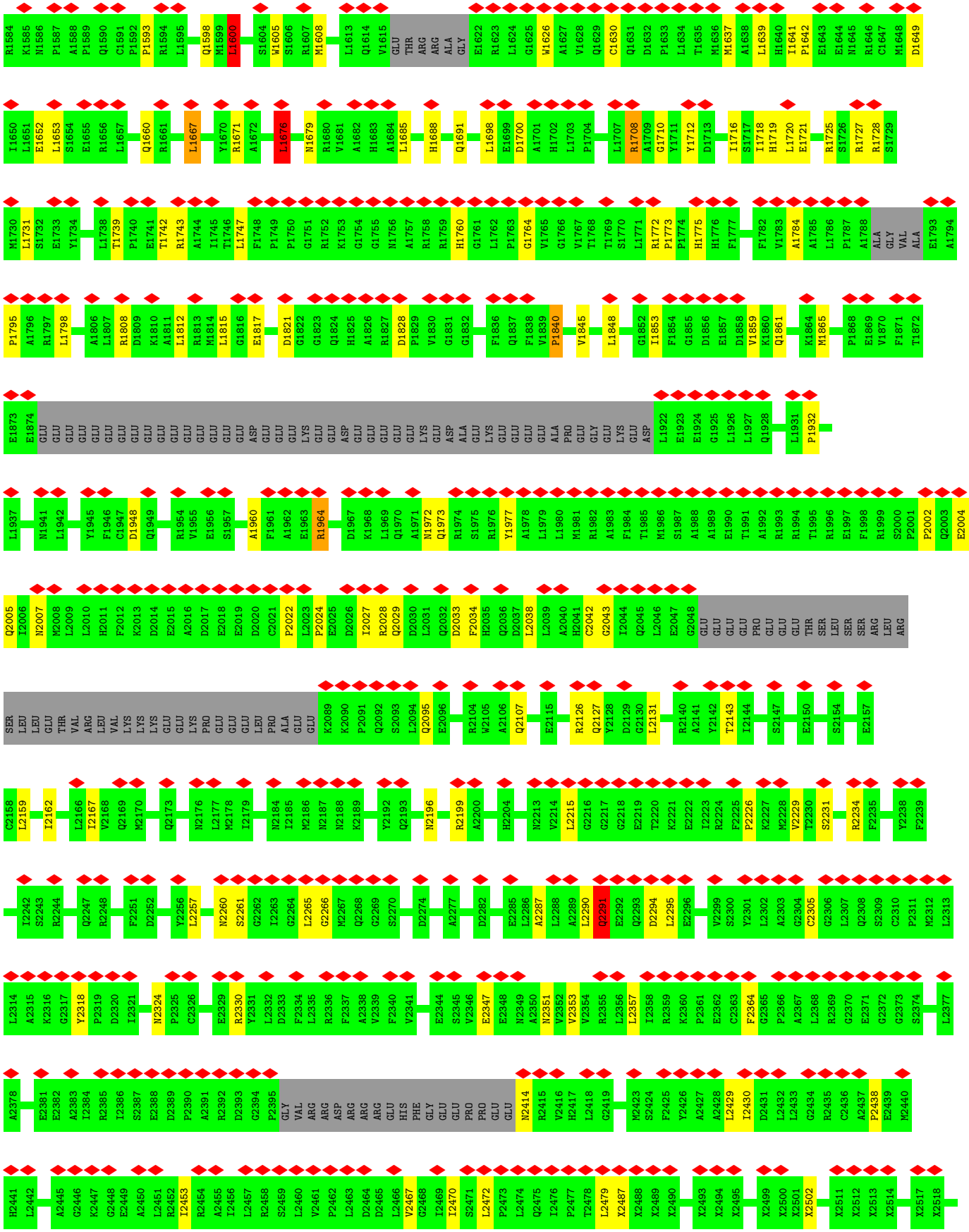

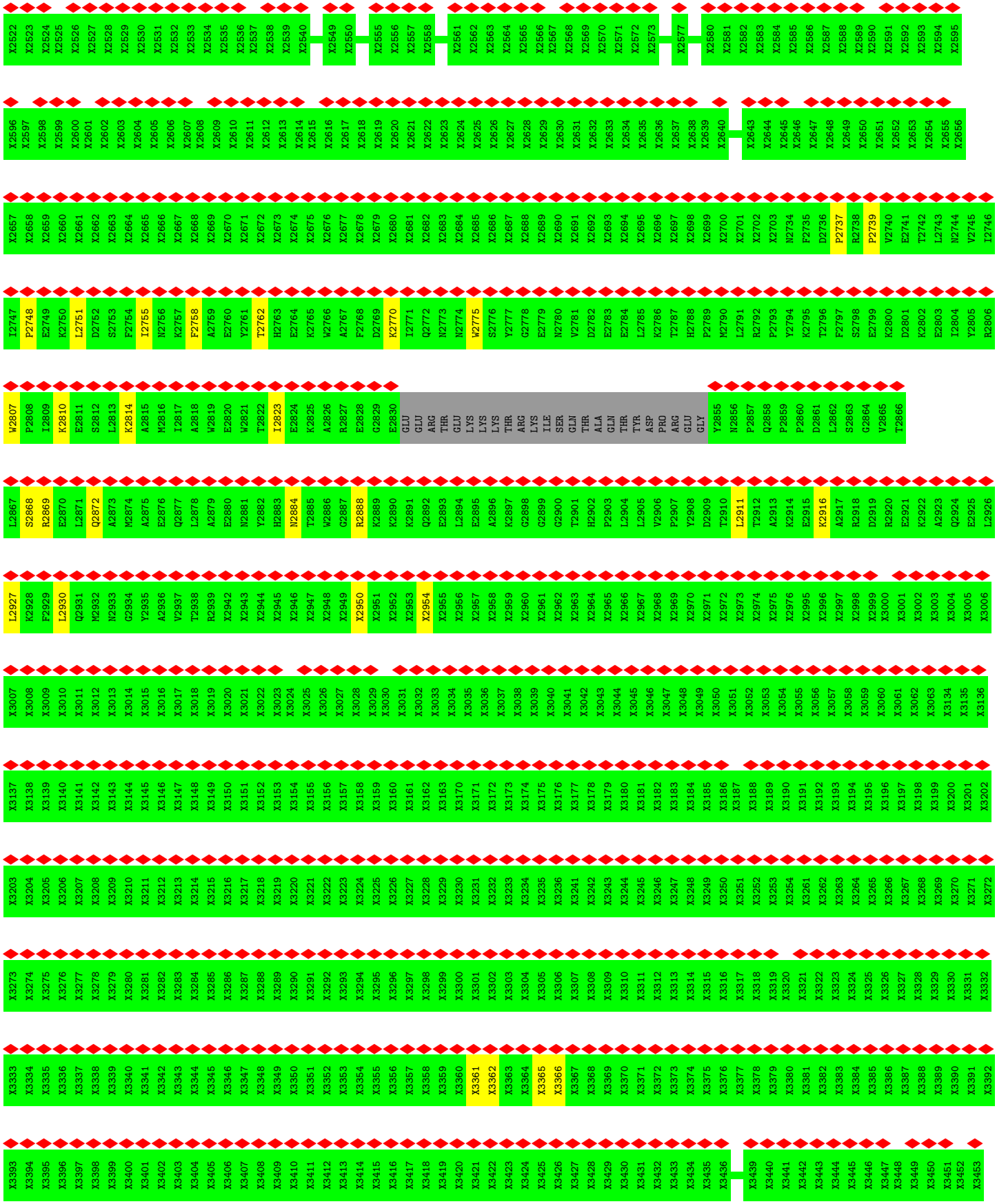
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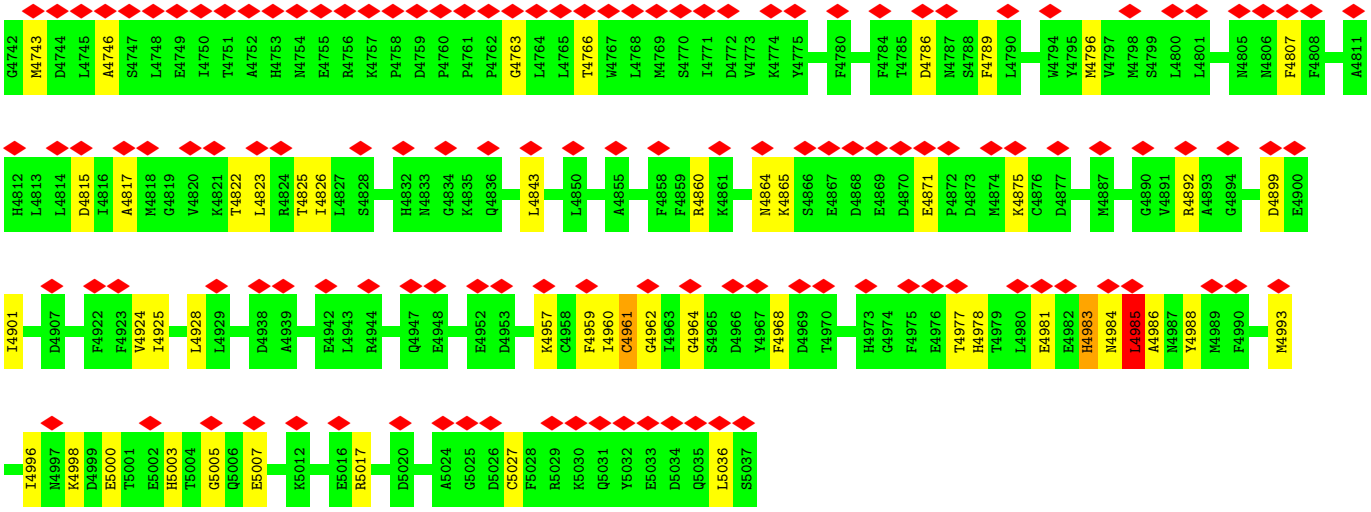

• Molecule 2: Ryanodine receptor 1

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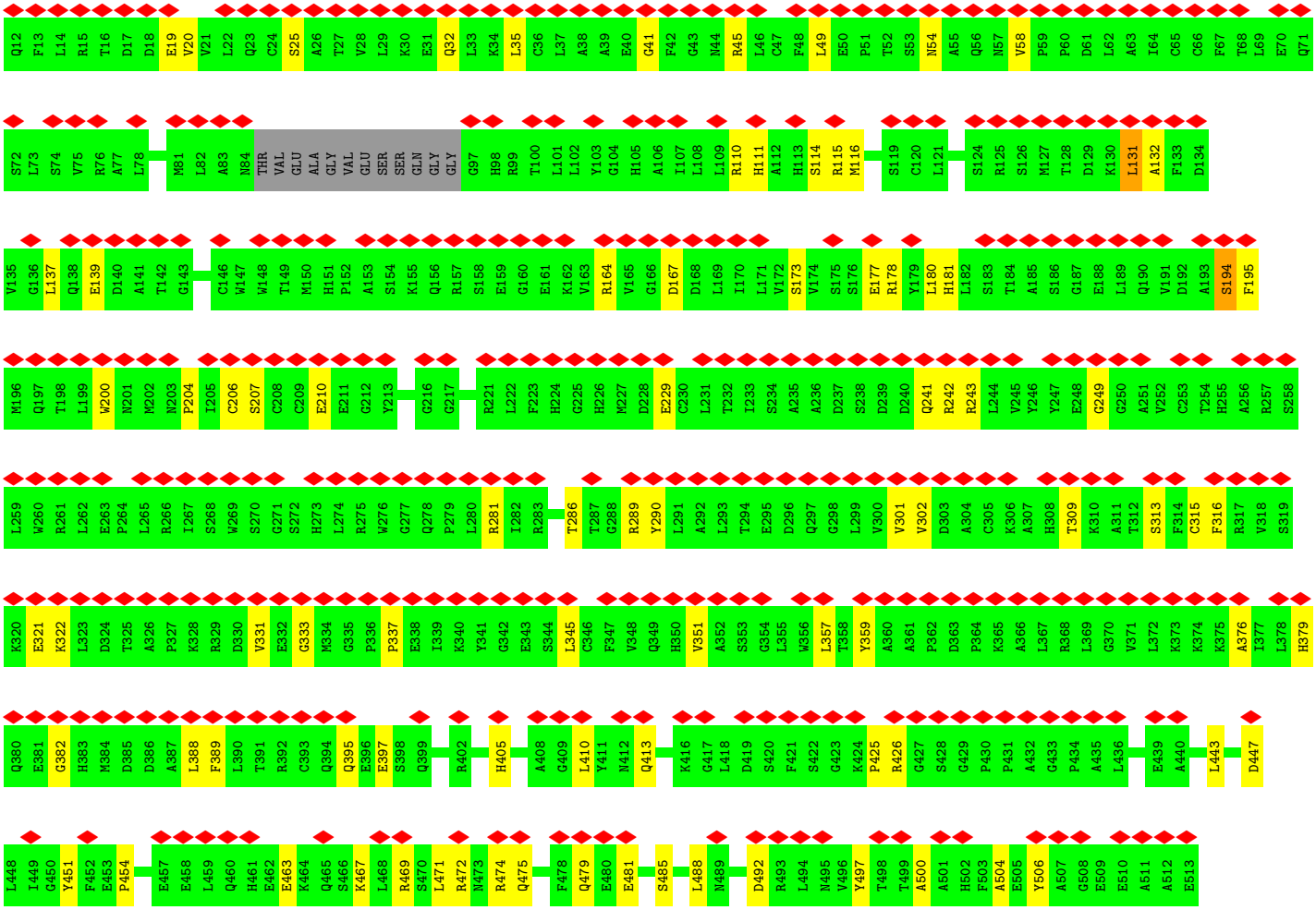

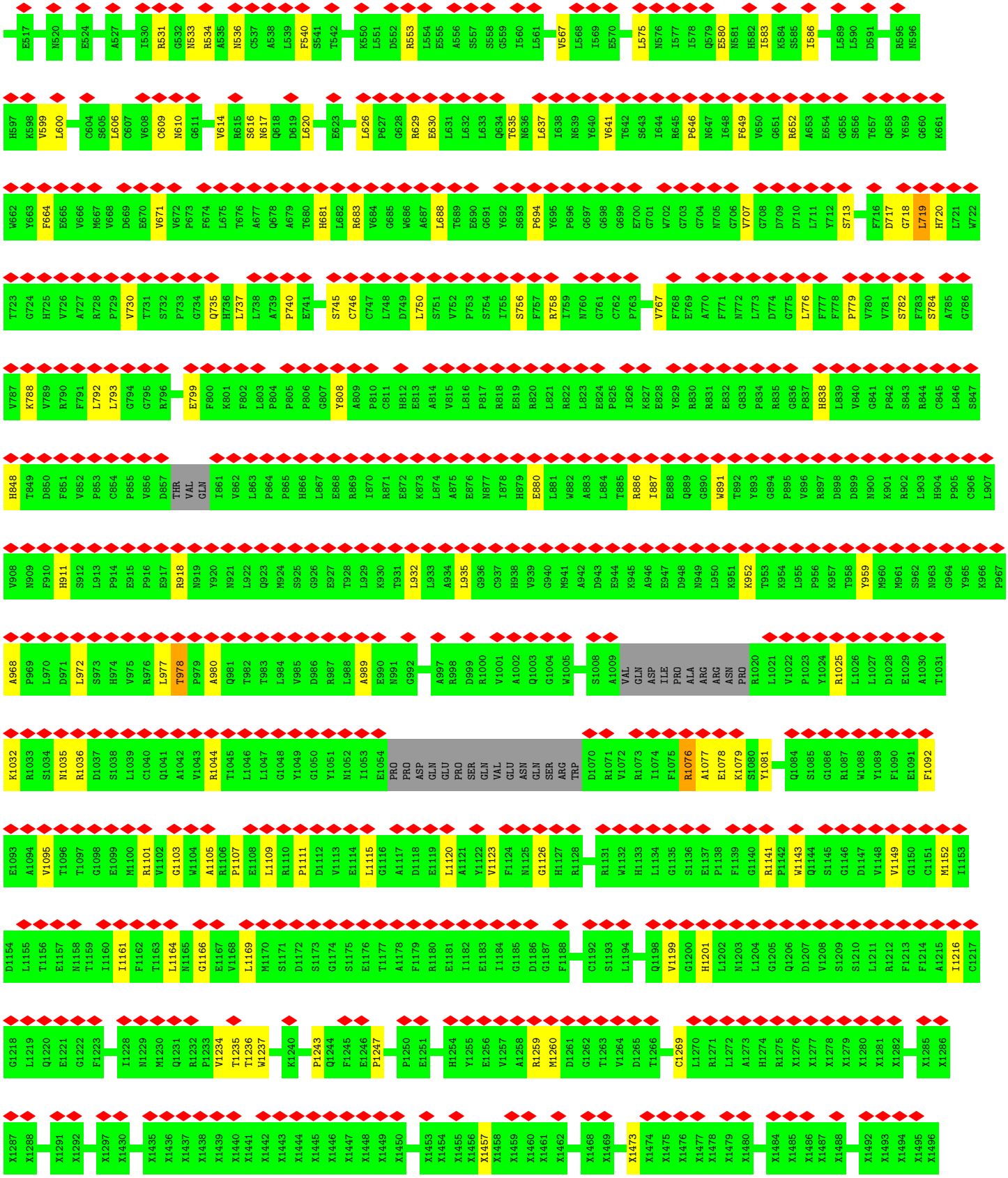
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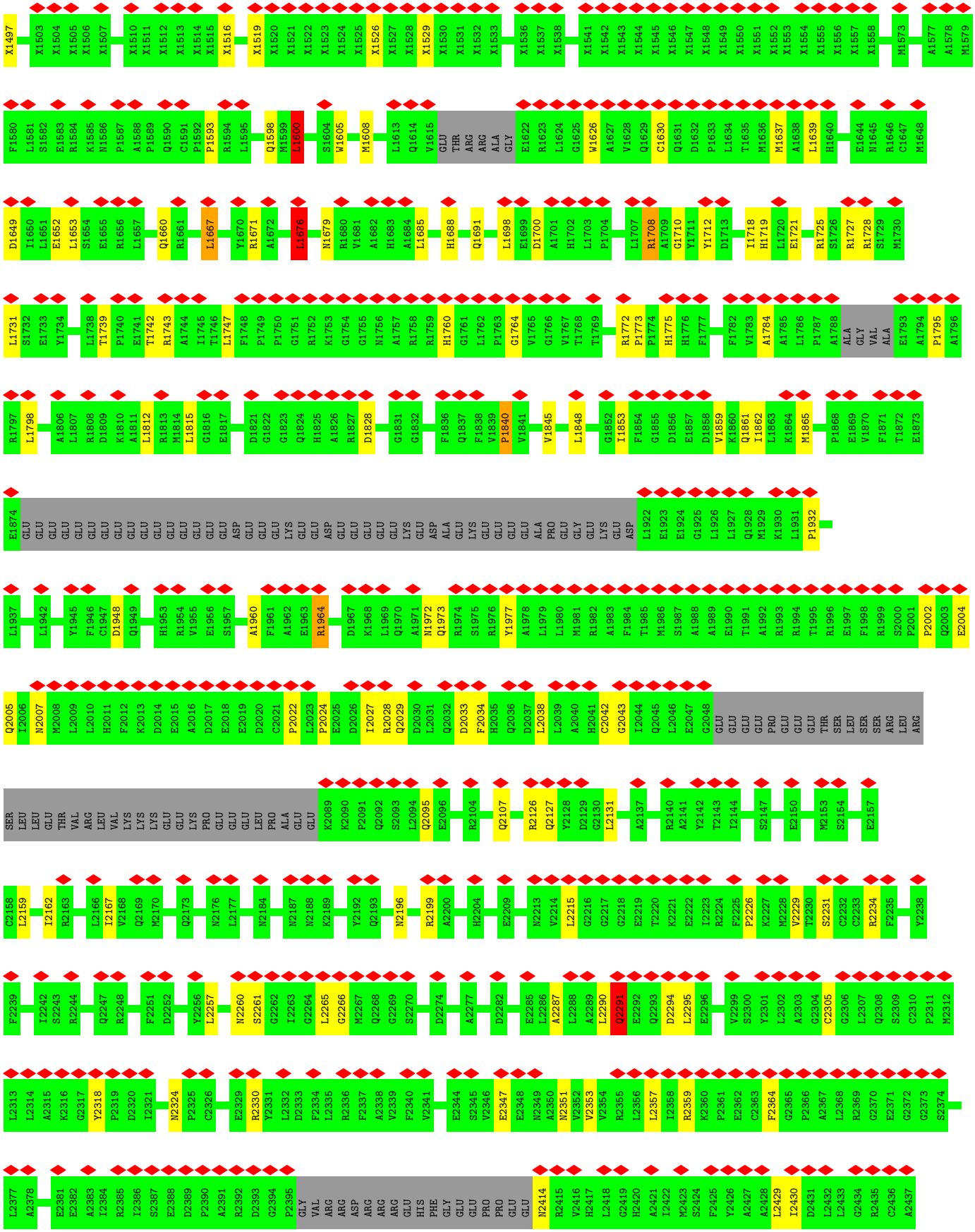

