wwPDB EM Validation Summary Report (i)

Mar 2, 2024 – 09:49 AM EST

PDB ID	:	5TAN
EMDB ID	:	EMD-8380
Title	:	Structure of rabbit RyR1 (Caffeine/ATP/Ca2+ dataset, class 3)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-10
Resolution	:	4.30 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (1)) were used in the production of this report:

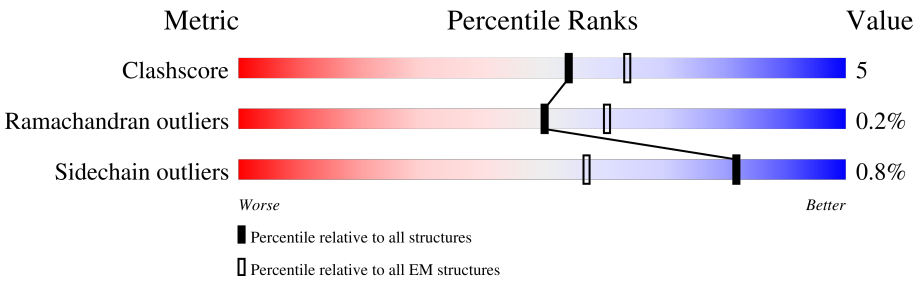
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.30 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	58% 81% 19% •
1	F	108	59% 81% 19% •
1	H	108	60% 81% 19% •
1	J	108	58% 81% 19% •
2	B	4416	46% 84% 11% 5%
2	E	4416	46% 83% 11% 5%
2	G	4416	46% 83% 11% 5%
2	I	4416	46% 84% 11% 5%

2 Entry composition (i)

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.

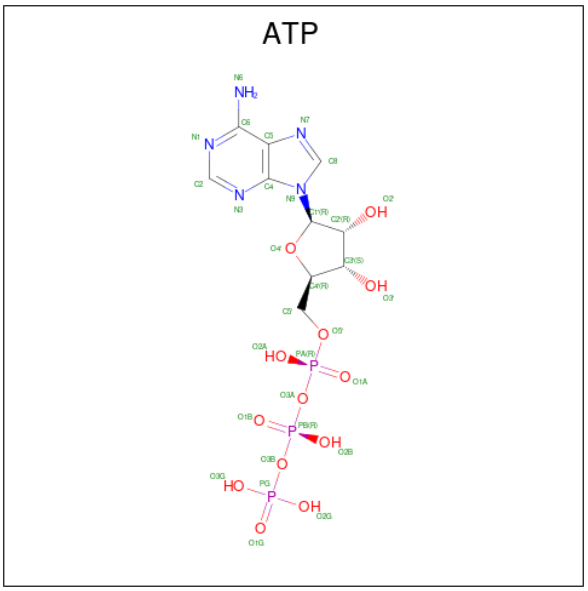
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 2 is a protein called Ryanodine receptor 1.

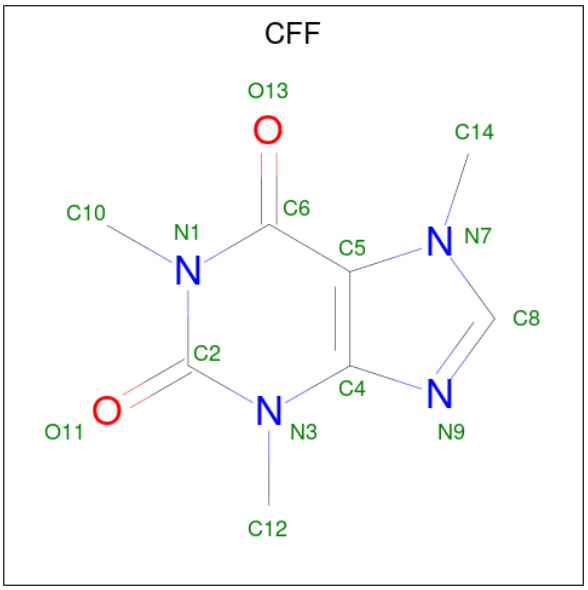
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	4194	29499	18686	5228	5428	157	0	0
2	E	4194	29499	18686	5228	5428	157	0	0
2	I	4194	29499	18686	5228	5428	157	0	0
2	G	4194	29499	18686	5228	5428	157	0	0

- 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	E	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	G	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
			Total	C	N	O	
4	B	1	14	8	4	2	0
4	E	1	14	8	4	2	0
4	I	1	14	8	4	2	0
4	G	1	14	8	4	2	0

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

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

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

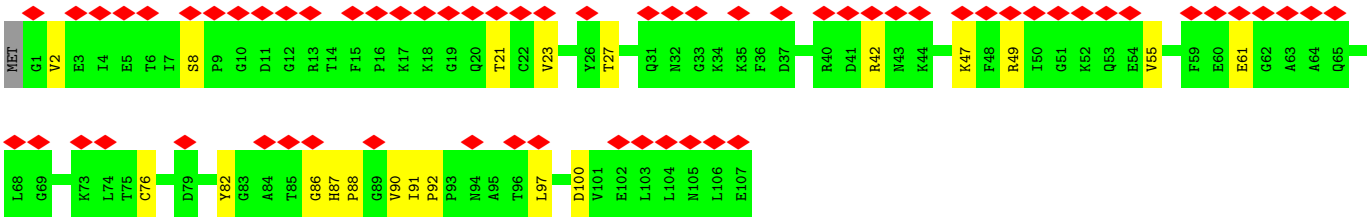
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
6	B	1	1	1	0
6	E	1	1	1	0
6	I	1	1	1	0
6	G	1	1	1	0

3 Residue-property plots (i)

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

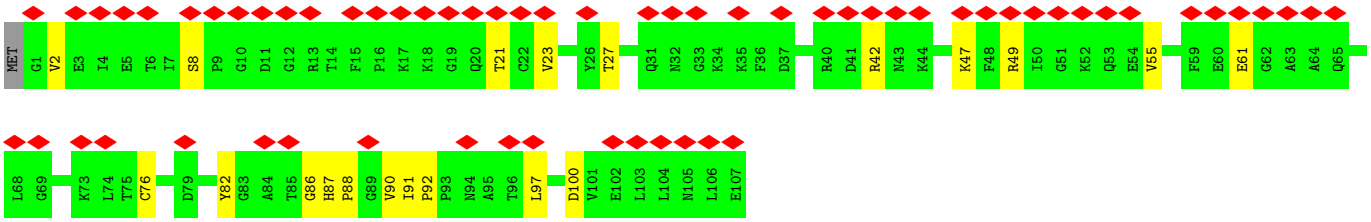
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