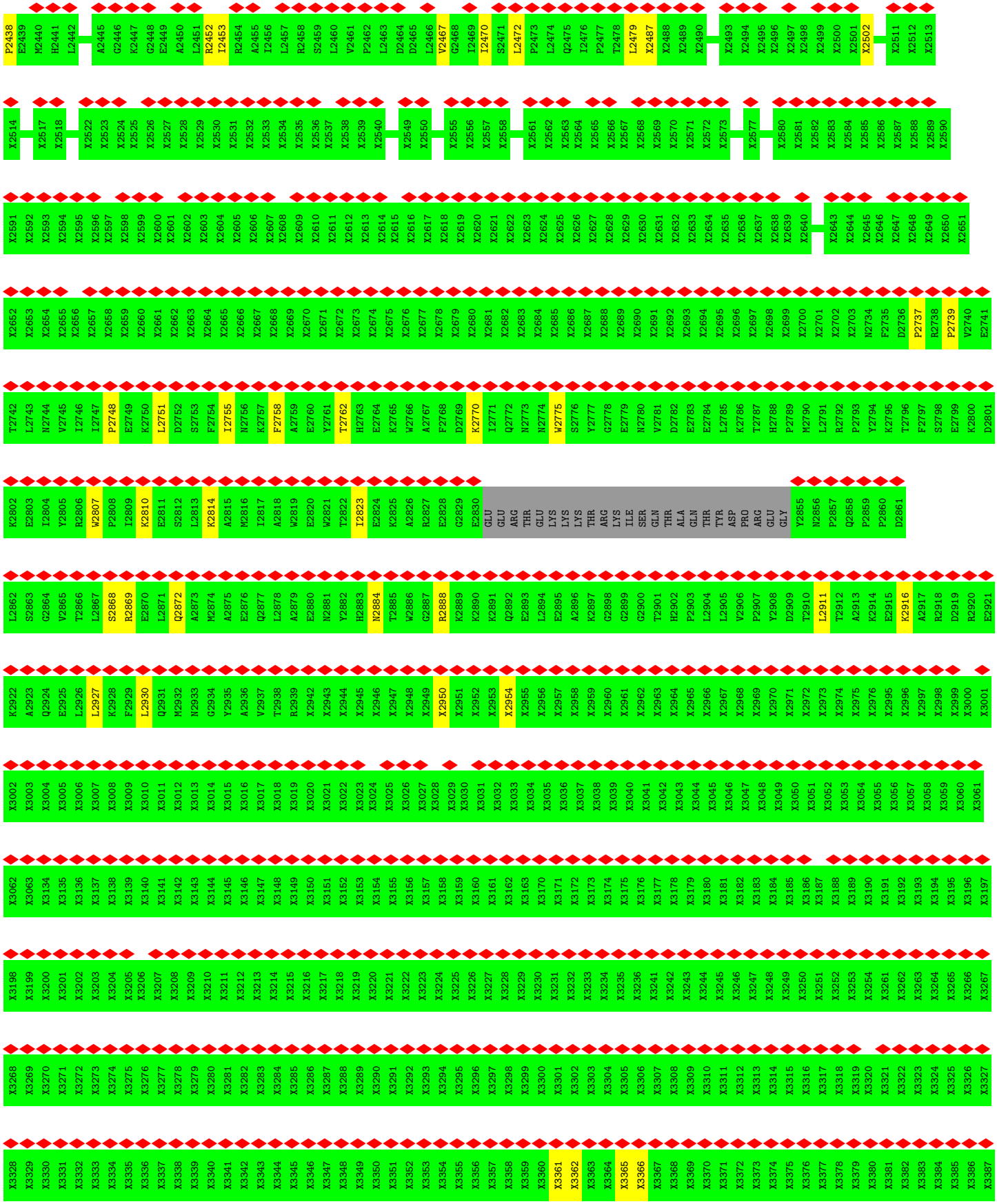
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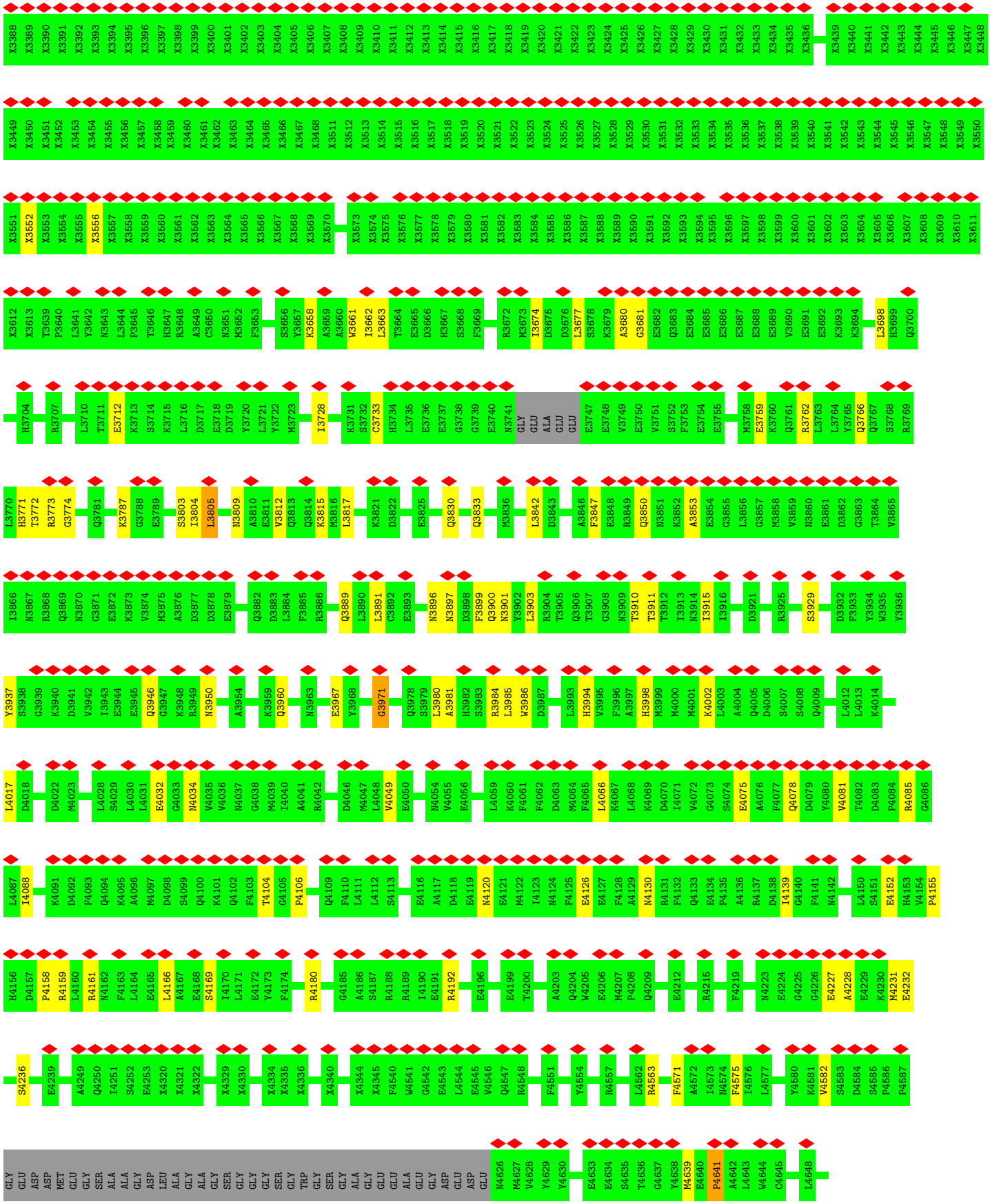
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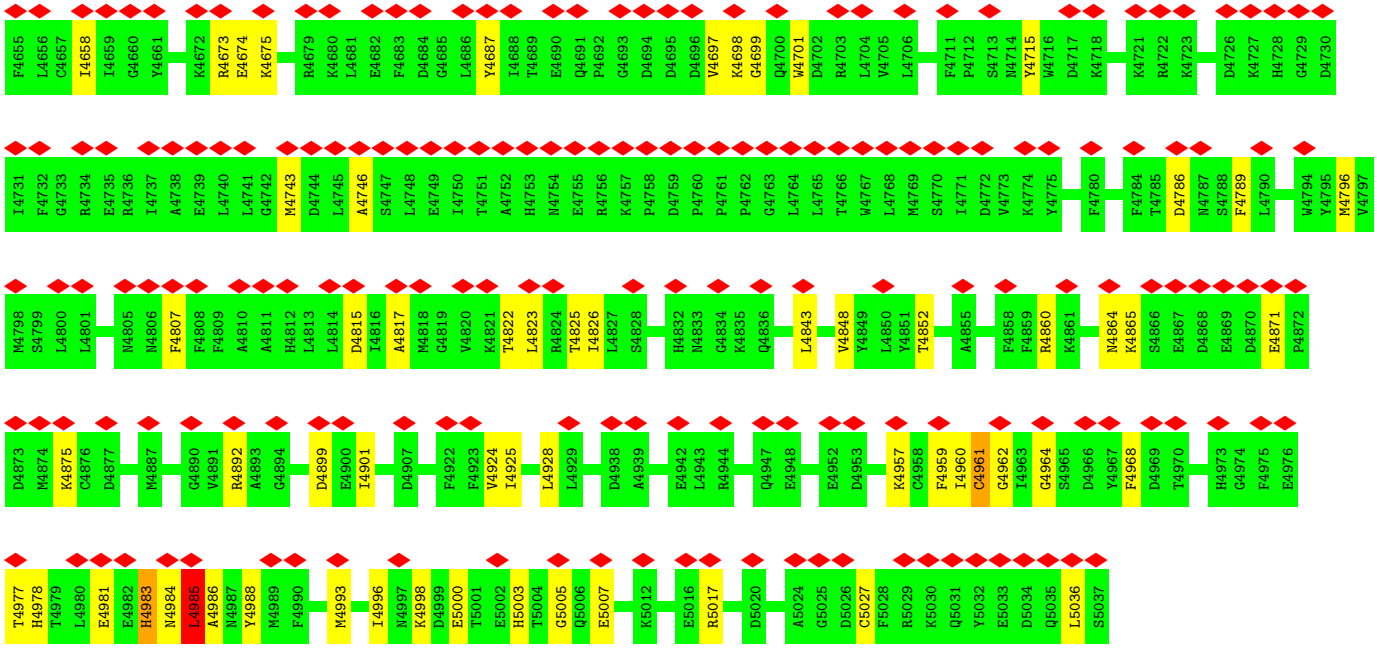
H3704 R3707 L3710 T3711 E3712 K3713 S3714 K3715 L3716 D3717 E3718 D3719 Y3720 L3721 Y3722 M3723 I3728 K3731 S3732 C3733 H3734 L3735 E3736 E3737 G3738 G3739 E3740 N3741 GLY GLU ALA GLU GLU E3747 E3748 V3749 E3750 V3751 S3752 F3753 E3754 E3755 M3758 E3759 K3760 Q3761 R3762 L3763 L3764 Y3765 Q3766 Q3767 S3768 R3769
L3770 H3771 T3772 R3773 G3774 Q3781 K3787 G3788 E3789 S3803 I3804 L3805 N3809 A3810 E3811 V3812 Q3813 Q3814 K3815 M3816 L3817 K3821 D3822 E3825 Q3830 Q3833 M3836 L3842 D3843 A3846 F3847 E3848 R3849 Q3850 N3851 K3852 A3853 E3854 G3855 L3856 G3857 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865
I3866 N3867 R3868 Q3869 N3870 G3871 E3872 K3873 V3874 M3875 A3876 D3877 D3878 E3879 Q3882 D3883 L3884 F3885 R3886 Q3889 L3890 L3891 G3892 E3893 N3896 N3897 D3898 F3899 Q3900 N3901 Y3902 L3903 R3904 T3905 Q3906 T3907 G3908 N3909 T3910 T3911 T3912 I3913 N3914 I3915 I3916 D3921 R3925 S3929 D3932 F3933 Y3934 W3935 Y3936
Y3937 S3938 G3939 K3940 D3941 V3942 I3943 E3944 E3945 Q3946 G3947 K3948 R3949 N3950 A3954 K3959 Q3960 N3963 E3967 Y3968 G3971 Q3978 S3979 L3980 A3981 H3982 S3983 R3984 L3985 W3986 D3987 L3993 H3994 V3995 F3996 A3997 H3998 M3999 M4000 M4001 K4002 L4003 A4004 Q4005 D4006 S4007 S4008 Q4009 L4012 L4013 K4014
L4017 D4018 D4022 M4023 L4028 S4029 L4030 L4031 E4032 G4033 N4034 V4035 V4036 N4037 G4038 M4039 I4040 A4041 R4042 D4046 M4047 L4048 V4049 E4050 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 K4091 D4092 F4093 Q4094 K4095 A4096 M4097 D4098 S4099 Q4100 K4101 Q4102 F4103 T4104 G4105 P4106 Q4109 F4110 L4111 L4112 S4113 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 L4150 S4151 E4152 H4153 V4154 P4155
H4156 D4157 P4158 R4159 L4160 R4161 N4162 F4163 L4164 E4165 L4166 A4167 E4168 S4169 I4170 L4171 E4172 Y4173 F4174 R4180 G4185 A4186 S4187 R4188 R4189 I4190 E4191 R4192 E4196 E4199 T4200 A4203 Q4204 W4205 E4206 M4207 P4208 Q4209 E4212 R4215 F4219 N4223 E4224 G4225 G4226 E4227 A4228 E4229 K4230 M4231 E4232
S4236 E4239 A4249 Q4250 I4251 S4252 E4253 X4320 X4321 X4322 X4329 X4330 X4334 X4335 X4336 X4340 X4344 X4345 F4540 W4541 G4542 E4543 L4544 E4545 V4546 Q4547 R4548 F4551 Y4554 R4557 L4562 R4563 F4571 A4572 I4573 N4574 F4575 I4576 L4577 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 ASP GLU N4626 M4627 V4628 Y4629 Y4630 E4633 E4634 S4635 T4636 G4637 Y4638 M4639 E4640 P4641 A4642 L4643 W4644 C4645 L4648


F4655 L4656 C4657 I4658 I4659 G4660 Y4661 K4672 R4673 E4674 K4675 R4679 K4680 L4681 E4682 F4683 D4684 G4685 L4686 Y4687 I4688 T4689 E4690 Q4691 P4692 G4693 D4694 D4695 D4696 V4697 K4698 G4699 Q4700 W4701 D4702 R4703 L4704 V4705 L4706 F4711 P4712 S4713 N4714 Y4715 W4716 D4717 K4718 K4721 R4722 K4723 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 F4780 F4784 T4785 D4786 N4787 S4788 F4789 L4790 W4794 Y4795 M4796 V4797
M4798 S4799 L4800 L4801 N4805 N4806 F4807 F4808 F4809 A4810 A4811 H4812 L4813 L4814 D4815 I4816 A4817 M4818 G4819 V4820 K4821 T4822 L4823 R4824 T4825 I4826 L4827 S4828 H4832 N4833 G4834 K4835 Q4836 L4843 V4848 Y4849 L4850 Y4851 T4852 A4855 F4858 F4859 R4860 K4861 N4864 K4865 S4866 E4867 D4868 E4869 D4870 E4871 P4872
D4873 M4874 K4875 C4876 D4877 M4887 G4890 V4891 R4892 A4893 G4894 D4899 E4900 I4901 D4907 F4922 F4923 V4924 I4925 L4928 L4929 D4938 A4939 E4942 L4943 R4944 Q4947 E4948 E4952 D4953 K4957 C4958 F4959 I4960 C4961 G4962 I4963 G4964 S4965 D4966 Y4967 F4968 D4969 T4970 H4973 G4974 F4975 E4976
T4977 H4978 T4979 L4980 E4981 E4982 H4983 N4984 L4985 A4986 N4987 Y4988 M4989 F4990 M4993 I4996 N4997 K4998 D4999 E5000 T5001 E5002 H5003 T5004 G5005 Q5006 E5007 K5012 E5016 R5017 D5020 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	0.060	Depositor
Minimum map value	-0.032	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: ATP, CA, ZN, CFF

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	0.31	0/834	0.53	0/1123
1	F	0.31	0/834	0.53	0/1123
1	H	0.31	0/834	0.53	0/1123
1	J	0.31	0/834	0.53	0/1123
2	B	0.30	0/25428	0.54	10/34534 (0.0%)
2	E	0.30	0/25428	0.54	10/34534 (0.0%)
2	G	0.30	0/25428	0.54	10/34534 (0.0%)
2	I	0.30	0/25428	0.54	10/34534 (0.0%)
All	All	0.30	0/105048	0.54	40/142628 (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	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	56

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	131	LEU	CA-CB-CG	7.69	132.98	115.30
2	B	131	LEU	CA-CB-CG	7.67	132.95	115.30
2	E	131	LEU	CA-CB-CG	7.67	132.93	115.30
2	G	131	LEU	CA-CB-CG	7.65	132.90	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	4985	LEU	CA-CB-CG	6.48	130.20	115.30
2	B	4985	LEU	CA-CB-CG	6.47	130.19	115.30
2	G	4985	LEU	CA-CB-CG	6.46	130.16	115.30
2	E	4985	LEU	CA-CB-CG	6.46	130.16	115.30
2	I	1676	LEU	CA-CB-CG	6.45	130.14	115.30
2	B	1676	LEU	CA-CB-CG	6.45	130.14	115.30
2	E	1676	LEU	CA-CB-CG	6.45	130.12	115.30
2	G	1676	LEU	CA-CB-CG	6.44	130.12	115.30
2	G	1600	LEU	CA-CB-CG	6.37	129.95	115.30
2	B	1600	LEU	CA-CB-CG	6.37	129.94	115.30
2	I	1600	LEU	CA-CB-CG	6.37	129.94	115.30
2	E	1600	LEU	CA-CB-CG	6.35	129.91	115.30
2	G	4901	ILE	CG1-CB-CG2	-6.05	98.08	111.40
2	B	4901	ILE	CG1-CB-CG2	-6.05	98.08	111.40
2	I	4901	ILE	CG1-CB-CG2	-6.05	98.09	111.40
2	E	4901	ILE	CG1-CB-CG2	-6.05	98.10	111.40
2	G	977	LEU	CA-CB-CG	5.51	127.97	115.30
2	E	977	LEU	CA-CB-CG	5.50	127.95	115.30
2	B	977	LEU	CA-CB-CG	5.50	127.94	115.30
2	I	977	LEU	CA-CB-CG	5.49	127.93	115.30
2	G	719	LEU	CA-CB-CG	5.26	127.40	115.30
2	I	719	LEU	CA-CB-CG	5.25	127.39	115.30
2	B	719	LEU	CA-CB-CG	5.25	127.38	115.30
2	E	719	LEU	CA-CB-CG	5.24	127.35	115.30
2	I	4639	MET	C-N-CA	5.15	134.57	121.70
2	B	4639	MET	C-N-CA	5.15	134.57	121.70
2	E	4639	MET	C-N-CA	5.15	134.57	121.70
2	G	4639	MET	C-N-CA	5.13	134.52	121.70
2	G	1667	LEU	CA-CB-CG	5.09	127.01	115.30
2	B	1667	LEU	CA-CB-CG	5.08	126.99	115.30
2	E	1667	LEU	CA-CB-CG	5.08	126.98	115.30
2	I	688	LEU	CA-CB-CG	5.07	126.97	115.30
2	I	1667	LEU	CA-CB-CG	5.07	126.96	115.30
2	E	688	LEU	CA-CB-CG	5.06	126.94	115.30
2	B	688	LEU	CA-CB-CG	5.06	126.93	115.30
2	G	688	LEU	CA-CB-CG	5.05	126.93	115.30

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	194	SER	Peptide
2	B	2291	GLN	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4641	PRO	Peptide
2	B	4807	PHE	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	194	SER	Peptide
2	E	2291	GLN	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4641	PRO	Peptide
2	E	4807	PHE	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	194	SER	Peptide
2	G	2291	GLN	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4641	PRO	Peptide
2	G	4807	PHE	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
2	I	139	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	I	1676	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	194	SER	Peptide
2	I	2291	GLN	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4641	PRO	Peptide
2	I	4807	PHE	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	13	0
1	F	818	0	824	13	0
1	H	818	0	824	12	0
1	J	818	0	824	15	0
2	B	29499	0	24748	311	0
2	E	29499	0	24748	298	0
2	G	29499	0	24748	300	0
2	I	29499	0	24748	305	0
3	B	31	0	12	1	0
3	E	31	0	12	1	0
3	G	31	0	12	1	0
3	I	31	0	12	1	0
4	B	14	0	10	0	0
4	E	14	0	10	0	0
4	G	14	0	10	0	0
4	I	14	0	10	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
All	All	121456	0	102376	1234	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 6.

All (1234) 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:E:4968:PHE:CE2	2:E:4978:HIS:CE1	2.64	0.86
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	2.64	0.86
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.64	0.85
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	2.64	0.85
2:I:2318:TYR:HH	2:I:2414:ASN:N	1.81	0.78
2:G:2318:TYR:HH	2:G:2414:ASN:N	1.82	0.78
2:G:4968:PHE:HE2	2:G:4978:HIS:CE1	2.02	0.78
2:B:2318:TYR:HH	2:B:2414:ASN:N	1.83	0.77
2:E:4968:PHE:HE2	2:E:4978:HIS:CE1	2.02	0.77
2:E:2318:TYR:HH	2:E:2414:ASN:N	1.82	0.77
2:B:4968:PHE:HE2	2:B:4978:HIS:CE1	2.02	0.77
2:I:4968:PHE:HE2	2:I:4978:HIS:CE1	2.02	0.76
2:G:4985:LEU:HB2	3:G:5101:ATP:HN61	1.51	0.75
2:I:4985:LEU:HB2	3:I:5101:ATP:HN61	1.51	0.75
2:E:4985:LEU:HB2	3:E:5101:ATP:HN61	1.51	0.75
2:B:4985:LEU:HB2	3:B:5101:ATP:HN61	1.51	0.74
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.72	0.72
2:E:4957:LYS:HG2	2:E:4964:GLY:HA2	1.72	0.71
2:G:4957:LYS:HG2	2:G:4964:GLY:HA2	1.73	0.71
2:I:4957:LYS:HG2	2:I:4964:GLY:HA2	1.72	0.71
2:B:4957:LYS:HG2	2:B:4964:GLY:HA2	1.73	0.69
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.76	0.68
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.76	0.68
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.76	0.67
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.76	0.67
2:B:2266:GLY:O	2:B:2330:ARG:NH2	2.28	0.67
2:E:379:HIS:HD2	2:E:382:GLY:H	1.43	0.66
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.60	0.66
2:I:2266:GLY:O	2:I:2330:ARG:NH2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2266:GLY:O	2:E:2330:ARG:NH2	2.28	0.66
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.60	0.66
2:G:2266:GLY:O	2:G:2330:ARG:NH2	2.28	0.65
2:B:379:HIS:HD2	2:B:382:GLY:H	1.43	0.65
2:B:4823:LEU:HD23	2:I:4843:LEU:HD12	1.79	0.65
2:G:379:HIS:HD2	2:G:382:GLY:H	1.43	0.65
2:G:4860:ARG:HD2	2:I:4582:VAL:HG11	1.79	0.65
2:B:4983:HIS:CD2	2:B:4983:HIS:H	2.16	0.64
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.61	0.64
2:E:4983:HIS:CD2	2:E:4983:HIS:H	2.16	0.64
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.80	0.63
2:G:4983:HIS:CD2	2:G:4983:HIS:H	2.16	0.63
2:I:379:HIS:HD2	2:I:382:GLY:H	1.43	0.63
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.81	0.63
2:B:4843:LEU:HD12	2:E:4823:LEU:HD23	1.80	0.63
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.81	0.63
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.80	0.63
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.81	0.63
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.81	0.63
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.60	0.63
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.16	0.62
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.82	0.62
2:B:3762:ARG:O	2:B:3766:GLN:NE2	2.33	0.62
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.82	0.62
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.33	0.62
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.82	0.62
2:E:132:ALA:HA	2:E:194:SER:HB2	1.82	0.62
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.81	0.62
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.33	0.62
2:G:626:LEU:HD23	2:G:630:GLU:H	1.65	0.61
2:I:626:LEU:HD23	2:I:630:GLU:H	1.65	0.61
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.82	0.61
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.82	0.61
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.82	0.61
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.82	0.61
2:E:626:LEU:HD23	2:E:630:GLU:H	1.65	0.61
2:B:132:ALA:HA	2:B:194:SER:HB2	1.82	0.61
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.33	0.61
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.81	0.61
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.34	0.61
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:132:ALA:HA	2:I:194:SER:HB2	1.82	0.61
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.33	0.61
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.82	0.61
2:E:111:HIS:HD2	2:E:114:SER:H	1.48	0.61
2:B:626:LEU:HD23	2:B:630:GLU:H	1.65	0.61
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.82	0.61
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.82	0.61
2:G:111:HIS:HD2	2:G:114:SER:H	1.48	0.61
2:I:4978:HIS:CE1	2:I:5027:CYS:SG	2.94	0.61
2:E:3762:ARG:O	2:E:3766:GLN:NE2	2.33	0.61
2:B:4978:HIS:CE1	2:B:5027:CYS:SG	2.94	0.61
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.82	0.61
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.34	0.61
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.34	0.61
2:G:132:ALA:HA	2:G:194:SER:HB2	1.82	0.60
2:G:4978:HIS:CE1	2:G:5027:CYS:SG	2.94	0.60
2:E:4978:HIS:CE1	2:E:5027:CYS:SG	2.94	0.60
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.83	0.60
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.82	0.60
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.82	0.60
2:B:111:HIS:HD2	2:B:114:SER:H	1.48	0.60
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.67	0.60
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.82	0.60
2:B:2452:ARG:HH12	2:I:177:GLU:HG3	1.66	0.60
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.83	0.60
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.82	0.60
2:B:609:CYS:SG	2:B:610:ASN:N	2.75	0.60
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.67	0.60
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.34	0.60
2:E:609:CYS:SG	2:E:610:ASN:N	2.75	0.60
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.67	0.60
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.67	0.60
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.83	0.60
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.67	0.60
2:I:359:TYR:HA	2:I:376:ALA:HA	1.84	0.60
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.67	0.60
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.67	0.59
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.83	0.59
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.84	0.59
1:F:34:LYS:HD3	2:E:629:ARG:HD2	1.85	0.59
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.34	0.59
2:B:359:TYR:HA	2:B:376:ALA:HA	1.84	0.59
2:G:609:CYS:SG	2:G:610:ASN:N	2.75	0.59
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.36	0.59
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.84	0.59
2:G:359:TYR:HA	2:G:376:ALA:HA	1.84	0.59
2:G:4823:LEU:HD23	2:E:4843:LEU:HD12	1.85	0.59
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.85	0.59
2:E:3733:CYS:HA	2:E:3766:GLN:HG2	1.85	0.59
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.67	0.59
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.84	0.59
2:G:3762:ARG:O	2:G:3766:GLN:NE2	2.33	0.59
2:I:609:CYS:SG	2:I:610:ASN:N	2.75	0.59
2:I:3762:ARG:O	2:I:3766:GLN:NE2	2.33	0.59
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.85	0.59
2:B:4957:LYS:HG2	2:B:4964:GLY:CA	2.33	0.59
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.84	0.59
2:I:111:HIS:HD2	2:I:114:SER:H	1.49	0.59
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.84	0.59
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.84	0.58
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.36	0.58
2:I:3981:ALA:HA	2:I:3986:TRP:HE1	1.67	0.58
2:E:641:VAL:HG11	2:E:681:HIS:HD1	1.68	0.58
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.34	0.58
2:G:4582:VAL:HG11	2:E:4860:ARG:HD2	1.85	0.58
2:E:359:TYR:HA	2:E:376:ALA:HA	1.84	0.58
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.36	0.58
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.36	0.58
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.37	0.58
2:E:3981:ALA:HA	2:E:3986:TRP:HE1	1.67	0.58
2:E:4977:THR:HG23	2:E:4981:GLU:HG3	1.85	0.58
2:G:3981:ALA:HA	2:G:3986:TRP:HE1	1.67	0.58
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.36	0.58
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.85	0.58
2:E:4957:LYS:HG2	2:E:4964:GLY:CA	2.33	0.58
2:G:4977:THR:HG23	2:G:4981:GLU:HG3	1.85	0.58
2:I:313:SER:HB3	2:I:351:VAL:HB	1.86	0.58
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.85	0.58
2:I:3733:CYS:HA	2:I:3766:GLN:HG2	1.85	0.58
2:B:4977:THR:HG23	2:B:4981:GLU:HG3	1.85	0.58
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.85	0.58
2:G:3733:CYS:HA	2:G:3766:GLN:HG2	1.85	0.58
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.86	0.58
2:E:313:SER:HB3	2:E:351:VAL:HB	1.86	0.58
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.86	0.58
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.84	0.58
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.86	0.57
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.86	0.57
2:B:641:VAL:HG11	2:B:681:HIS:HD1	1.68	0.57
2:B:3981:ALA:HA	2:B:3986:TRP:HE1	1.67	0.57
2:G:313:SER:HB3	2:G:351:VAL:HB	1.86	0.57
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.86	0.57
2:G:4957:LYS:HG2	2:G:4964:GLY:CA	2.33	0.57
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.85	0.57
2:B:3733:CYS:HA	2:B:3766:GLN:HG2	1.85	0.57
2:I:4957:LYS:HG2	2:I:4964:GLY:CA	2.33	0.57
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.70	0.57
2:G:173:SER:HB3	2:G:178:ARG:H	1.70	0.57
2:I:4977:THR:HG23	2:I:4981:GLU:HG3	1.85	0.57
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.87	0.57
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.86	0.57
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.86	0.57
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.86	0.57
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.86	0.57
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.86	0.57
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.70	0.57
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.86	0.57
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.86	0.57
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.87	0.57
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.37	0.57
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.86	0.57
2:I:173:SER:HB3	2:I:178:ARG:H	1.70	0.57
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.86	0.57
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.37	0.57
2:B:313:SER:HB3	2:B:351:VAL:HB	1.86	0.57
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.86	0.57
2:G:641:VAL:HG11	2:G:681:HIS:HD1	1.68	0.57
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.34	0.57
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.85	0.57
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.86	0.57
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.87	0.57
2:B:4978:HIS:HE1	2:B:5027:CYS:SG	2.28	0.57
2:E:173:SER:HB3	2:E:178:ARG:H	1.70	0.57
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.70	0.56
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.86	0.56
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.87	0.56
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.87	0.56
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.86	0.56
2:G:4843:LEU:HD12	2:I:4823:LEU:HD23	1.86	0.56
2:I:641:VAL:HG11	2:I:681:HIS:HD1	1.68	0.56
2:E:4978:HIS:HE1	2:E:5027:CYS:SG	2.28	0.56
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.86	0.56
2:B:173:SER:HB3	2:B:178:ARG:H	1.70	0.56
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.86	0.56
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.79	0.56
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.34	0.56
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.87	0.56
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.79	0.56
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.87	0.56
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.79	0.56
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.86	0.56
2:B:241:GLN:O	2:B:289:ARG:NH1	2.37	0.56
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.86	0.56
2:G:4978:HIS:HE1	2:G:5027:CYS:SG	2.28	0.56
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.71	0.56
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.38	0.56
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.86	0.56
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.38	0.56
2:I:4978:HIS:HE1	2:I:5027:CYS:SG	2.28	0.56
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.87	0.56
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.38	0.56
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.39	0.56
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.71	0.56
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.71	0.56
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.71	0.56
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.79	0.56
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.88	0.56
2:E:683:ARG:NH1	2:E:707:VAL:O	2.37	0.56
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.38	0.56
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.39	0.56
1:A:34:LYS:HD3	2:B:629:ARG:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:241:GLN:O	2:G:289:ARG:NH1	2.37	0.56
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.88	0.56
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.39	0.56
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.88	0.56
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.71	0.56
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.88	0.56
2:G:1164:LEU:HB3	2:G:1169:LEU:HD21	1.88	0.56
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.88	0.56
2:I:683:ARG:NH1	2:I:707:VAL:O	2.37	0.56
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.71	0.56
2:B:1164:LEU:HB3	2:B:1169:LEU:HD21	1.88	0.55
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.71	0.55
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.70	0.55
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.87	0.55
2:I:1164:LEU:HB3	2:I:1169:LEU:HD21	1.88	0.55
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.88	0.55
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.39	0.55
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.72	0.55
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.87	0.55
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.88	0.55
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.40	0.55
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.89	0.55
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.88	0.55
2:E:1164:LEU:HB3	2:E:1169:LEU:HD21	1.88	0.55
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.88	0.55
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.71	0.55
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.72	0.55
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.40	0.55
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.88	0.55
2:E:241:GLN:O	2:E:289:ARG:NH1	2.37	0.54
2:G:395:GLN:HG3	2:G:397:GLU:H	1.72	0.54
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.40	0.54
2:E:4180:ARG:NH1	2:E:4981:GLU:OE1	2.41	0.54
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.40	0.54
2:I:4180:ARG:NH1	2:I:4981:GLU:OE1	2.41	0.54
2:E:395:GLN:HG3	2:E:397:GLU:H	1.73	0.54
2:E:1032:LYS:O	2:E:1036:ARG:N	2.40	0.54
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.41	0.54
1:J:55:VAL:HA	2:I:1784:ALA:HA	1.90	0.54
2:E:111:HIS:CD2	2:E:114:SER:H	2.26	0.54
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:241:GLN:O	2:I:289:ARG:NH1	2.37	0.54
2:E:3733:CYS:HB2	2:E:3803:SER:HB3	1.90	0.54
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.72	0.54
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.90	0.54
2:I:2911:LEU:HB2	2:I:2916:LYS:HE3	1.90	0.54
2:E:4983:HIS:H	2:E:4983:HIS:HD2	1.56	0.54
2:G:242:ARG:NH1	2:G:481:GLU:OE1	2.41	0.54
2:E:2095:GLN:NE2	2:E:2127:GLN:O	2.39	0.54
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.41	0.53
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.90	0.53
2:G:111:HIS:CD2	2:G:114:SER:H	2.26	0.53
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.91	0.53
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.72	0.53
2:I:242:ARG:NH1	2:I:481:GLU:OE1	2.41	0.53
2:B:2911:LEU:HB2	2:B:2916:LYS:HE3	1.90	0.53
2:B:3733:CYS:HB2	2:B:3803:SER:HB3	1.90	0.53
2:G:2107:GLN:HG3	2:G:3681:GLY:HA2	1.90	0.53
2:G:4993:MET:HA	2:G:4996:ILE:HD12	1.90	0.53
2:I:2107:GLN:HG3	2:I:3681:GLY:HA2	1.90	0.53
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.90	0.53
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.42	0.53
2:G:4983:HIS:H	2:G:4983:HIS:HD2	1.56	0.53
2:E:243:ARG:NH1	2:E:301:VAL:O	2.38	0.53
2:B:4993:MET:HA	2:B:4996:ILE:HD12	1.90	0.53
2:G:3733:CYS:HB2	2:G:3803:SER:HB3	1.90	0.53
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.91	0.53
2:B:395:GLN:HG3	2:B:397:GLU:H	1.73	0.53
2:B:4180:ARG:NH1	2:B:4981:GLU:OE1	2.41	0.53
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.91	0.53
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.91	0.53
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.91	0.53
2:I:395:GLN:HG3	2:I:397:GLU:H	1.73	0.53
2:I:3733:CYS:HB2	2:I:3803:SER:HB3	1.90	0.53
2:E:2911:LEU:HB2	2:E:2916:LYS:HE3	1.90	0.53
2:B:242:ARG:NH1	2:B:481:GLU:OE1	2.41	0.53
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.42	0.53
2:G:4180:ARG:NH1	2:G:4981:GLU:OE1	2.41	0.53
2:I:180:LEU:O	2:I:200:TRP:NE1	2.37	0.53
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.74	0.53
2:E:242:ARG:NH1	2:E:481:GLU:OE1	2.41	0.53
2:E:606:LEU:O	2:E:617:ASN:ND2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:SER:O	2:B:32:GLN:NE2	2.42	0.53
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.74	0.53
2:E:2107:GLN:HG3	2:E:3681:GLY:HA2	1.90	0.53
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.42	0.53
2:B:2265:LEU:O	2:B:2330:ARG:NH1	2.42	0.53
2:G:606:LEU:O	2:G:617:ASN:ND2	2.42	0.53
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.41	0.53
2:I:606:LEU:O	2:I:617:ASN:ND2	2.42	0.53
2:I:2265:LEU:O	2:I:2330:ARG:NH1	2.42	0.53
2:E:4231:MET:CE	2:E:4960:ILE:HA	2.39	0.53
2:B:4231:MET:CE	2:B:4960:ILE:HA	2.39	0.52
2:G:180:LEU:O	2:G:200:TRP:NE1	2.37	0.52
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.73	0.52
2:E:4993:MET:HA	2:E:4996:ILE:HD12	1.90	0.52
2:B:683:ARG:NH1	2:B:707:VAL:O	2.37	0.52
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.73	0.52
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.41	0.52
2:B:4983:HIS:H	2:B:4983:HIS:HD2	1.56	0.52
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.43	0.52
2:I:4231:MET:CE	2:I:4960:ILE:HA	2.39	0.52
2:B:606:LEU:O	2:B:617:ASN:ND2	2.42	0.52
2:G:25:SER:O	2:G:32:GLN:NE2	2.42	0.52
2:G:243:ARG:NH1	2:G:301:VAL:O	2.38	0.52
2:G:776:LEU:HG	2:G:848:HIS:HA	1.92	0.52
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.73	0.52
2:G:2911:LEU:HB2	2:G:2916:LYS:HE3	1.90	0.52
2:E:4865:LYS:HG3	2:E:4875:LYS:HZ3	1.74	0.52
2:B:111:HIS:CD2	2:B:114:SER:H	2.26	0.52
2:B:180:LEU:O	2:B:200:TRP:NE1	2.37	0.52
2:G:683:ARG:NH1	2:G:707:VAL:O	2.37	0.52
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.91	0.52
1:J:21:THR:HA	1:J:49:ARG:HA	1.92	0.52
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.92	0.52
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.91	0.52
2:I:25:SER:O	2:I:32:GLN:NE2	2.42	0.52
2:I:4865:LYS:HG3	2:I:4875:LYS:HZ3	1.73	0.52
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.92	0.52
2:B:2318:TYR:OH	2:B:2414:ASN:N	2.42	0.52
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.92	0.52
2:G:793:LEU:HD11	2:G:1626:TRP:HE1	1.75	0.52
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2265:LEU:O	2:G:2330:ARG:NH1	2.43	0.52
2:I:793:LEU:HD11	2:I:1626:TRP:HE1	1.75	0.52
2:I:4993:MET:HA	2:I:4996:ILE:HD12	1.90	0.52
2:B:776:LEU:HG	2:B:848:HIS:HA	1.92	0.52
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.41	0.52
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.91	0.52
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.92	0.52
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.73	0.52
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.91	0.52
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.41	0.52
2:I:243:ARG:NH1	2:I:301:VAL:O	2.38	0.52
2:I:776:LEU:HG	2:I:848:HIS:HA	1.92	0.52
2:E:25:SER:O	2:E:32:GLN:NE2	2.42	0.52
1:A:82:TYR:O	1:A:86:GLY:N	2.43	0.52
2:B:1032:LYS:O	2:B:1036:ARG:N	2.40	0.52
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.92	0.52
2:G:4231:MET:CE	2:G:4960:ILE:HA	2.39	0.52
2:E:2265:LEU:O	2:E:2330:ARG:NH1	2.42	0.52
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.43	0.52
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.91	0.51
2:B:20:VAL:HG12	2:B:204:PRO:HA	1.92	0.51
2:B:179:TYR:OH	2:E:2359:ARG:NH1	2.43	0.51
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.74	0.51
2:G:20:VAL:HG12	2:G:204:PRO:HA	1.92	0.51
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.92	0.51
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.92	0.51
2:I:4983:HIS:H	2:I:4983:HIS:HD2	1.56	0.51
2:E:776:LEU:HG	2:E:848:HIS:HA	1.92	0.51
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.91	0.51
1:H:21:THR:HA	1:H:49:ARG:HA	1.92	0.51
2:I:111:HIS:CD2	2:I:114:SER:H	2.26	0.51
2:I:880:GLU:OE1	2:I:968:ALA:N	2.43	0.51
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.91	0.51
2:E:2479:LEU:O	2:E:2487:UNK:N	2.44	0.51
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.91	0.51
2:B:2107:GLN:HG3	2:B:3681:GLY:HA2	1.90	0.51
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.43	0.51
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.43	0.51
2:G:1032:LYS:O	2:G:1036:ARG:N	2.40	0.51
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.43	0.51
2:E:331:VAL:HG12	2:E:333:GLY:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:793:LEU:HD11	2:E:1626:TRP:HE1	1.75	0.51
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.40	0.51
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.93	0.51
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.43	0.51
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.92	0.51
2:E:20:VAL:HG12	2:E:204:PRO:HA	1.92	0.51
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.74	0.51
2:E:2318:TYR:OH	2:E:2414:ASN:N	2.42	0.51
1:F:21:THR:HA	1:F:49:ARG:HA	1.92	0.51
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.44	0.51
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.76	0.51
2:G:331:VAL:HG12	2:G:333:GLY:H	1.76	0.51
2:G:2318:TYR:OH	2:G:2414:ASN:N	2.42	0.51
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	1.92	0.51
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.92	0.51
2:I:1032:LYS:O	2:I:1036:ARG:N	2.40	0.51
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.44	0.51
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.76	0.51
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.92	0.51
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.43	0.51
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.76	0.51
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.92	0.51
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.44	0.51
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.40	0.51
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.93	0.51
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.44	0.51
2:I:345:LEU:HD23	2:I:389:PHE:HB3	1.93	0.51
2:E:1865:MET:SD	2:E:1865:MET:N	2.84	0.51
1:F:55:VAL:HA	2:E:1784:ALA:HA	1.93	0.51
1:J:82:TYR:O	1:J:86:GLY:N	2.43	0.51
2:B:164:ARG:N	2:B:167:ASP:OD2	2.43	0.51
2:G:1865:MET:SD	2:G:1865:MET:N	2.84	0.51
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	1.92	0.51
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.43	0.51
2:E:345:LEU:HD23	2:E:389:PHE:HB3	1.93	0.51
1:H:55:VAL:HA	2:G:1784:ALA:HA	1.93	0.51
2:B:793:LEU:HD11	2:B:1626:TRP:HE1	1.75	0.51
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.93	0.51
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.43	0.51
2:G:911:HIS:O	2:G:918:ARG:NH2	2.44	0.51
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:82:TYR:O	1:F:86:GLY:N	2.43	0.51
2:B:1865:MET:SD	2:B:1865:MET:N	2.84	0.51
2:G:315:CYS:SG	2:G:316:PHE:N	2.84	0.51
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.43	0.51
2:I:20:VAL:HG12	2:I:204:PRO:HA	1.92	0.51
2:B:345:LEU:HD23	2:B:389:PHE:HB3	1.93	0.50
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.44	0.50
2:B:4983:HIS:HB2	2:B:4988:TYR:HE2	1.77	0.50
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.91	0.50
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.91	0.50
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.93	0.50
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.43	0.50
2:B:315:CYS:SG	2:B:316:PHE:N	2.84	0.50
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	1.92	0.50
2:G:345:LEU:HD23	2:G:389:PHE:HB3	1.93	0.50
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.93	0.50
2:I:315:CYS:SG	2:I:316:PHE:N	2.84	0.50
2:E:315:CYS:SG	2:E:316:PHE:N	2.84	0.50
2:E:4081:VAL:HB	2:E:4088:ILE:HD12	1.94	0.50
2:B:652:ARG:HD2	2:B:750:LEU:HB3	1.94	0.50
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.44	0.50
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.40	0.50
2:G:3903:LEU:HG	2:G:3915:ILE:HD12	1.94	0.50
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.44	0.50
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.93	0.50
2:B:2359:ARG:NH1	2:I:179:TYR:OH	2.44	0.50
2:I:652:ARG:HD2	2:I:750:LEU:HB3	1.93	0.50
2:I:1457:UNK:N	2:I:1497:UNK:O	2.45	0.50
2:I:2159:LEU:HA	2:I:2162:ILE:HD12	1.94	0.50
2:I:4231:MET:HE1	2:I:4960:ILE:HA	1.94	0.50
2:I:4983:HIS:HB2	2:I:4988:TYR:HE2	1.77	0.50
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.92	0.50
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	1.93	0.50
2:E:3903:LEU:HG	2:E:3915:ILE:HD12	1.93	0.50
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	1.93	0.50
2:I:1865:MET:SD	2:I:1865:MET:N	2.84	0.50
2:I:4081:VAL:HB	2:I:4088:ILE:HD12	1.94	0.50
2:E:206:CYS:SG	2:E:207:SER:N	2.84	0.50
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.44	0.50
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	1.92	0.50
2:B:2364:PHE:HD1	2:B:2429:LEU:HD21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2364:PHE:HD1	2:G:2429:LEU:HD21	1.76	0.50
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.93	0.50
1:A:21:THR:HA	1:A:49:ARG:HA	1.92	0.50
2:B:290:TYR:O	2:B:302:VAL:N	2.45	0.50
2:B:331:VAL:HG12	2:B:333:GLY:H	1.76	0.50
2:B:1457:UNK:N	2:B:1497:UNK:O	2.45	0.50
2:B:2159:LEU:HA	2:B:2162:ILE:HD12	1.94	0.50
2:I:2479:LEU:O	2:I:2487:UNK:N	2.44	0.50
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.44	0.50
1:H:34:LYS:HD3	2:G:629:ARG:HD2	1.94	0.50
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.47	0.50
2:E:1457:UNK:N	2:E:1497:UNK:O	2.45	0.50
2:E:4983:HIS:HB2	2:E:4988:TYR:HE2	1.77	0.50
1:H:82:TYR:O	1:H:86:GLY:N	2.44	0.50
2:G:2479:LEU:O	2:G:2487:UNK:N	2.44	0.50
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.93	0.50
2:E:911:HIS:O	2:E:918:ARG:NH2	2.44	0.50
2:B:2479:LEU:O	2:B:2487:UNK:N	2.44	0.49
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.94	0.49
2:G:164:ARG:N	2:G:167:ASP:OD2	2.43	0.49
2:G:206:CYS:SG	2:G:207:SER:N	2.84	0.49
2:G:1457:UNK:N	2:G:1497:UNK:O	2.45	0.49
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.45	0.49
2:B:978:THR:HB	2:B:980:ALA:H	1.78	0.49
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.45	0.49
2:I:2364:PHE:HD1	2:I:2429:LEU:HD21	1.76	0.49
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.93	0.49
2:G:652:ARG:HB2	2:G:750:LEU:HD13	1.94	0.49
2:G:880:GLU:OE1	2:G:968:ALA:N	2.43	0.49
2:I:978:THR:HB	2:I:980:ALA:H	1.78	0.49
2:E:164:ARG:N	2:E:167:ASP:OD2	2.43	0.49
2:E:652:ARG:HB2	2:E:750:LEU:HD13	1.94	0.49
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.94	0.49
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.93	0.49
2:B:3903:LEU:HG	2:B:3915:ILE:HD12	1.94	0.49
2:G:652:ARG:HD2	2:G:750:LEU:HB3	1.93	0.49
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.94	0.49
2:G:3900:GLN:NE2	2:G:3967:GLU:O	2.46	0.49
2:I:290:TYR:O	2:I:302:VAL:N	2.45	0.49
2:I:331:VAL:HG12	2:I:333:GLY:H	1.76	0.49
2:I:3903:LEU:HG	2:I:3915:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:290:TYR:O	2:E:302:VAL:N	2.45	0.49
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.47	0.49
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.44	0.49
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.45	0.49
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.47	0.49
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.40	0.49
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.84	0.49
2:B:3759:GLU:HA	2:B:3762:ARG:HE	1.78	0.49
2:B:3900:GLN:NE2	2:B:3967:GLU:O	2.46	0.49
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.41	0.49
2:I:649:PHE:HB3	2:I:776:LEU:HD13	1.95	0.49
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.95	0.49
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.93	0.49
2:E:3759:GLU:HA	2:E:3762:ARG:HE	1.78	0.49
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.76	0.49
2:B:206:CYS:SG	2:B:207:SER:N	2.84	0.49
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.95	0.49
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.44	0.49
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.84	0.49
2:I:2095:GLN:NE2	2:I:2127:GLN:O	2.39	0.49
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.95	0.49
2:E:2159:LEU:HA	2:E:2162:ILE:HD12	1.94	0.49
2:G:4081:VAL:HB	2:G:4088:ILE:HD12	1.94	0.49
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.95	0.49
2:I:3759:GLU:HA	2:I:3762:ARG:HE	1.78	0.49
2:E:652:ARG:HD2	2:E:750:LEU:HB3	1.93	0.49
2:E:978:THR:HB	2:E:980:ALA:H	1.78	0.49
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.78	0.49
2:B:652:ARG:HB2	2:B:750:LEU:HD13	1.94	0.49
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.47	0.49
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	1.93	0.49
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.95	0.49
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.78	0.49
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	1.93	0.49
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.95	0.49
2:E:3900:GLN:NE2	2:E:3967:GLU:O	2.46	0.49
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.93	0.49
2:G:290:TYR:O	2:G:302:VAL:N	2.45	0.49
2:G:4983:HIS:HB2	2:G:4988:TYR:HE2	1.77	0.49
2:I:4786:ASP:OD2	2:I:4789:PHE:N	2.39	0.49
2:E:2364:PHE:HD1	2:E:2429:LEU:HD21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4983:HIS:CD2	2:E:4983:HIS:N	2.81	0.49
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.95	0.49
2:B:4081:VAL:HB	2:B:4088:ILE:HD12	1.94	0.49
2:G:649:PHE:HB3	2:G:776:LEU:HD13	1.95	0.49
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.95	0.49
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.95	0.49
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	1.95	0.49
2:B:4786:ASP:OD2	2:B:4789:PHE:N	2.39	0.48
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.95	0.48
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.84	0.48
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.94	0.48
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.95	0.48
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.95	0.48
2:B:2758:PHE:O	2:B:2762:THR:N	2.46	0.48
2:E:41:GLY:O	2:E:45:ARG:NH1	2.47	0.48
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	1.96	0.48
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.95	0.48
2:G:2159:LEU:HA	2:G:2162:ILE:HD12	1.94	0.48
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.95	0.48
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	1.95	0.48
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.94	0.48
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.45	0.48
2:E:880:GLU:OE1	2:E:968:ALA:N	2.43	0.48
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.93	0.48
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.78	0.48
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.78	0.48
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	1.95	0.48
2:G:3759:GLU:HA	2:G:3762:ARG:HE	1.78	0.48
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	1.96	0.48
2:I:3900:GLN:NE2	2:I:3967:GLU:O	2.46	0.48
2:E:180:LEU:O	2:E:200:TRP:NE1	2.37	0.48
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	1.95	0.48
2:B:41:GLY:O	2:B:45:ARG:NH1	2.47	0.48
2:B:649:PHE:HB3	2:B:776:LEU:HD13	1.95	0.48
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.44	0.48
2:I:2318:TYR:OH	2:I:2414:ASN:N	2.42	0.48
2:G:978:THR:HB	2:G:980:ALA:H	1.77	0.48
2:G:1243:PRO:HB2	2:G:1600:LEU:HD22	1.95	0.48
2:G:1676:LEU:HD23	2:G:2167:ILE:HG23	1.96	0.48
2:G:4865:LYS:HG3	2:G:4875:LYS:HZ3	1.77	0.48
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.95	0.48
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.95	0.48
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	1.95	0.48
2:I:41:GLY:O	2:I:45:ARG:NH1	2.47	0.48
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.95	0.48
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.95	0.48
2:E:4968:PHE:CE2	2:E:4978:HIS:ND1	2.82	0.48
2:I:206:CYS:SG	2:I:207:SER:N	2.84	0.48
2:I:652:ARG:HB2	2:I:750:LEU:HD13	1.94	0.48
2:E:649:PHE:HB3	2:E:776:LEU:HD13	1.95	0.48
2:B:4968:PHE:CE2	2:B:4978:HIS:ND1	2.82	0.48
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.95	0.48
2:G:1948:ASP:OD1	2:G:2126:ARG:NH2	2.46	0.48
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.95	0.48
2:I:164:ARG:N	2:I:167:ASP:OD2	2.43	0.48
2:I:4817:ALA:HA	2:I:4823:LEU:HD22	1.96	0.48
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.42	0.48
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.96	0.48
2:G:41:GLY:O	2:G:45:ARG:NH1	2.47	0.48
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.96	0.48
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.96	0.48
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.94	0.47
2:G:3994:HIS:O	2:G:3998:HIS:ND1	2.39	0.47
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.96	0.47
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.47	0.47
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.82	0.47
2:E:2758:PHE:O	2:E:2762:THR:N	2.46	0.47
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.95	0.47
2:E:4571:PHE:O	2:E:4575:PHE:N	2.46	0.47
2:E:4817:ALA:HA	2:E:4823:LEU:HD22	1.96	0.47
2:B:54:ASN:O	2:B:58:VAL:N	2.44	0.47
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.95	0.47
2:G:2095:GLN:NE2	2:G:2127:GLN:O	2.39	0.47
2:G:4817:ALA:HA	2:G:4823:LEU:HD22	1.96	0.47
2:I:500:ALA:HB1	2:I:504:ALA:HB2	1.96	0.47
2:E:1516:UNK:N	2:E:1529:UNK:O	2.48	0.47
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.47	0.47
2:B:116:MET:HB2	2:B:137:LEU:HD12	1.97	0.47
2:B:177:GLU:HG3	2:E:2452:ARG:HH12	1.79	0.47
2:G:500:ALA:HB1	2:G:504:ALA:HB2	1.97	0.47
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1516:UNK:N	2:I:1529:UNK:O	2.48	0.47
2:B:4066:LEU:HD12	2:B:4169:SER:HB2	1.96	0.47
2:G:1516:UNK:N	2:G:1529:UNK:O	2.48	0.47
2:G:4998:LYS:NZ	2:G:5007:GLU:OE1	2.38	0.47
2:I:1236:THR:OG1	2:I:1608:MET:SD	2.73	0.47
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	1.95	0.47
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.96	0.47
2:B:4075:GLU:HA	2:B:4078:GLN:HB2	1.97	0.47
2:B:4817:ALA:HA	2:B:4823:LEU:HD22	1.96	0.47
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.97	0.47
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.97	0.47
2:E:500:ALA:HB1	2:E:504:ALA:HB2	1.97	0.47
2:B:500:ALA:HB1	2:B:504:ALA:HB2	1.96	0.47
2:B:1516:UNK:N	2:B:1529:UNK:O	2.48	0.47
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.47	0.47
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.97	0.47
2:G:4983:HIS:CD2	2:G:4983:HIS:N	2.81	0.47
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	1.97	0.47
2:E:4075:GLU:HA	2:E:4078:GLN:HB2	1.97	0.47
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.96	0.47
2:B:4983:HIS:CD2	2:B:4983:HIS:N	2.81	0.47
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.73	0.47
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.95	0.47
2:I:4075:GLU:HA	2:I:4078:GLN:HB2	1.97	0.47
2:E:116:MET:HB2	2:E:137:LEU:HD12	1.96	0.47
2:E:3994:HIS:O	2:E:3998:HIS:ND1	2.39	0.47
2:E:4066:LEU:HD12	2:E:4169:SER:HB2	1.97	0.47
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.97	0.47
2:B:2231:SER:HA	2:B:2234:ARG:HG2	1.97	0.47
2:B:3842:LEU:O	2:B:3929:SER:OG	2.33	0.47
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.80	0.47
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.97	0.47
2:G:4075:GLU:HA	2:G:4078:GLN:HB2	1.97	0.47
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.80	0.47
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.84	0.47
2:I:2215:LEU:HD23	2:I:2260:ASN:HB3	1.97	0.47
2:E:479:GLN:HE21	2:E:536:ASN:ND2	2.13	0.47
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	1.97	0.47
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.97	0.47
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.73	0.47
2:G:479:GLN:HE21	2:G:536:ASN:ND2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2215:LEU:HD23	2:G:2260:ASN:HB3	1.97	0.47
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.47	0.47
2:I:2353:VAL:O	2:I:2357:LEU:N	2.48	0.47
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.96	0.47
2:B:614:VAL:HG22	2:B:616:SER:H	1.80	0.47
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.97	0.47
2:G:116:MET:HB2	2:G:137:LEU:HD12	1.97	0.47
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.40	0.47
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.97	0.47
2:I:2347:GLU:O	2:I:2351:ASN:N	2.48	0.47
2:E:2215:LEU:HD23	2:E:2260:ASN:HB3	1.97	0.47
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.96	0.47
2:B:3994:HIS:O	2:B:3998:HIS:ND1	2.39	0.46
2:B:4571:PHE:O	2:B:4575:PHE:N	2.46	0.46
2:B:4823:LEU:HA	2:B:4826:ILE:HD12	1.97	0.46
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.96	0.46
2:G:4152:GLU:OE1	2:G:4192:ARG:NH2	2.48	0.46
2:I:2231:SER:HA	2:I:2234:ARG:HG2	1.97	0.46
2:I:3980:LEU:HD22	2:I:3985:LEU:HD22	1.98	0.46
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.80	0.46
2:E:4823:LEU:HA	2:E:4826:ILE:HD12	1.97	0.46
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.96	0.46
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.96	0.46
2:I:3971:GLY:N	2:I:4032:GLU:OE2	2.48	0.46
2:E:3674:ILE:HD11	2:E:3728:ILE:HG22	1.97	0.46
2:E:3842:LEU:O	2:E:3929:SER:OG	2.33	0.46
2:E:4152:GLU:OE1	2:E:4192:ARG:NH2	2.48	0.46
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.81	0.46
2:B:2347:GLU:O	2:B:2351:ASN:N	2.48	0.46
2:B:3980:LEU:HD22	2:B:3985:LEU:HD22	1.97	0.46
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.82	0.46
2:I:614:VAL:HG22	2:I:616:SER:H	1.80	0.46
2:I:1948:ASP:OD1	2:I:2126:ARG:NH2	2.46	0.46
2:B:880:GLU:OE1	2:B:968:ALA:N	2.43	0.46
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.95	0.46
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	1.97	0.46
2:G:2353:VAL:O	2:G:2357:LEU:N	2.48	0.46
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	1.95	0.46
2:I:4066:LEU:HD12	2:I:4169:SER:HB2	1.96	0.46
2:E:1948:ASP:OD1	2:E:2126:ARG:NH2	2.46	0.46
2:B:3971:GLY:N	2:B:4032:GLU:OE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4152:GLU:OE1	2:B:4192:ARG:NH2	2.48	0.46
2:I:4961:CYS:HB3	2:I:4983:HIS:CE1	2.51	0.46
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.96	0.46
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.50	0.46
2:B:243:ARG:NH1	2:B:301:VAL:O	2.38	0.46
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.49	0.46
2:B:2215:LEU:HD23	2:B:2260:ASN:HB3	1.97	0.46
2:B:2868:SER:O	2:B:2872:GLN:N	2.49	0.46
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	1.97	0.46
2:G:1077:ALA:HB1	2:G:1234:VAL:HG11	1.98	0.46
2:G:2868:SER:O	2:G:2872:GLN:N	2.49	0.46
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.49	0.46
2:E:2231:SER:HA	2:E:2234:ARG:HG2	1.97	0.46
2:E:2868:SER:O	2:E:2872:GLN:N	2.49	0.46
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.49	0.46
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	1.97	0.46
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.49	0.46
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	1.97	0.46
2:I:4152:GLU:OE1	2:I:4192:ARG:NH2	2.48	0.46
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.97	0.46
2:B:3773:ARG:HG3	2:B:3815:LYS:HZ3	1.81	0.46
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.49	0.46
2:B:4961:CYS:HB3	2:B:4983:HIS:CE1	2.51	0.46
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.49	0.46
2:G:2452:ARG:HH12	2:E:177:GLU:HG3	1.81	0.46
2:G:3980:LEU:HD22	2:G:3985:LEU:HD22	1.98	0.46
2:G:4066:LEU:HD12	2:G:4169:SER:HB2	1.96	0.46
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.98	0.46
2:G:4961:CYS:HB3	2:G:4983:HIS:CE1	2.51	0.46
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.50	0.46
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.81	0.46
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.81	0.46
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.98	0.46
2:B:1948:ASP:OD1	2:B:2126:ARG:NH2	2.46	0.46
2:G:54:ASN:O	2:G:58:VAL:N	2.44	0.46
2:G:4843:LEU:HD22	2:G:4928:LEU:HD11	1.98	0.46
2:I:1077:ALA:HB1	2:I:1234:VAL:HG11	1.98	0.46
2:E:838:HIS:HA	2:E:1201:HIS:HB3	1.98	0.46
2:E:1236:THR:OG1	2:E:1608:MET:SD	2.73	0.46
2:E:4961:CYS:HB3	2:E:4983:HIS:CE1	2.51	0.46
2:B:911:HIS:O	2:B:918:ARG:NH2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2095:GLN:NE2	2:B:2127:GLN:O	2.39	0.46
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.50	0.46
2:G:3361:UNK:O	2:G:3365:UNK:N	2.49	0.46
2:I:2868:SER:O	2:I:2872:GLN:N	2.49	0.46
2:I:4998:LYS:NZ	2:I:5007:GLU:OE1	2.38	0.46
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.81	0.45
2:B:838:HIS:HA	2:B:1201:HIS:HB3	1.98	0.45
2:B:1077:ALA:HB1	2:B:1234:VAL:HG11	1.98	0.45
2:B:4899:ASP:OD1	2:E:4892:ARG:NH2	2.48	0.45
2:G:471:LEU:O	2:G:475:GLN:N	2.47	0.45
2:G:580:GLU:HG3	2:G:620:LEU:HD22	1.99	0.45
2:G:2231:SER:HA	2:G:2234:ARG:HG2	1.97	0.45
2:I:3361:UNK:O	2:I:3365:UNK:N	2.49	0.45
2:E:614:VAL:HG22	2:E:616:SER:H	1.80	0.45
2:E:3980:LEU:HD22	2:E:3985:LEU:HD22	1.98	0.45
2:E:4843:LEU:HD22	2:E:4928:LEU:HD11	1.98	0.45
2:I:116:MET:HB2	2:I:137:LEU:HD12	1.96	0.45
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.98	0.45
2:E:2353:VAL:O	2:E:2357:LEU:N	2.48	0.45
1:J:34:LYS:HD3	2:I:629:ARG:HD2	1.97	0.45
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.81	0.45
2:B:2353:VAL:O	2:B:2357:LEU:N	2.48	0.45
2:B:2950:UNK:O	2:B:2954:UNK:N	2.50	0.45
2:B:3361:UNK:O	2:B:3365:UNK:N	2.49	0.45
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.33	0.45
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	1.99	0.45
2:G:2347:GLU:O	2:G:2351:ASN:N	2.48	0.45
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.49	0.45
2:G:4571:PHE:O	2:G:4575:PHE:N	2.46	0.45
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.41	0.45
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.97	0.45
2:I:3842:LEU:O	2:I:3929:SER:OG	2.33	0.45
2:I:4823:LEU:HA	2:I:4826:ILE:HD12	1.97	0.45
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.99	0.45
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.80	0.45
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.81	0.45
2:G:451:TYR:O	2:G:474:ARG:NH1	2.49	0.45
2:I:911:HIS:O	2:I:918:ARG:NH2	2.44	0.45
2:E:1077:ALA:HB1	2:E:1234:VAL:HG11	1.98	0.45
2:E:2347:GLU:O	2:E:2351:ASN:N	2.48	0.45
2:E:4231:MET:HE1	2:E:4960:ILE:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.97	0.45
2:G:2950:UNK:O	2:G:2954:UNK:N	2.50	0.45
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.50	0.45
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	1.99	0.45
2:E:3773:ARG:HG3	2:E:3815:LYS:HZ3	1.81	0.45
2:B:580:GLU:HG3	2:B:620:LEU:HD22	1.99	0.45
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.98	0.45
2:G:614:VAL:HG22	2:G:616:SER:H	1.80	0.45
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.35	0.45
2:G:4823:LEU:HA	2:G:4826:ILE:HD12	1.97	0.45
2:I:2950:UNK:O	2:I:2954:UNK:N	2.50	0.45
2:I:4822:THR:O	2:I:4825:THR:OG1	2.31	0.45
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.35	0.45
2:E:2950:UNK:O	2:E:2954:UNK:N	2.50	0.45
2:B:479:GLN:HE21	2:B:536:ASN:ND2	2.13	0.45
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	1.99	0.45
2:B:1973:GLN:O	2:B:1977:TYR:N	2.49	0.45
2:B:2810:LYS:HE2	2:B:2814:LYS:HE3	1.99	0.45
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.98	0.45
2:G:2758:PHE:O	2:G:2762:THR:N	2.46	0.45
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	1.97	0.45
2:G:3971:GLY:N	2:G:4032:GLU:OE2	2.48	0.45
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.99	0.45
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.49	0.45
2:I:4697:VAL:O	2:I:4701:TRP:N	2.49	0.45
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.99	0.45
2:I:2810:LYS:HE2	2:I:2814:LYS:HE3	1.99	0.45
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.97	0.45
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.82	0.45
2:G:1078:GLU:HB3	2:G:1081:TYR:HD2	1.82	0.45
2:G:4959:PHE:O	2:G:4959:PHE:CG	2.70	0.45
2:I:580:GLU:HG3	2:I:620:LEU:HD22	1.99	0.45
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.82	0.45
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.43	0.45
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.99	0.45
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	1.99	0.45
2:E:3361:UNK:O	2:E:3365:UNK:N	2.49	0.45
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.97	0.45
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.99	0.45
2:B:3971:GLY:H	2:B:5005:GLY:HA3	1.82	0.45
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:838:HIS:HA	2:G:1201:HIS:HB3	1.98	0.45
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.35	0.45
2:I:2758:PHE:O	2:I:2762:THR:N	2.47	0.45
2:I:3971:GLY:H	2:I:5005:GLY:HA3	1.82	0.45
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.34	0.45
2:E:471:LEU:O	2:E:475:GLN:N	2.47	0.45
2:E:2004:GLU:HA	2:E:2007:ASN:HB2	1.99	0.45
2:E:4697:VAL:O	2:E:4701:TRP:N	2.50	0.45
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	1.99	0.44
2:B:4843:LEU:HD22	2:B:4928:LEU:HD11	1.98	0.44
2:B:4892:ARG:NH2	2:I:4899:ASP:OD1	2.49	0.44
2:B:4959:PHE:O	2:B:4959:PHE:CG	2.70	0.44
2:G:3773:ARG:HG3	2:G:3815:LYS:HZ3	1.82	0.44
2:G:3842:LEU:O	2:G:3929:SER:OG	2.33	0.44
2:G:4959:PHE:O	2:G:4959:PHE:CD1	2.70	0.44
2:I:54:ASN:O	2:I:58:VAL:N	2.44	0.44
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.82	0.44
2:I:838:HIS:HA	2:I:1201:HIS:HB3	1.98	0.44
2:I:2004:GLU:HA	2:I:2007:ASN:HB2	1.99	0.44
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.43	0.44
2:G:3971:GLY:H	2:G:5005:GLY:HA3	1.82	0.44
2:I:451:TYR:O	2:I:474:ARG:NH1	2.49	0.44
2:I:887:ILE:HG21	2:I:959:TYR:HA	2.00	0.44
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.98	0.44
2:I:4571:PHE:O	2:I:4575:PHE:N	2.46	0.44
2:I:4843:LEU:HD22	2:I:4928:LEU:HD11	1.98	0.44
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.82	0.44
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	1.99	0.44
1:A:7:ILE:N	1:A:71:ARG:O	2.47	0.44
2:B:1247:PRO:HA	2:B:1598:GLN:HA	2.00	0.44
2:B:4231:MET:HE1	2:B:4960:ILE:HA	2.00	0.44
2:I:3891:LEU:HB3	2:I:3899:PHE:CE2	2.53	0.44
2:E:357:LEU:HD12	2:E:388:LEU:HD11	2.00	0.44
2:E:2810:LYS:HE2	2:E:2814:LYS:HE3	1.99	0.44
2:E:3971:GLY:H	2:E:5005:GLY:HA3	1.82	0.44
1:H:87:HIS:HA	1:H:88:PRO:HD3	1.88	0.44
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.42	0.44
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.41	0.44
2:B:1078:GLU:HB3	2:B:1081:TYR:HD2	1.82	0.44
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.35	0.44
2:G:583:ILE:HA	2:G:586:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:756:SER:HB3	2:G:767:VAL:HG22	2.00	0.44
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.99	0.44
2:G:2810:LYS:HE2	2:G:2814:LYS:HE3	1.99	0.44
2:G:3891:LEU:HB3	2:G:3899:PHE:CE2	2.53	0.44
2:G:4697:VAL:O	2:G:4701:TRP:N	2.49	0.44
2:I:479:GLN:HE21	2:I:536:ASN:ND2	2.13	0.44
2:E:4158:PRO:HA	2:E:4161:ARG:HB2	2.00	0.44
2:E:4959:PHE:O	2:E:4959:PHE:CG	2.70	0.44
2:B:357:LEU:HD12	2:B:388:LEU:HD11	2.00	0.44
2:B:887:ILE:HG21	2:B:959:TYR:HA	2.00	0.44
2:G:485:SER:HA	2:G:488:LEU:HB2	1.99	0.44
2:G:4786:ASP:OD2	2:G:4789:PHE:N	2.39	0.44
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.98	0.44
1:F:87:HIS:HA	1:F:88:PRO:HD3	1.88	0.44
2:B:2004:GLU:HA	2:B:2007:ASN:HB2	1.99	0.44
2:B:3552:UNK:O	2:B:3556:UNK:N	2.51	0.44
2:I:583:ILE:HA	2:I:586:ILE:HD12	2.00	0.44
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.99	0.44
2:E:887:ILE:HG21	2:E:959:TYR:HA	2.00	0.44
2:E:3552:UNK:O	2:E:3556:UNK:N	2.51	0.44
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.83	0.44
2:B:583:ILE:HA	2:B:586:ILE:HD12	2.00	0.44
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.41	0.44
2:G:1973:GLN:O	2:G:1977:TYR:N	2.49	0.44
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	1.99	0.44
2:I:485:SER:HA	2:I:488:LEU:HB2	1.99	0.44
2:E:756:SER:HB3	2:E:767:VAL:HG22	2.00	0.44
2:E:1247:PRO:HA	2:E:1598:GLN:HA	2.00	0.44
2:E:4563:ARG:NH1	2:E:4815:ASP:OD1	2.51	0.44
1:J:92:PRO:HD3	2:I:627:PRO:HB2	2.00	0.44
2:G:3552:UNK:O	2:G:3556:UNK:N	2.51	0.44
2:G:4231:MET:HE1	2:G:4960:ILE:HA	2.00	0.44
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.81	0.44
2:I:3552:UNK:O	2:I:3556:UNK:N	2.51	0.44
2:I:4959:PHE:O	2:I:4959:PHE:CG	2.70	0.44
2:B:4924:VAL:HG23	2:B:4925:ILE:HG12	2.00	0.44
2:G:887:ILE:HG21	2:G:959:TYR:HA	2.00	0.44
2:G:1247:PRO:HA	2:G:1598:GLN:HA	2.00	0.44
2:G:2257:LEU:O	2:G:2261:SER:N	2.51	0.44
2:G:4563:ARG:NH1	2:G:4815:ASP:OD1	2.51	0.44
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4563:ARG:NH1	2:I:4815:ASP:OD1	2.51	0.44
2:E:1973:GLN:O	2:E:1977:TYR:N	2.49	0.44
2:E:3891:LEU:HB3	2:E:3899:PHE:CE2	2.53	0.44
2:B:3891:LEU:HB3	2:B:3899:PHE:CE2	2.53	0.43
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.42	0.43
2:G:488:LEU:O	2:G:492:ASP:N	2.48	0.43
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.82	0.43
2:E:286:THR:HA	2:E:405:HIS:HB2	2.00	0.43
2:E:4786:ASP:OD2	2:E:4789:PHE:N	2.39	0.43
1:A:55:VAL:HA	2:B:1784:ALA:HA	1.99	0.43
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.83	0.43
2:B:4959:PHE:O	2:B:4959:PHE:CD1	2.70	0.43
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.82	0.43
2:I:357:LEU:HD12	2:I:388:LEU:HD11	2.00	0.43
2:I:756:SER:HB3	2:I:767:VAL:HG22	2.00	0.43
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.82	0.43
2:I:4959:PHE:O	2:I:4959:PHE:CD1	2.70	0.43
2:E:485:SER:HA	2:E:488:LEU:HB2	1.99	0.43
2:E:580:GLU:HG3	2:E:620:LEU:HD22	1.99	0.43
2:B:45:ARG:NH2	2:B:447:ASP:OD1	2.48	0.43
2:B:451:TYR:O	2:B:474:ARG:NH1	2.49	0.43
2:I:475:GLN:NE2	2:I:531:ARG:O	2.42	0.43
2:I:2257:LEU:O	2:I:2261:SER:N	2.51	0.43
2:E:425:PRO:HA	2:E:506:TYR:HD1	1.83	0.43
2:E:4959:PHE:O	2:E:4959:PHE:CD1	2.70	0.43
2:E:5000:GLU:HA	2:E:5003:HIS:CD2	2.53	0.43
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.34	0.43
2:G:357:LEU:HD12	2:G:388:LEU:HD11	2.00	0.43
2:G:1166:GLY:HA3	2:G:1216:ILE:HD13	2.01	0.43
2:G:4158:PRO:HA	2:G:4161:ARG:HB2	2.00	0.43
2:G:4822:THR:O	2:G:4825:THR:OG1	2.31	0.43
2:G:5000:GLU:HA	2:G:5003:HIS:CD2	2.53	0.43
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.01	0.43
2:I:876:GLU:O	2:I:880:GLU:N	2.50	0.43
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.54	0.43
2:E:488:LEU:O	2:E:492:ASP:N	2.48	0.43
2:E:583:ILE:HA	2:E:586:ILE:HD12	2.00	0.43
2:E:2257:LEU:O	2:E:2261:SER:N	2.51	0.43
2:B:161:GLU:HA	2:E:3984:ARG:HH22	1.84	0.43
2:B:2257:LEU:O	2:B:2261:SER:N	2.51	0.43
2:B:4563:ARG:NH1	2:B:4815:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4865:LYS:HG3	2:B:4875:LYS:HZ3	1.82	0.43
2:B:5000:GLU:HA	2:B:5003:HIS:CD2	2.53	0.43
2:G:286:THR:HA	2:G:405:HIS:HB2	2.00	0.43
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.54	0.43
2:E:1078:GLU:HB3	2:E:1081:TYR:HD2	1.82	0.43
2:E:4822:THR:O	2:E:4825:THR:OG1	2.31	0.43
2:G:2004:GLU:HA	2:G:2007:ASN:HB2	1.99	0.43
2:I:4924:VAL:HG23	2:I:4925:ILE:HG12	2.00	0.43
2:I:4983:HIS:CD2	2:I:4983:HIS:N	2.81	0.43
2:I:5000:GLU:HA	2:I:5003:HIS:CD2	2.53	0.43
2:E:1166:GLY:HA3	2:E:1216:ILE:HD13	2.01	0.43
2:B:425:PRO:HA	2:B:506:TYR:HD1	1.83	0.43
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.99	0.43
2:G:161:GLU:HA	2:I:3984:ARG:HH22	1.83	0.43
2:I:1247:PRO:HA	2:I:1598:GLN:HA	2.00	0.43
2:I:1973:GLN:O	2:I:1977:TYR:N	2.49	0.43
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.33	0.43
2:E:309:THR:O	2:E:313:SER:OG	2.37	0.43
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.54	0.43
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	2.01	0.43
2:B:3771:HIS:O	2:B:3774:GLY:N	2.48	0.43
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	2.01	0.43
2:I:45:ARG:NH2	2:I:447:ASP:OD1	2.48	0.43
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.01	0.43
2:B:485:SER:HA	2:B:488:LEU:HB2	1.99	0.43
2:B:681:HIS:HB3	2:B:784:SER:HB3	2.01	0.43
2:B:4158:PRO:HA	2:B:4161:ARG:HB2	2.00	0.43
2:G:181:HIS:CE1	2:G:195:PHE:HB2	2.54	0.43
2:E:4236:SER:OG	2:E:4675:LYS:NZ	2.46	0.43
1:J:23:VAL:H	1:J:105:ASN:HB3	1.84	0.43
1:J:87:HIS:HA	1:J:88:PRO:HD3	1.88	0.43
2:B:1166:GLY:HA3	2:B:1216:ILE:HD13	2.01	0.43
2:G:425:PRO:HA	2:G:506:TYR:HD1	1.83	0.43
2:G:2107:GLN:NE2	2:G:3680:ALA:O	2.52	0.43
2:E:181:HIS:CE1	2:E:195:PHE:HB2	2.54	0.43
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.54	0.43
2:B:286:THR:HA	2:B:405:HIS:HB2	2.00	0.42
2:B:2107:GLN:NE2	2:B:3680:ALA:O	2.52	0.42
2:G:309:THR:O	2:G:313:SER:OG	2.37	0.42
2:G:707:VAL:HG23	2:G:713:SER:HB2	2.01	0.42
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2107:GLN:NE2	2:I:3680:ALA:O	2.52	0.42
2:E:3771:HIS:O	2:E:3774:GLY:N	2.48	0.42
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.33	0.42
2:I:425:PRO:HA	2:I:506:TYR:HD1	1.83	0.42
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.84	0.42
2:E:4924:VAL:HG23	2:E:4925:ILE:HG12	2.00	0.42
2:B:181:HIS:CE1	2:B:195:PHE:HB2	2.54	0.42
2:B:488:LEU:O	2:B:492:ASP:N	2.48	0.42
2:B:756:SER:HB3	2:B:767:VAL:HG22	2.00	0.42
2:B:1817:GLU:O	2:B:1821:ASP:N	2.49	0.42
2:B:4658:ILE:HD11	2:B:4796:MET:HG3	2.01	0.42
2:G:4658:ILE:HD11	2:G:4796:MET:HG3	2.00	0.42
2:I:1817:GLU:O	2:I:1821:ASP:N	2.49	0.42
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.41	0.42
2:E:3897:ASN:O	2:E:3901:ASN:ND2	2.52	0.42
2:G:3804:ILE:HG22	2:G:3812:VAL:HG21	2.02	0.42
2:I:181:HIS:CE1	2:I:195:PHE:HB2	2.54	0.42
2:I:707:VAL:HG23	2:I:713:SER:HB2	2.01	0.42
2:I:1166:GLY:HA3	2:I:1216:ILE:HD13	2.01	0.42
2:I:4158:PRO:HA	2:I:4161:ARG:HB2	2.00	0.42
2:E:707:VAL:HG23	2:E:713:SER:HB2	2.01	0.42
1:F:23:VAL:H	1:F:105:ASN:HB3	1.85	0.42
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.85	0.42
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.01	0.42
2:G:1739:THR:H	2:G:1742:THR:HB	1.84	0.42
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.43	0.42
2:G:4892:ARG:NH2	2:E:4899:ASP:OD1	2.52	0.42
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	2.01	0.42
2:E:3971:GLY:N	2:E:4032:GLU:OE2	2.48	0.42
1:A:23:VAL:H	1:A:105:ASN:HB3	1.84	0.42
1:J:34:LYS:HE3	2:I:634:GLN:HB3	2.00	0.42
2:B:983:THR:O	2:B:987:ARG:N	2.52	0.42
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.53	0.42
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.53	0.42
2:G:1815:LEU:HD22	2:G:1845:VAL:HG21	2.02	0.42
2:I:3362:UNK:O	2:I:3366:UNK:N	2.53	0.42
2:I:3804:ILE:HG22	2:I:3812:VAL:HG21	2.02	0.42
2:E:475:GLN:NE2	2:E:531:ARG:O	2.42	0.42
2:E:2107:GLN:NE2	2:E:3680:ALA:O	2.52	0.42
2:B:3804:ILE:HG22	2:B:3812:VAL:HG21	2.02	0.42
2:B:4017:LEU:HD22	2:B:4139:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:475:GLN:NE2	2:G:531:ARG:O	2.42	0.42
2:G:792:LEU:HD22	2:G:799:GLU:H	1.83	0.42
2:G:1972:ASN:HD21	2:G:2024:PRO:HB3	1.85	0.42
2:I:286:THR:HA	2:I:405:HIS:HB2	2.00	0.42
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.42	0.42
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.53	0.42
2:I:1739:THR:H	2:I:1742:THR:HB	1.85	0.42
2:E:1078:GLU:HB2	2:E:1235:THR:HG22	2.02	0.42
2:E:3362:UNK:O	2:E:3366:UNK:N	2.53	0.42
2:E:4017:LEU:HD22	2:E:4139:ILE:HG12	2.02	0.42
1:H:23:VAL:H	1:H:105:ASN:HB3	1.85	0.42
2:B:309:THR:O	2:B:313:SER:OG	2.37	0.42
2:B:471:LEU:O	2:B:475:GLN:N	2.47	0.42
2:B:540:PHE:HD2	2:B:567:VAL:HG11	1.85	0.42
2:B:792:LEU:HD22	2:B:799:GLU:H	1.83	0.42
2:B:3362:UNK:O	2:B:3366:UNK:N	2.53	0.42
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.84	0.42
2:G:3362:UNK:O	2:G:3366:UNK:N	2.53	0.42
2:G:3897:ASN:O	2:G:3901:ASN:ND2	2.52	0.42
2:G:4231:MET:HE3	2:G:4960:ILE:HA	2.02	0.42
2:E:1739:THR:H	2:E:1742:THR:HB	1.85	0.42
2:E:1815:LEU:HD22	2:E:1845:VAL:HG21	2.02	0.42
2:E:3804:ILE:HG22	2:E:3812:VAL:HG21	2.02	0.42
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.88	0.42
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.41	0.42
2:G:4017:LEU:HD22	2:G:4139:ILE:HG12	2.02	0.42
2:G:4924:VAL:HG23	2:G:4925:ILE:HG12	2.00	0.42
2:I:540:PHE:HD2	2:I:567:VAL:HG11	1.85	0.42
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.53	0.42
2:E:1972:ASN:HD21	2:E:2024:PRO:HB3	1.85	0.42
1:J:57:LYS:HB2	1:J:80:VAL:HB	2.02	0.42
2:B:454:PRO:HG2	2:B:531:ARG:HH12	1.85	0.42
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.84	0.42
2:B:707:VAL:HG23	2:B:713:SER:HB2	2.01	0.42
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	2.02	0.42
2:G:730:VAL:O	2:G:735:GLN:NE2	2.53	0.42
2:G:932:LEU:HA	2:G:935:LEU:HD12	2.02	0.42
2:I:924:MET:O	2:I:928:THR:OG1	2.34	0.42
2:I:1747:LEU:HD13	2:I:1760:HIS:CE1	2.55	0.42
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	2.02	0.42
2:E:45:ARG:NH2	2:E:447:ASP:OD1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:54:ASN:O	2:E:58:VAL:N	2.44	0.42
2:E:454:PRO:HG2	2:E:531:ARG:HH12	1.85	0.42
2:E:792:LEU:HD22	2:E:799:GLU:H	1.83	0.42
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	2.02	0.42
2:B:730:VAL:O	2:B:735:GLN:NE2	2.53	0.41
2:B:1972:ASN:HD21	2:B:2024:PRO:HB3	1.85	0.41
2:B:4984:ASN:C	2:B:4986:ALA:H	2.23	0.41
2:I:3897:ASN:O	2:I:3901:ASN:ND2	2.52	0.41
2:E:730:VAL:O	2:E:735:GLN:NE2	2.53	0.41
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.86	0.41
2:B:1078:GLU:HB2	2:B:1235:THR:HG22	2.02	0.41
2:B:1747:LEU:HD13	2:B:1760:HIS:CE1	2.55	0.41
2:G:1817:GLU:O	2:G:1821:ASP:N	2.49	0.41
1:A:57:LYS:HB2	1:A:80:VAL:HB	2.02	0.41
2:B:2467:VAL:HA	2:B:2470:ILE:HD12	2.03	0.41
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	2.02	0.41
2:I:1972:ASN:HD21	2:I:2024:PRO:HB3	1.85	0.41
2:I:3677:LEU:O	2:I:3698:LEU:N	2.51	0.41
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	2.02	0.41
2:E:2467:VAL:HA	2:E:2470:ILE:HD12	2.03	0.41
2:B:3897:ASN:O	2:B:3901:ASN:ND2	2.52	0.41
2:G:540:PHE:HD2	2:G:567:VAL:HG11	1.85	0.41
2:G:2143:THR:O	2:G:3651:ASN:ND2	2.49	0.41
2:I:792:LEU:HD22	2:I:799:GLU:H	1.83	0.41
2:I:1101:ARG:HH21	2:I:1115:LEU:HB3	1.86	0.41
2:E:451:TYR:O	2:E:474:ARG:NH1	2.49	0.41
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	2.02	0.41
2:E:4658:ILE:HD11	2:E:4796:MET:HG3	2.01	0.41
2:B:475:GLN:NE2	2:B:531:ARG:O	2.42	0.41
2:B:1269:CYS:HA	2:B:1473:UNK:HA	2.02	0.41
2:B:4231:MET:HE3	2:B:4960:ILE:HA	2.02	0.41
2:G:4899:ASP:OD1	2:I:4892:ARG:NH2	2.52	0.41
2:G:4984:ASN:C	2:G:4986:ALA:H	2.23	0.41
2:I:599:VAL:HG23	2:I:600:LEU:HD12	2.03	0.41
2:I:1815:LEU:HD22	2:I:1845:VAL:HG21	2.02	0.41
2:I:2305:CYS:HA	2:I:2324:ASN:HD22	1.86	0.41
2:E:3847:PHE:HD1	2:E:3850:GLN:HE21	1.69	0.41
1:J:7:ILE:N	1:J:71:ARG:O	2.47	0.41
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	2.02	0.41
2:G:45:ARG:NH2	2:G:447:ASP:OD1	2.48	0.41
2:G:599:VAL:HG23	2:G:600:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1269:CYS:HA	2:G:1473:UNK:HA	2.02	0.41
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	2.03	0.41
2:G:3847:PHE:HD1	2:G:3850:GLN:HE21	1.69	0.41
2:I:309:THR:O	2:I:313:SER:OG	2.37	0.41
2:I:3847:PHE:HD1	2:I:3850:GLN:HE21	1.69	0.41
2:I:4984:ASN:C	2:I:4986:ALA:H	2.23	0.41
2:E:1101:ARG:HH21	2:E:1115:LEU:HB3	1.86	0.41
2:E:1747:LEU:HD13	2:E:1760:HIS:CE1	2.55	0.41
2:B:1101:ARG:HH21	2:B:1115:LEU:HB3	1.86	0.41
2:B:4821:LYS:HE2	2:B:4821:LYS:HB3	1.95	0.41
2:G:1078:GLU:HB2	2:G:1235:THR:HG22	2.02	0.41
2:G:1747:LEU:HD13	2:G:1760:HIS:CE1	2.55	0.41
2:I:1078:GLU:HB2	2:I:1235:THR:HG22	2.02	0.41
2:I:4658:ILE:HD11	2:I:4796:MET:HG3	2.01	0.41
2:E:932:LEU:HA	2:E:935:LEU:HD12	2.02	0.41
2:E:4848:VAL:O	2:E:4852:THR:OG1	2.28	0.41
2:E:4928:LEU:HD13	2:E:4928:LEU:HA	1.90	0.41
2:B:1815:LEU:HD22	2:B:1845:VAL:HG21	2.02	0.41
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.85	0.41
2:I:892:THR:N	2:I:902:ARG:O	2.52	0.41
2:I:4017:LEU:HD22	2:I:4139:ILE:HG12	2.02	0.41
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.85	0.41
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	2.03	0.41
1:F:7:ILE:N	1:F:71:ARG:O	2.47	0.41
2:B:932:LEU:HA	2:B:935:LEU:HD12	2.02	0.41
2:B:1739:THR:H	2:B:1742:THR:HB	1.85	0.41
2:B:1859:VAL:HA	2:B:1862:ILE:HG12	2.03	0.41
2:B:3677:LEU:O	2:B:3698:LEU:N	2.51	0.41
2:B:4222:VAL:HG23	2:B:4950:VAL:HG12	2.02	0.41
2:G:1859:VAL:HA	2:G:1862:ILE:HG12	2.03	0.41
2:G:2305:CYS:HA	2:G:2324:ASN:HD22	1.86	0.41
2:G:4558:ASN:OD1	2:G:4558:ASN:N	2.54	0.41
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.33	0.41
2:I:730:VAL:O	2:I:735:GLN:NE2	2.53	0.41
2:I:1716:ILE:HG23	2:I:1720:LEU:HD13	2.03	0.41
2:I:3771:HIS:O	2:I:3774:GLY:N	2.48	0.41
2:E:540:PHE:HD2	2:E:567:VAL:HG11	1.85	0.41
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.03	0.41
2:E:2034:PHE:O	2:E:2038:LEU:N	2.54	0.41
1:H:57:LYS:HB2	1:H:80:VAL:HB	2.02	0.41
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3847:PHE:HD1	2:B:3850:GLN:HE21	1.69	0.41
2:G:119:SER:HA	2:G:146:CYS:HA	2.03	0.41
2:I:1808:ARG:NH1	2:I:1853:ILE:O	2.54	0.41
2:I:2143:THR:O	2:I:3651:ASN:ND2	2.49	0.41
2:E:2196:ASN:OD1	2:E:2199:ARG:NH1	2.44	0.41
2:E:3677:LEU:O	2:E:3698:LEU:N	2.51	0.41
2:E:4998:LYS:NZ	2:E:5007:GLU:OE1	2.38	0.41
2:B:16:THR:OG1	2:B:97:GLY:O	2.39	0.40
2:B:512:ALA:HA	2:B:515:TRP:HB2	2.03	0.40
2:B:1657:LEU:HD13	2:B:1657:LEU:HA	1.95	0.40
2:B:4822:THR:O	2:B:4825:THR:OG1	2.31	0.40
2:G:615:ARG:NH2	2:G:1677:GLY:O	2.41	0.40
2:G:1141:ARG:H	2:G:1141:ARG:HD2	1.86	0.40
2:I:16:THR:OG1	2:I:97:GLY:O	2.39	0.40
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.85	0.40
2:I:1641:ILE:HA	2:I:1642:PRO:HD3	1.92	0.40
2:E:1269:CYS:HA	2:E:1473:UNK:HA	2.02	0.40
2:E:2305:CYS:HA	2:E:2324:ASN:HD22	1.86	0.40
1:F:57:LYS:HB2	1:F:80:VAL:HB	2.02	0.40
2:B:2029:GLN:O	2:B:2033:ASP:N	2.50	0.40
2:B:4697:VAL:O	2:B:4701:TRP:N	2.50	0.40
2:G:1973:GLN:HA	2:G:1976:ARG:HB3	2.04	0.40
2:G:3781:GLN:HA	2:G:3784:SER:HB3	2.04	0.40
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	2.02	0.40
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	2.03	0.40
2:I:2029:GLN:O	2:I:2033:ASP:N	2.50	0.40
2:I:3994:HIS:O	2:I:3998:HIS:ND1	2.39	0.40
2:B:1685:LEU:HD22	2:B:1718:ILE:HG21	2.03	0.40
2:B:2305:CYS:HA	2:B:2324:ASN:HD22	1.86	0.40
2:B:2437:ALA:HA	2:B:2438:PRO:HD3	1.95	0.40
2:B:4710:SER:HB3	2:B:4713:SER:HB3	2.03	0.40
2:G:983:THR:O	2:G:987:ARG:N	2.52	0.40
2:I:471:LEU:O	2:I:475:GLN:N	2.47	0.40
2:I:1685:LEU:HD22	2:I:1718:ILE:HG21	2.03	0.40
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	2.04	0.40
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.86	0.40
2:G:512:ALA:HA	2:G:515:TRP:HB2	2.03	0.40
2:G:1592:PRO:HA	2:G:1593:PRO:HD3	1.98	0.40
2:G:1716:ILE:HG23	2:G:1720:LEU:HD13	2.03	0.40
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.86	0.40
2:I:932:LEU:HA	2:I:935:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:983:THR:O	2:I:987:ARG:N	2.52	0.40
2:I:3773:ARG:HG3	2:I:3815:LYS:HZ3	1.86	0.40
2:I:3781:GLN:HA	2:I:3784:SER:HB3	2.04	0.40
2:E:4984:ASN:C	2:E:4986:ALA:H	2.23	0.40
2:B:119:SER:HA	2:B:146:CYS:HA	2.03	0.40
2:B:594:GLY:H	2:B:1594:ARG:HD3	1.87	0.40
2:B:907:LEU:O	2:B:963:ASN:ND2	2.40	0.40
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	2.03	0.40
2:B:2587:UNK:O	2:B:2591:UNK:N	2.55	0.40
2:G:1101:ARG:HH21	2:G:1115:LEU:HB3	1.86	0.40
2:I:2034:PHE:O	2:I:2038:LEU:N	2.54	0.40
2:I:2467:VAL:HA	2:I:2470:ILE:HD12	2.03	0.40
2:E:321:GLU:HB3	2:E:322:LYS:H	1.76	0.40
2:E:472:ARG:HA	2:E:475:GLN:HB2	2.03	0.40
2:E:599:VAL:HG23	2:E:600:LEU:HD12	2.02	0.40
2:E:2029:GLN:O	2:E:2033:ASP:N	2.50	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%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2890 (89%)	338 (10%)	7 (0%)	47	81
2	E	3235/4416 (73%)	2888 (89%)	340 (10%)	7 (0%)	47	81
2	G	3235/4416 (73%)	2889 (89%)	339 (10%)	7 (0%)	47	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	I	3235/4416 (73%)	2889 (89%)	339 (10%)	7 (0%)	47 81
All	All	13360/18096 (74%)	11932 (89%)	1400 (10%)	28 (0%)	50 81

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	G	1708	ARG
2	I	1708	ARG
2	E	1708	ARG
2	E	4985	LEU
2	B	4962	GLY
2	B	4985	LEU
2	G	4641	PRO
2	G	4962	GLY
2	G	4985	LEU
2	I	4641	PRO
2	I	4962	GLY
2	I	4985	LEU
2	E	4962	GLY
2	B	1840	PRO
2	B	4641	PRO
2	G	1840	PRO
2	I	1840	PRO
2	E	1840	PRO
2	E	4641	PRO
2	B	2291	GLN
2	G	2291	GLN
2	I	2291	GLN
2	E	2291	GLN
2	B	1932	PRO
2	G	1932	PRO
2	I	1932	PRO
2	E	1932	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%)	2474 (99%)	19 (1%)	81 89
2	E	2493/3022 (82%)	2474 (99%)	19 (1%)	81 89
2	G	2493/3022 (82%)	2474 (99%)	19 (1%)	81 89
2	I	2493/3022 (82%)	2474 (99%)	19 (1%)	81 89
All	All	10324/12444 (83%)	10248 (99%)	76 (1%)	84 90

All (76) 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	978	THR
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	3663	LEU
2	B	3787	LYS
2	B	3805	LEU
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4166	LEU
2	B	4961	CYS
2	B	4983	HIS
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	978	THR
2	G	1076	ARG
2	G	1141	ARG

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Mol	Chain	Res	Type
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	3663	LEU
2	G	3787	LYS
2	G	3805	LEU
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4166	LEU
2	G	4961	CYS
2	G	4983	HIS
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	978	THR
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3663	LEU
2	I	3787	LYS
2	I	3805	LEU
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4166	LEU
2	I	4961	CYS
2	I	4983	HIS
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	978	THR
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3663	LEU

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Mol	Chain	Res	Type
2	E	3787	LYS
2	E	3805	LEU
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4166	LEU
2	E	4961	CYS
2	E	4983	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (132) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	43	ASN
1	F	87	HIS
1	A	43	ASN
1	A	87	HIS
1	H	43	ASN
1	H	87	HIS
1	J	43	ASN
1	J	87	HIS
2	B	57	ASN
2	B	71	GLN
2	B	111	HIS
2	B	224	HIS
2	B	273	HIS
2	B	379	HIS
2	B	413	GLN
2	B	479	GLN
2	B	725	HIS
2	B	838	HIS
2	B	1598	GLN
2	B	1691	GLN
2	B	1719	HIS
2	B	1760	HIS
2	B	1775	HIS
2	B	2127	GLN
2	B	3809	ASN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN

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Mol	Chain	Res	Type
2	B	3960	GLN
2	B	4034	ASN
2	B	4054	ASN
2	B	4120	ASN
2	B	4142	ASN
2	B	4806	ASN
2	B	4833	ASN
2	B	4978	HIS
2	B	4983	HIS
2	B	5003	HIS
2	G	57	ASN
2	G	71	GLN
2	G	111	HIS
2	G	224	HIS
2	G	273	HIS
2	G	379	HIS
2	G	413	GLN
2	G	479	GLN
2	G	725	HIS
2	G	838	HIS
2	G	1598	GLN
2	G	1691	GLN
2	G	1719	HIS
2	G	1760	HIS
2	G	1775	HIS
2	G	2127	GLN
2	G	3809	ASN
2	G	3889	GLN
2	G	3896	ASN
2	G	3900	GLN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	4034	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4142	ASN
2	G	4806	ASN
2	G	4833	ASN
2	G	4978	HIS
2	G	4983	HIS
2	G	5003	HIS

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Mol	Chain	Res	Type
2	I	57	ASN
2	I	71	GLN
2	I	111	HIS
2	I	224	HIS
2	I	273	HIS
2	I	379	HIS
2	I	413	GLN
2	I	479	GLN
2	I	725	HIS
2	I	838	HIS
2	I	1598	GLN
2	I	1691	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	2127	GLN
2	I	3809	ASN
2	I	3889	GLN
2	I	3896	ASN
2	I	3900	GLN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	4034	ASN
2	I	4054	ASN
2	I	4120	ASN
2	I	4142	ASN
2	I	4806	ASN
2	I	4833	ASN
2	I	4978	HIS
2	I	4983	HIS
2	I	5003	HIS
2	E	57	ASN
2	E	71	GLN
2	E	111	HIS
2	E	224	HIS
2	E	273	HIS
2	E	379	HIS
2	E	413	GLN
2	E	479	GLN
2	E	725	HIS
2	E	838	HIS
2	E	1598	GLN

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Mol	Chain	Res	Type
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	2127	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	4034	ASN
2	E	4054	ASN
2	E	4120	ASN
2	E	4142	ASN
2	E	4806	ASN
2	E	4833	ASN
2	E	4978	HIS
2	E	4983	HIS
2	E	5003	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ATP	B	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.62	5 (16%)
3	ATP	I	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.62	5 (16%)
4	CFF	B	5102	-	8,15,15	2.47	3 (37%)	8,23,23	1.30	1 (12%)
4	CFF	G	5102	-	8,15,15	2.48	3 (37%)	8,23,23	1.30	1 (12%)
3	ATP	E	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.62	5 (16%)
3	ATP	G	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.62	5 (16%)
4	CFF	I	5102	-	8,15,15	2.48	3 (37%)	8,23,23	1.30	1 (12%)
4	CFF	E	5102	-	8,15,15	2.48	3 (37%)	8,23,23	1.29	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	5101	-	-	5/18/38/38	0/3/3/3
3	ATP	I	5101	-	-	5/18/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
4	CFF	G	5102	-	-	-	0/2/2/2
3	ATP	E	5101	-	-	5/18/38/38	0/3/3/3
3	ATP	G	5101	-	-	5/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	-	0/2/2/2
4	CFF	E	5102	-	-	-	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	5102	CFF	C5-C4	-4.39	1.33	1.39
4	E	5102	CFF	C5-C4	-4.39	1.33	1.39
4	B	5102	CFF	C5-C4	-4.35	1.33	1.39
4	G	5102	CFF	C5-C4	-4.34	1.33	1.39
4	G	5102	CFF	C6-N1	-4.21	1.32	1.38
4	B	5102	CFF	C6-N1	-4.18	1.32	1.38
4	E	5102	CFF	C6-N1	-4.18	1.32	1.38
4	I	5102	CFF	C6-N1	-4.17	1.32	1.38
4	I	5102	CFF	O13-C6	-2.38	1.18	1.24
3	I	5101	ATP	C5-C4	2.36	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5101	ATP	C5-C4	2.36	1.47	1.40
4	B	5102	CFF	O13-C6	-2.36	1.18	1.24
3	E	5101	ATP	C5-C4	2.35	1.47	1.40
4	G	5102	CFF	O13-C6	-2.35	1.18	1.24
3	G	5101	ATP	C5-C4	2.35	1.47	1.40
4	E	5102	CFF	O13-C6	-2.34	1.18	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	5101	ATP	PA-O3A-PB	-3.69	120.15	132.83
3	G	5101	ATP	PA-O3A-PB	-3.69	120.18	132.83
3	E	5101	ATP	PA-O3A-PB	-3.68	120.18	132.83
3	I	5101	ATP	PA-O3A-PB	-3.67	120.22	132.83
3	I	5101	ATP	C3'-C2'-C1'	3.55	106.33	100.98
3	E	5101	ATP	C3'-C2'-C1'	3.55	106.32	100.98
3	B	5101	ATP	C3'-C2'-C1'	3.55	106.32	100.98
3	G	5101	ATP	C3'-C2'-C1'	3.52	106.28	100.98
3	B	5101	ATP	PB-O3B-PG	-3.39	121.20	132.83
3	I	5101	ATP	PB-O3B-PG	-3.39	121.21	132.83
3	G	5101	ATP	PB-O3B-PG	-3.38	121.22	132.83
3	E	5101	ATP	PB-O3B-PG	-3.37	121.25	132.83
3	E	5101	ATP	C4-C5-N7	-3.06	106.20	109.40
3	I	5101	ATP	C4-C5-N7	-3.06	106.21	109.40
3	B	5101	ATP	C4-C5-N7	-3.03	106.24	109.40
3	G	5101	ATP	C4-C5-N7	-3.02	106.25	109.40
3	E	5101	ATP	N3-C2-N1	-2.87	124.20	128.68
3	B	5101	ATP	N3-C2-N1	-2.85	124.23	128.68
3	G	5101	ATP	N3-C2-N1	-2.84	124.25	128.68
3	I	5101	ATP	N3-C2-N1	-2.83	124.26	128.68
4	E	5102	CFF	C14-N7-C8	-2.80	111.94	125.43
4	B	5102	CFF	C14-N7-C8	-2.80	111.96	125.43
4	G	5102	CFF	C14-N7-C8	-2.79	111.98	125.43
4	I	5102	CFF	C14-N7-C8	-2.79	111.99	125.43

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	G	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	E	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C4'-C5'-O5'-PA
3	G	5101	ATP	C4'-C5'-O5'-PA
3	I	5101	ATP	C4'-C5'-O5'-PA
3	E	5101	ATP	C4'-C5'-O5'-PA
3	B	5101	ATP	C5'-O5'-PA-O3A
3	G	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O3A
3	E	5101	ATP	C5'-O5'-PA-O3A
3	B	5101	ATP	C5'-O5'-PA-O2A
3	G	5101	ATP	C5'-O5'-PA-O2A
3	I	5101	ATP	C5'-O5'-PA-O2A
3	E	5101	ATP	C5'-O5'-PA-O2A
3	B	5101	ATP	O4'-C4'-C5'-O5'
3	G	5101	ATP	O4'-C4'-C5'-O5'
3	I	5101	ATP	O4'-C4'-C5'-O5'
3	E	5101	ATP	O4'-C4'-C5'-O5'

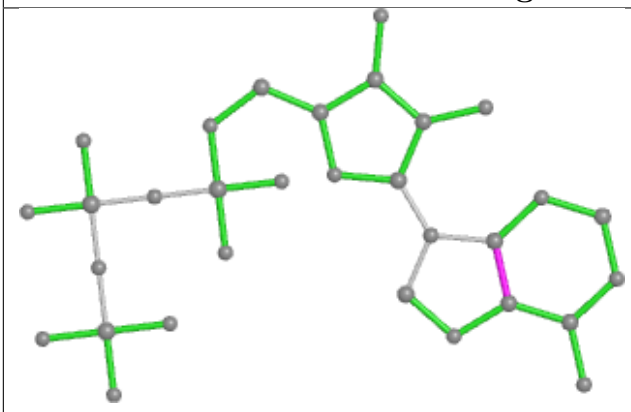
There are no ring outliers.

4 monomers are involved in 4 short contacts:

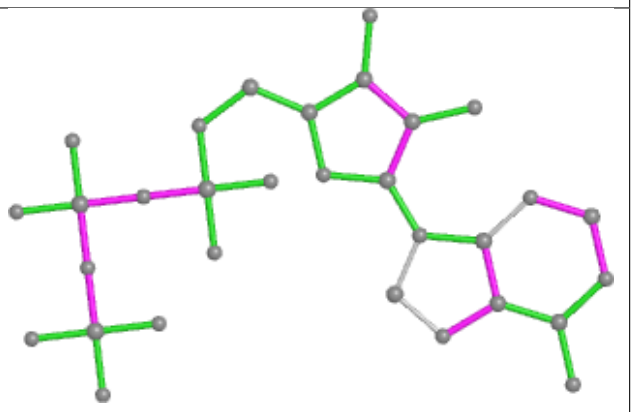
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	1	0
3	I	5101	ATP	1	0
3	E	5101	ATP	1	0
3	G	5101	ATP	1	0

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

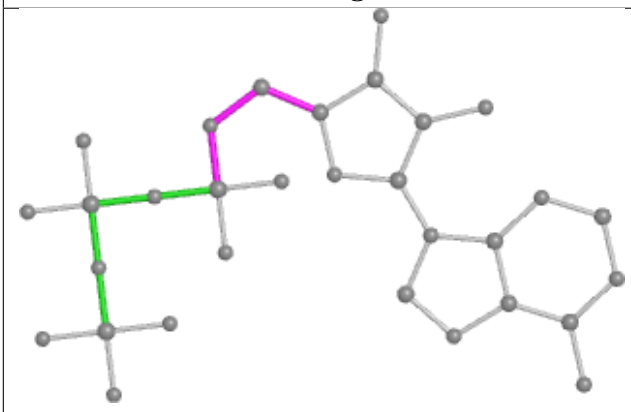
Ligand ATP B 5101



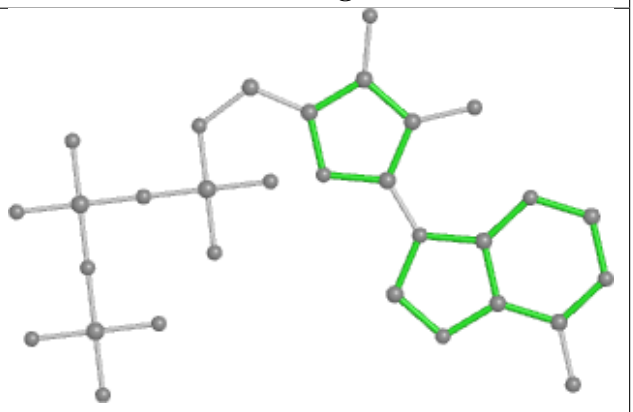
Bond lengths



Bond angles

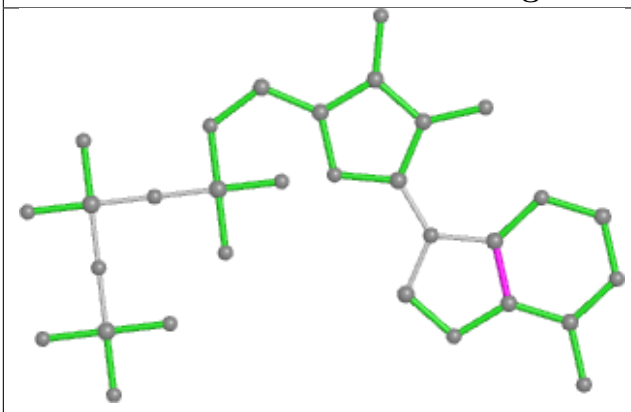


Torsions

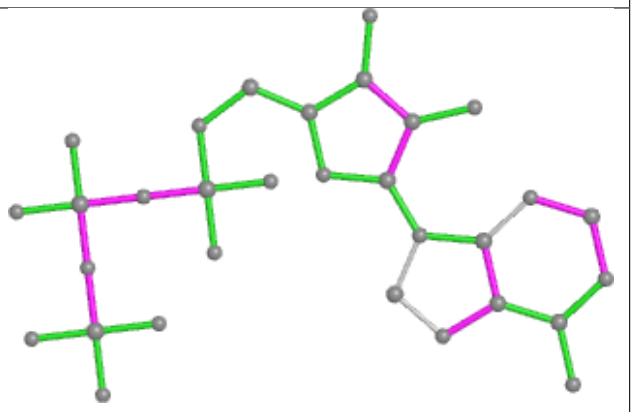


Rings

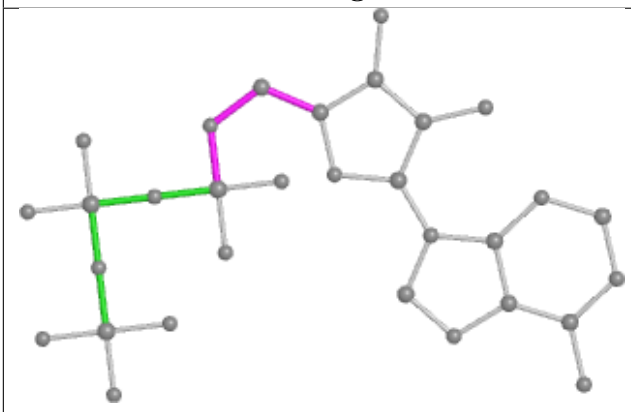
Ligand ATP I 5101



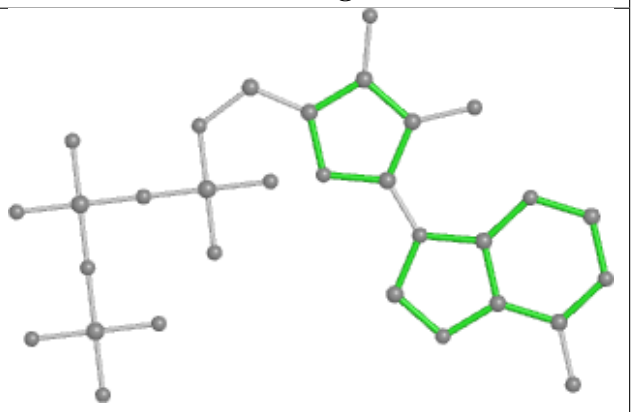
Bond lengths



Bond angles

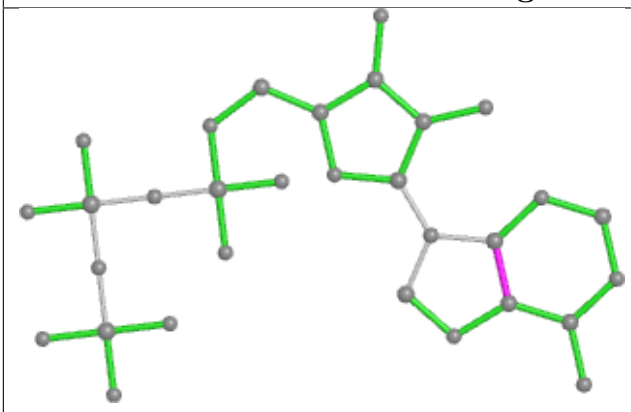


Torsions

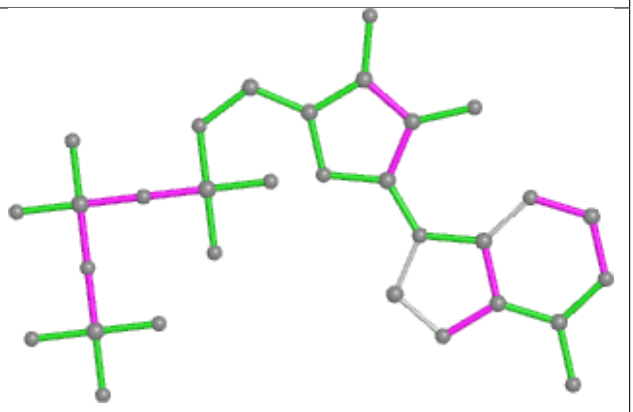


Rings

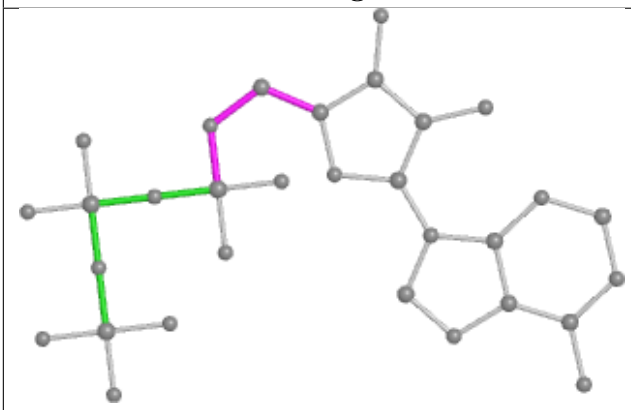
Ligand ATP E 5101



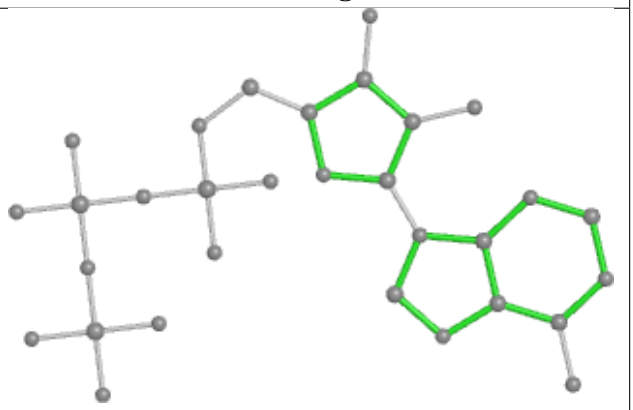
Bond lengths



Bond angles

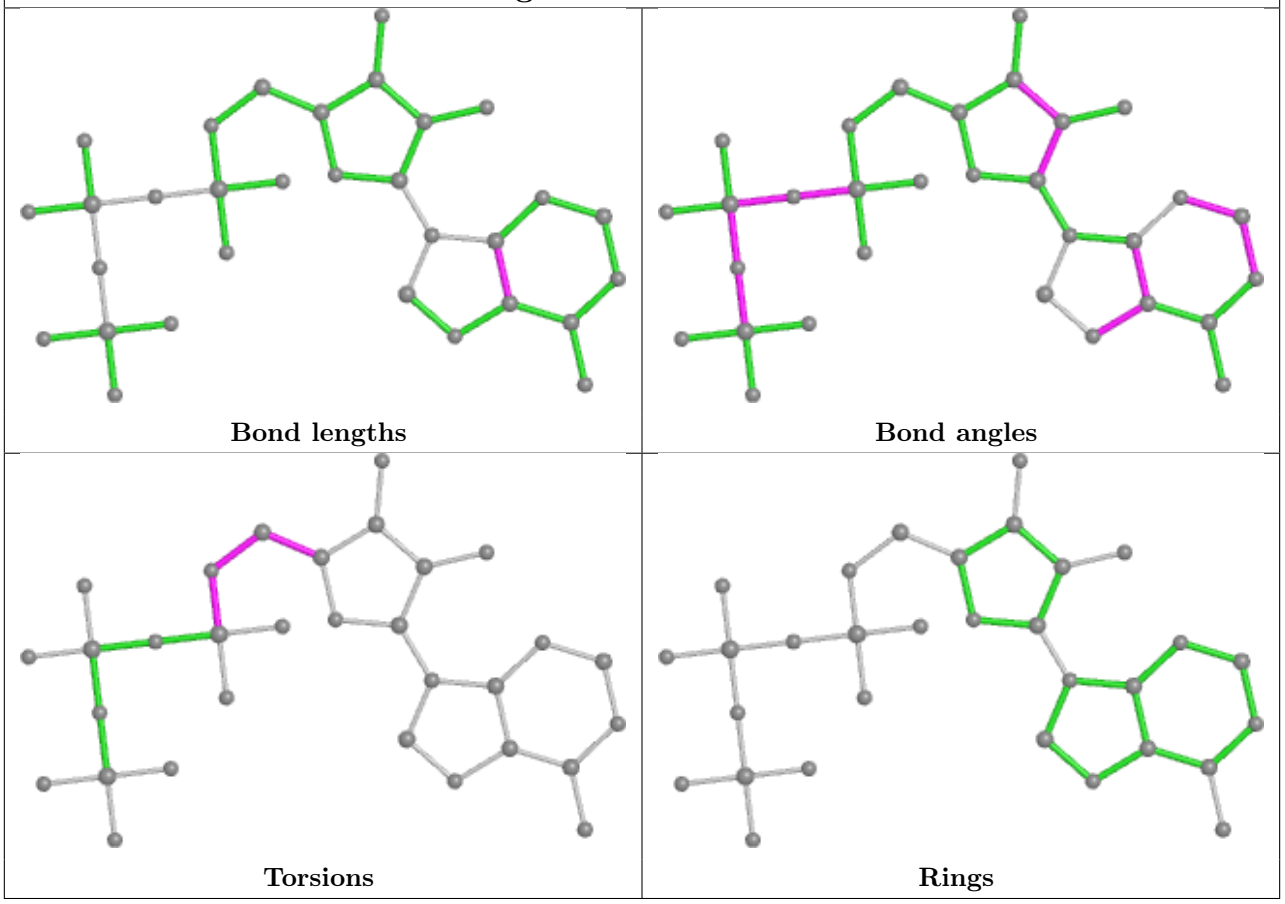


Torsions



Rings

Ligand ATP G 5101



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	G	14
2	I	14
2	E	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	73.47
1	G	4345:UNK	C	4540:PHE	N	73.47

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	73.47
1	E	4345:UNK	C	4540:PHE	N	73.47
1	B	3613:UNK	C	3639:THR	N	45.62
1	G	3613:UNK	C	3639:THR	N	45.62
1	I	3613:UNK	C	3639:THR	N	45.62
1	E	3613:UNK	C	3639:THR	N	45.62
1	B	4253:GLU	C	4320:UNK	N	27.90
1	G	4253:GLU	C	4320:UNK	N	27.90
1	I	4253:GLU	C	4320:UNK	N	27.90
1	E	4253:GLU	C	4320:UNK	N	27.90
1	B	3163:UNK	C	3170:UNK	N	15.83
1	G	3163:UNK	C	3170:UNK	N	15.83
1	I	3163:UNK	C	3170:UNK	N	15.83
1	E	3163:UNK	C	3170:UNK	N	15.83
1	B	3063:UNK	C	3134:UNK	N	14.87
1	G	3063:UNK	C	3134:UNK	N	14.87
1	I	3063:UNK	C	3134:UNK	N	14.87
1	E	3063:UNK	C	3134:UNK	N	14.87
1	B	3468:UNK	C	3511:UNK	N	14.52
1	G	3468:UNK	C	3511:UNK	N	14.52
1	I	3468:UNK	C	3511:UNK	N	14.52
1	E	3468:UNK	C	3511:UNK	N	14.52
1	B	2703:UNK	C	2734:ASN	N	13.45
1	G	2703:UNK	C	2734:ASN	N	13.45
1	I	2703:UNK	C	2734:ASN	N	13.45
1	E	2703:UNK	C	2734:ASN	N	13.45
1	B	3236:UNK	C	3241:UNK	N	12.87
1	G	3236:UNK	C	3241:UNK	N	12.87
1	I	3236:UNK	C	3241:UNK	N	12.87
1	E	3236:UNK	C	3241:UNK	N	12.87
1	B	1564:UNK	C	1573:MET	N	12.40
1	G	1564:UNK	C	1573:MET	N	12.40
1	I	1564:UNK	C	1573:MET	N	12.40
1	E	1564:UNK	C	1573:MET	N	12.40
1	B	2976:UNK	C	2995:UNK	N	12.24
1	G	2976:UNK	C	2995:UNK	N	12.24
1	I	2976:UNK	C	2995:UNK	N	12.24
1	E	2976:UNK	C	2995:UNK	N	12.24
1	B	3254:UNK	C	3261:UNK	N	8.57
1	G	3254:UNK	C	3261:UNK	N	8.57
1	I	3254:UNK	C	3261:UNK	N	8.57
1	E	3254:UNK	C	3261:UNK	N	8.57

Continued on next page...

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1297:UNK	C	1430:UNK	N	5.81
1	G	1297:UNK	C	1430:UNK	N	5.81
1	I	1297:UNK	C	1430:UNK	N	5.81
1	E	1297:UNK	C	1430:UNK	N	5.81
1	B	2939:ARG	C	2942:UNK	N	3.33
1	G	2939:ARG	C	2942:UNK	N	3.33
1	I	2939:ARG	C	2942:UNK	N	3.33
1	E	2939:ARG	C	2942:UNK	N	3.33
1	B	2479:LEU	C	2487:UNK	N	3.30
1	G	2479:LEU	C	2487:UNK	N	3.30
1	I	2479:LEU	C	2487:UNK	N	3.30
1	E	2479:LEU	C	2487:UNK	N	3.30

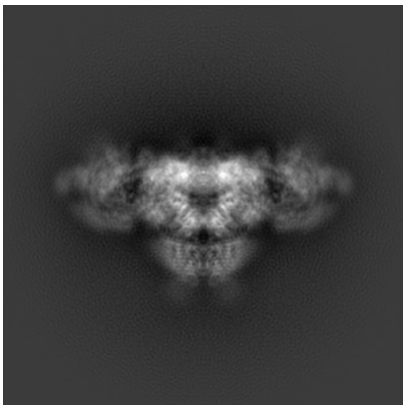
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8376. These allow visual inspection of the internal detail of the map and identification of artifacts.

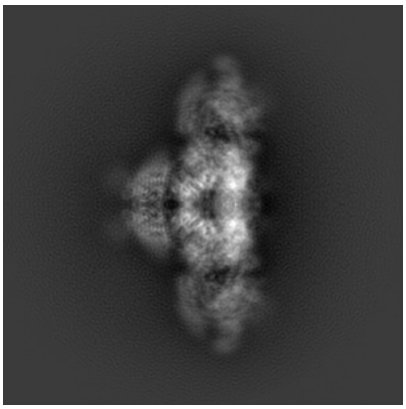
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

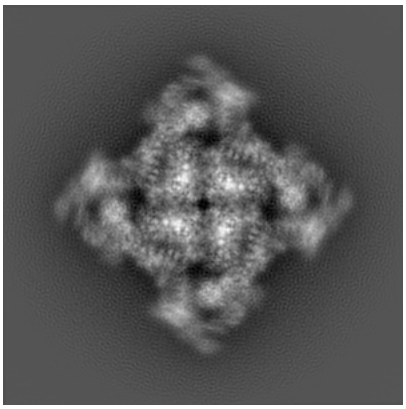
6.1.1 Primary map



X

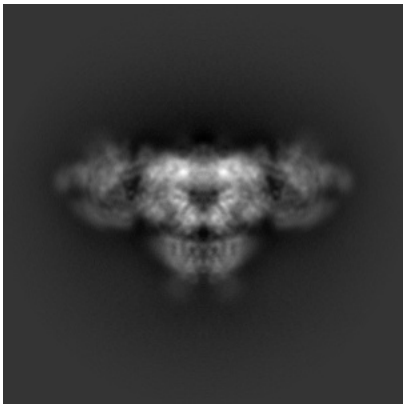


Y

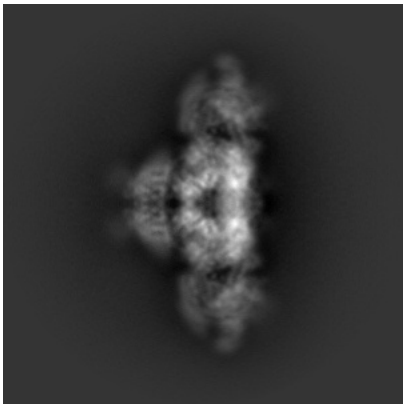


Z

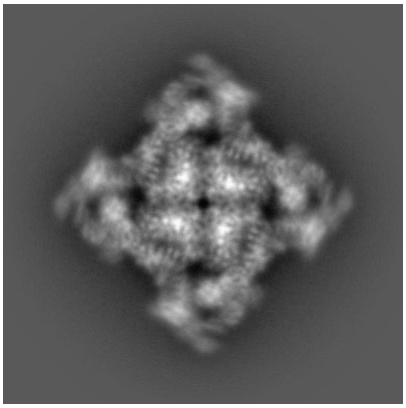
6.1.2 Raw map



X



Y

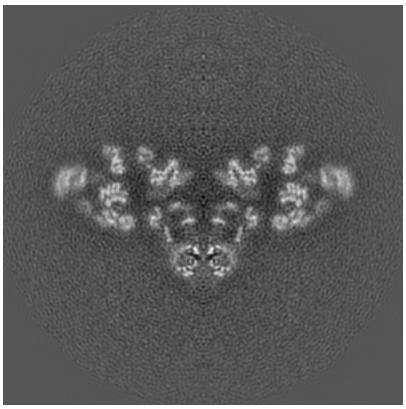


Z

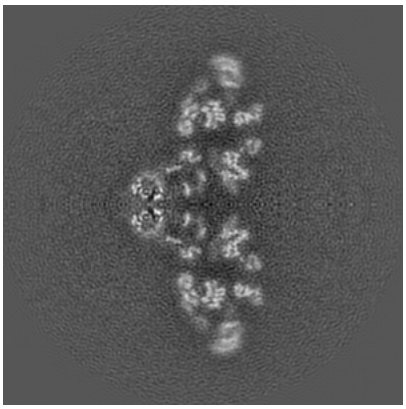
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

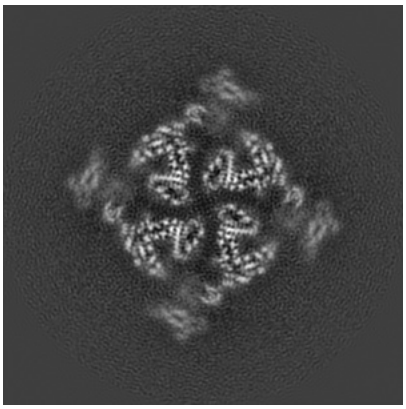
6.2.1 Primary map



X Index: 200

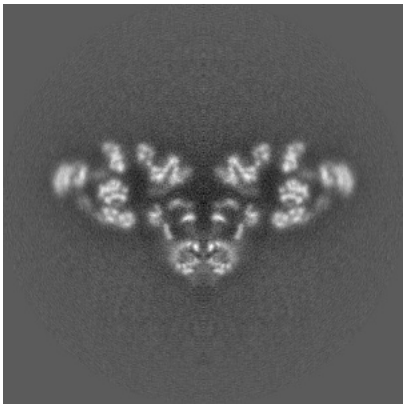


Y Index: 200

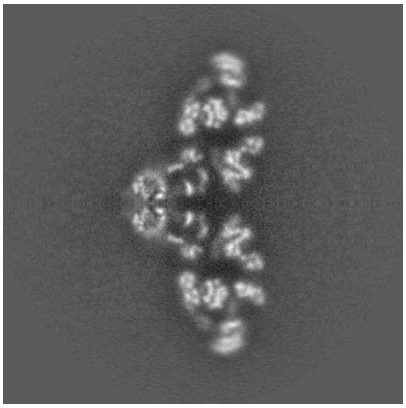


Z Index: 200

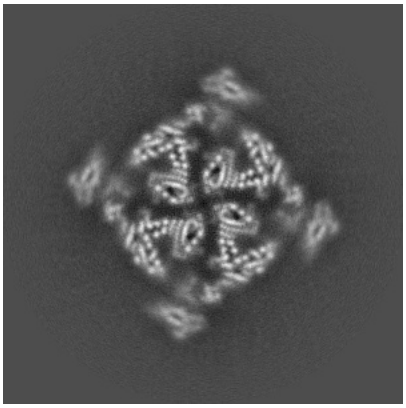
6.2.2 Raw map



X Index: 200



Y Index: 200

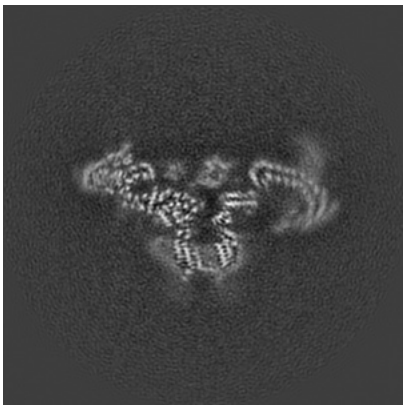


Z Index: 200

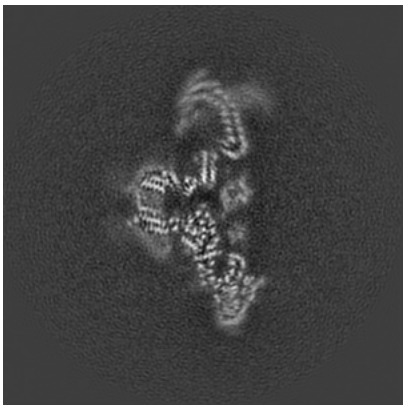
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

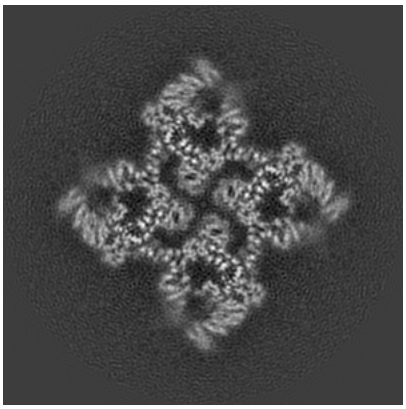
6.3.1 Primary map



X Index: 225

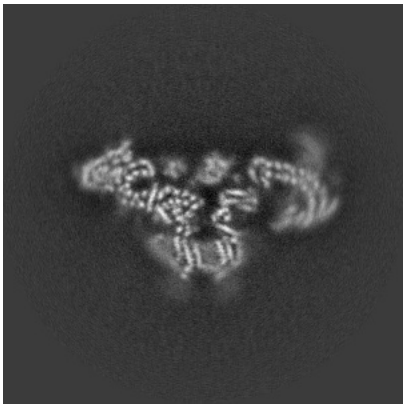


Y Index: 175

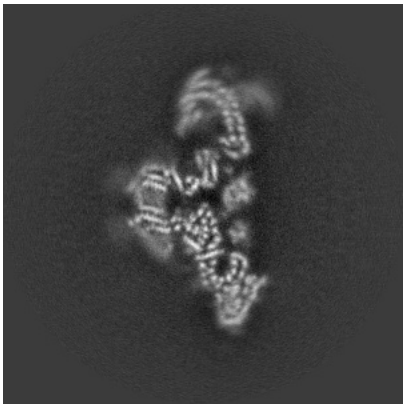


Z Index: 232

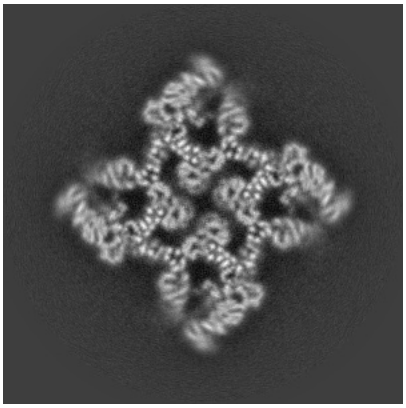
6.3.2 Raw map



X Index: 224



Y Index: 176



Z Index: 232

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.

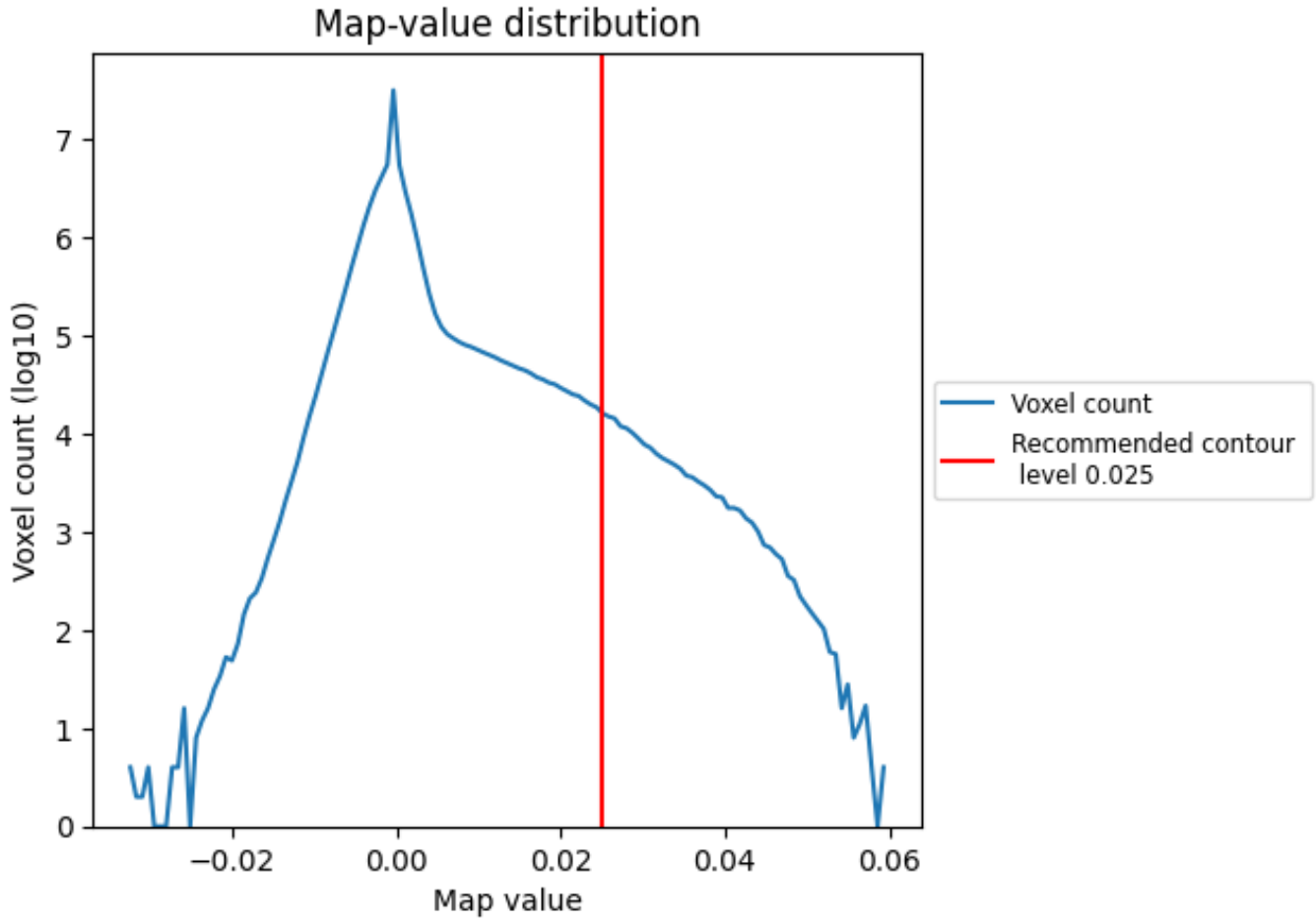
6.5 Mask visualisation (i)

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

7 Map analysis

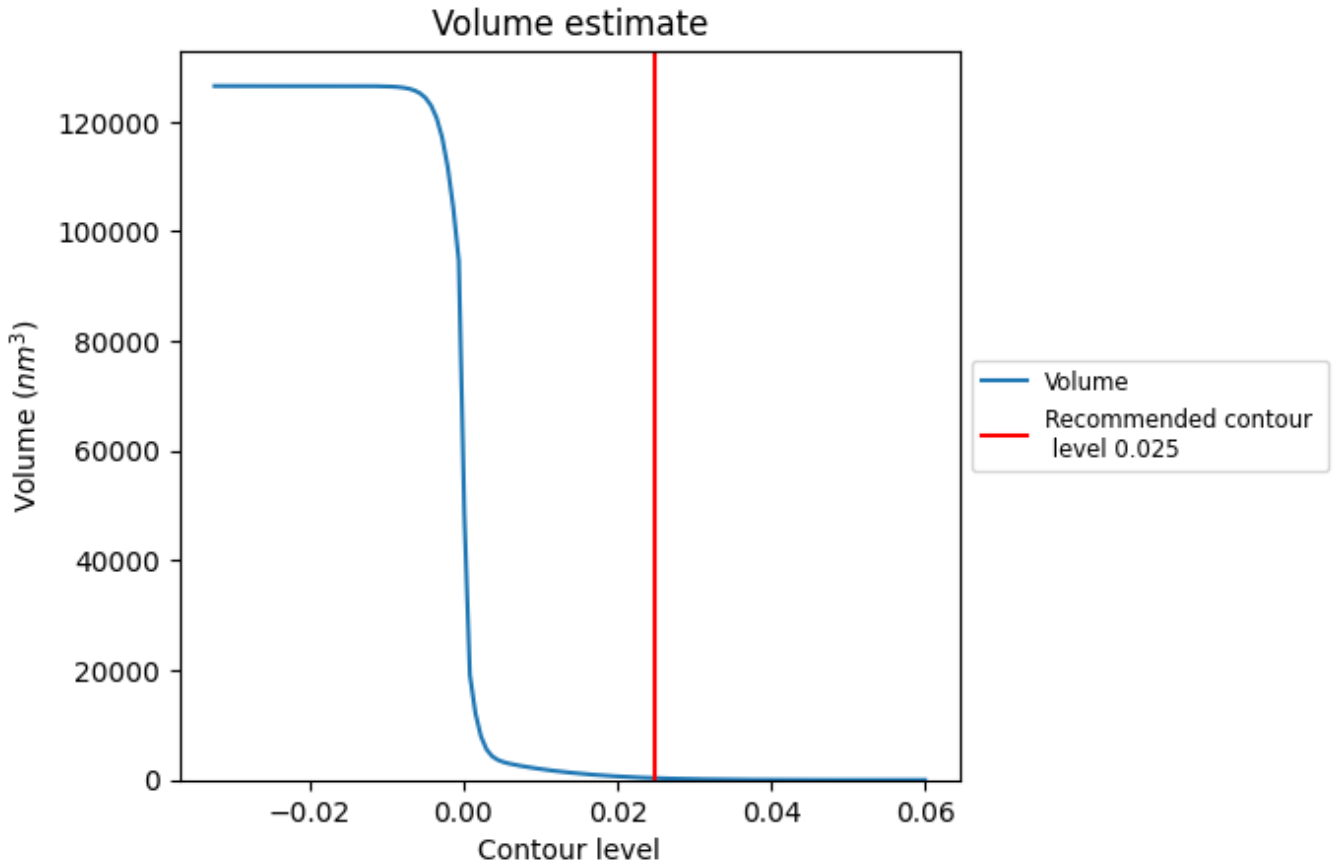
This section contains the results of statistical analysis of the map.

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.

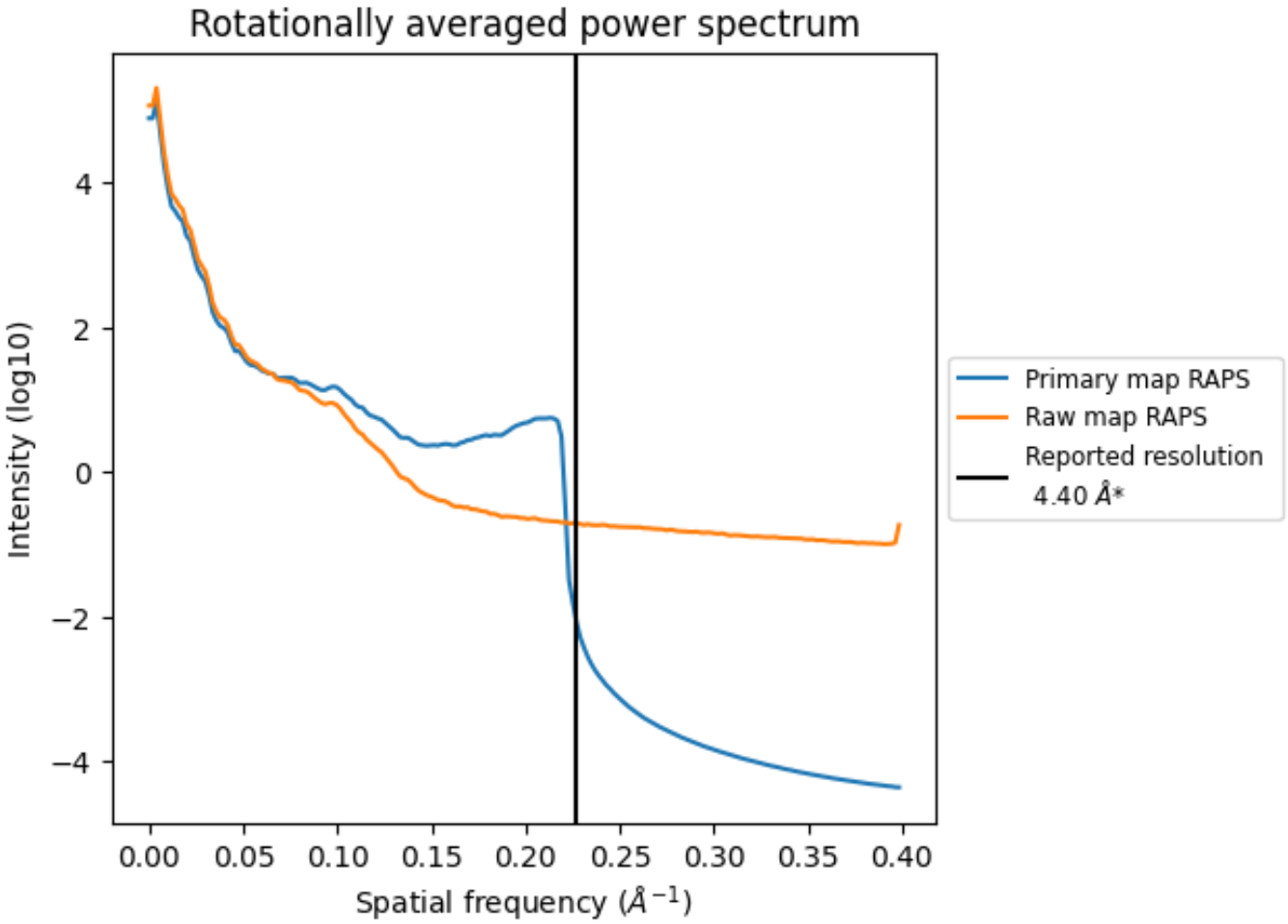
7.2 Volume estimate



The volume at the recommended contour level is 331 nm^3; this corresponds to an approximate mass of 299 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)

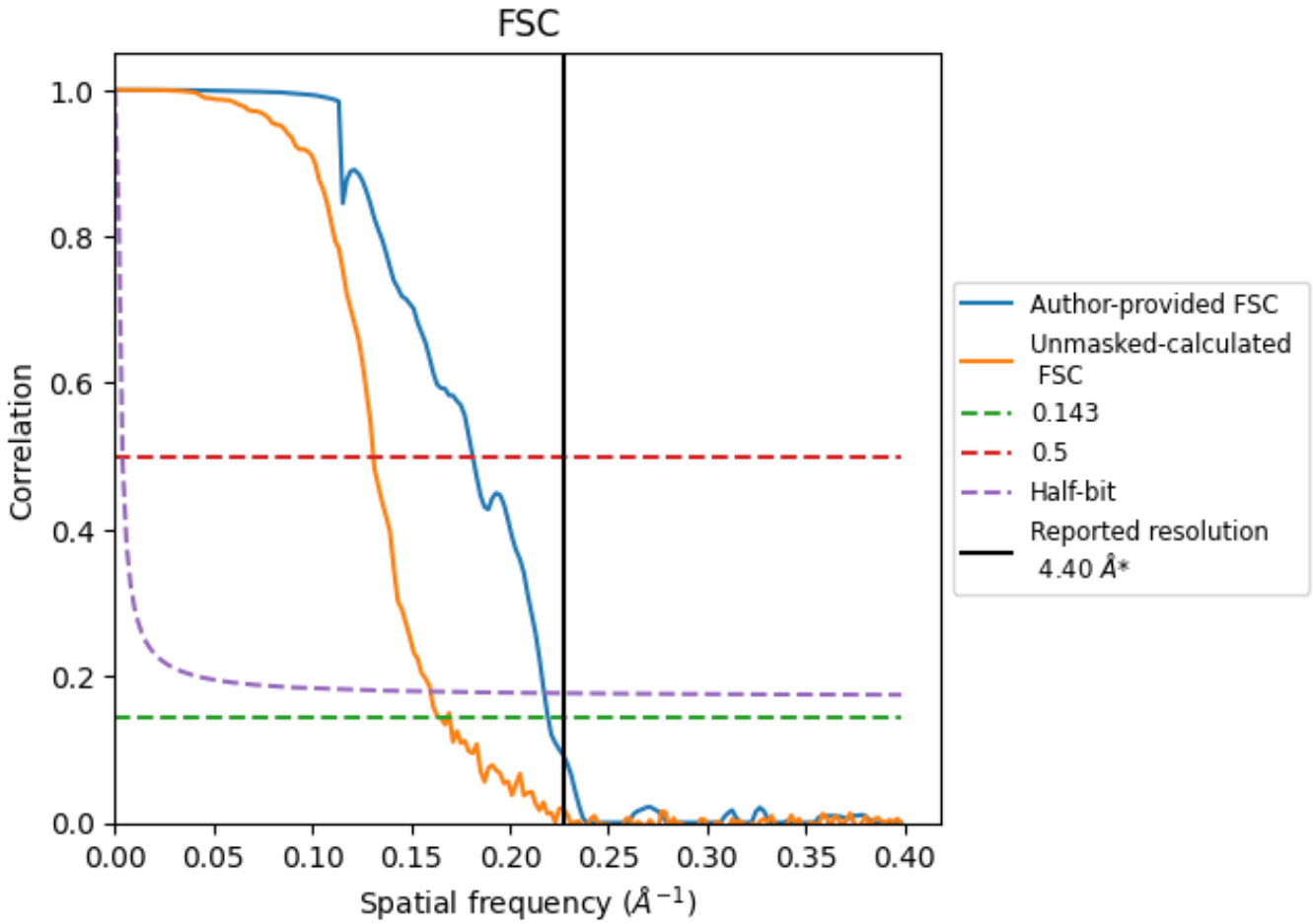


*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

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 0.227 Å^{-1}

8.2 Resolution estimates (i)

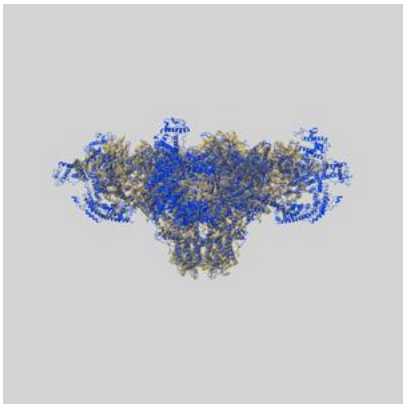
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.56	5.52	4.60
Unmasked-calculated*	6.06	7.64	6.25

*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 6.06 differs from the reported value 4.4 by more than 10 %

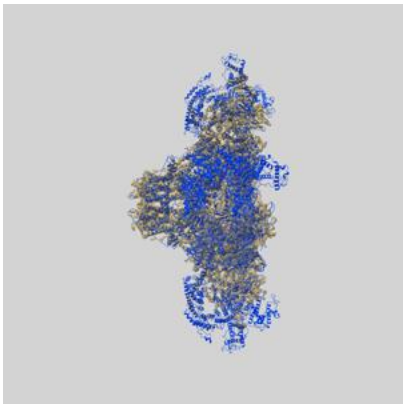
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8376 and PDB model 5T9V. Per-residue inclusion information can be found in section 3 on page 6.

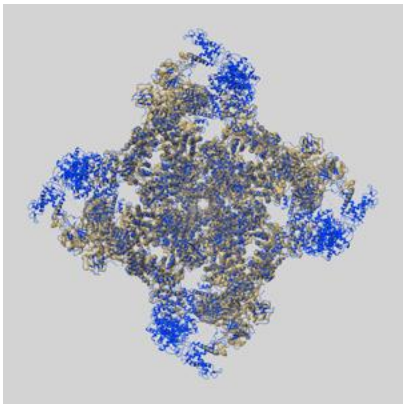
9.1 Map-model overlay



X



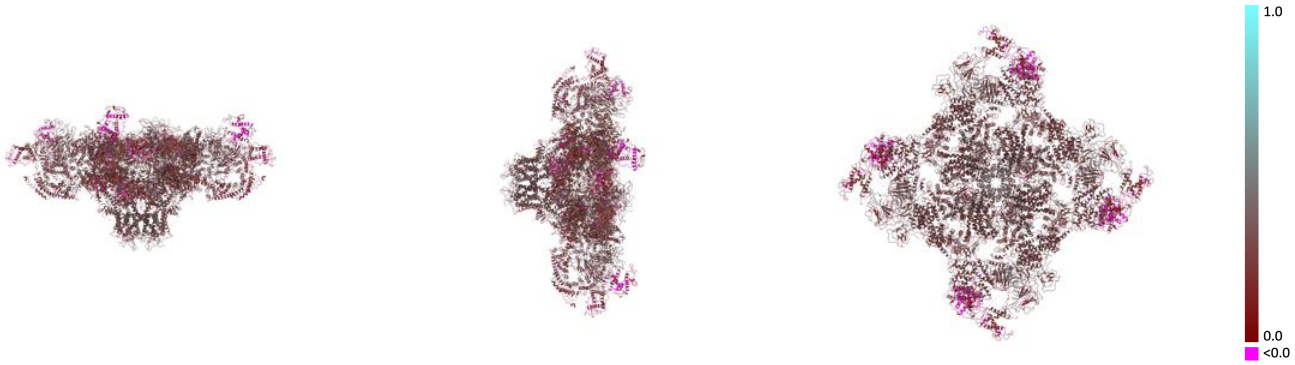
Y



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.

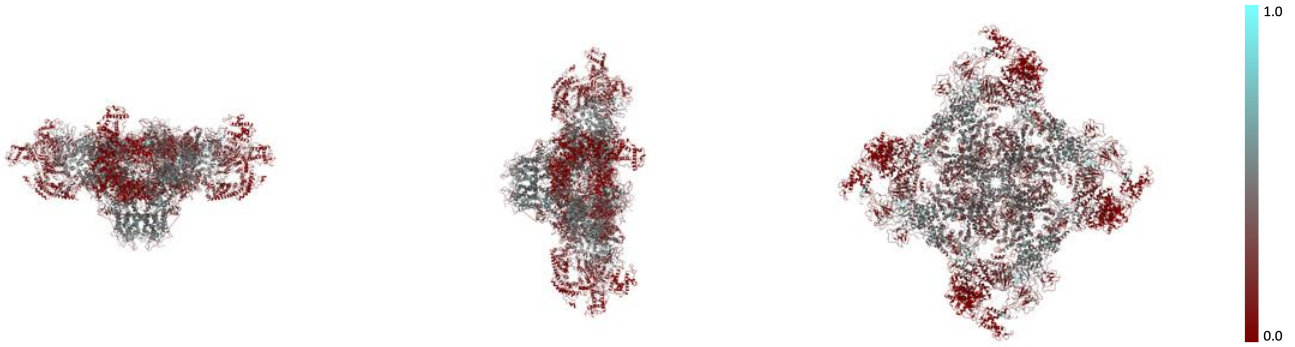
9.2 Q-score mapped to coordinate model (i)



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.

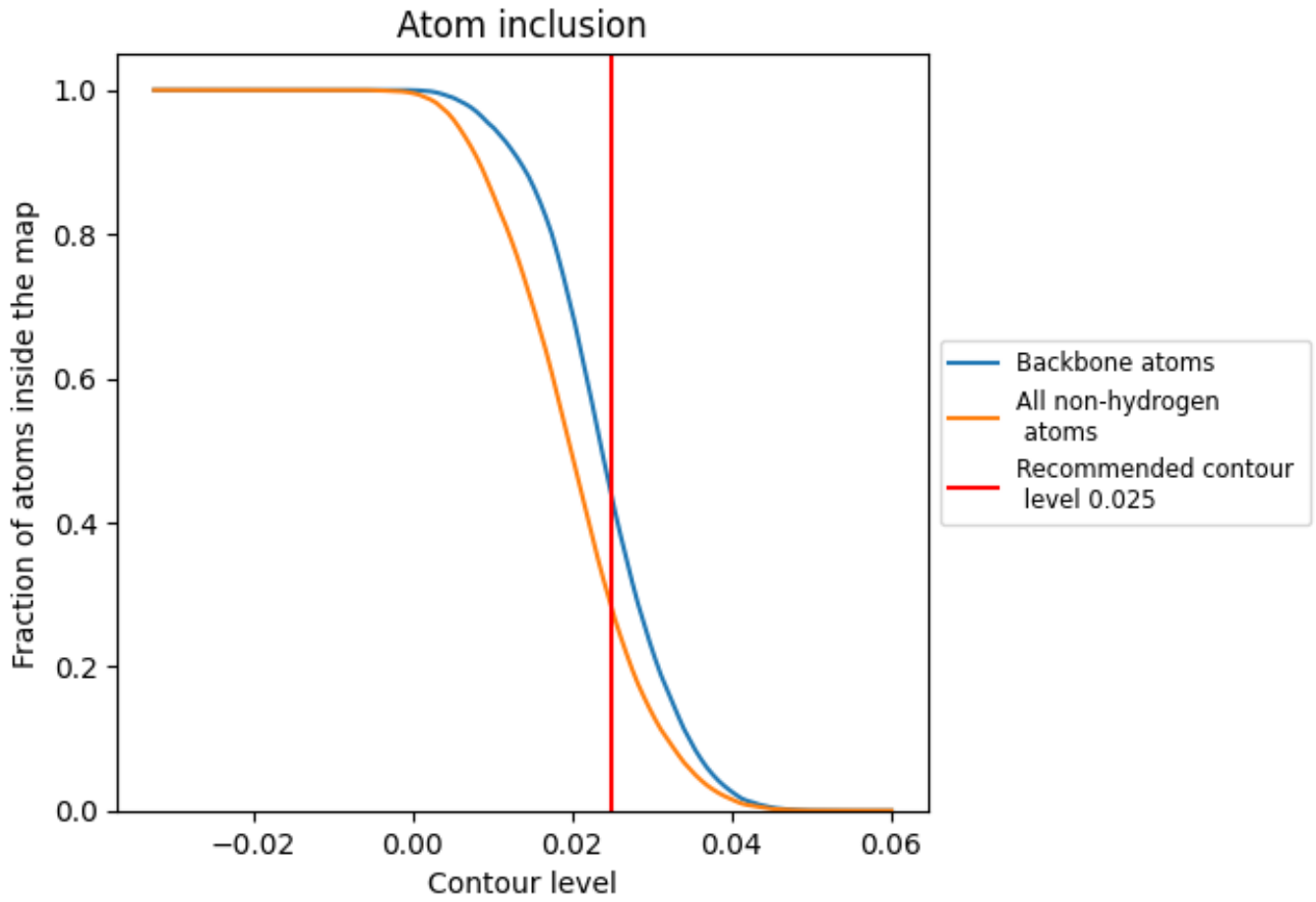
9.3 Atom inclusion mapped to coordinate model (i)



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, 43% of all backbone atoms, 28% 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	0.2799	0.2680
A	0.2692	0.3040
B	0.2808	0.2690
E	0.2796	0.2650
F	0.2680	0.3070
G	0.2801	0.2680
H	0.2705	0.3040
I	0.2803	0.2660
J	0.2717	0.3050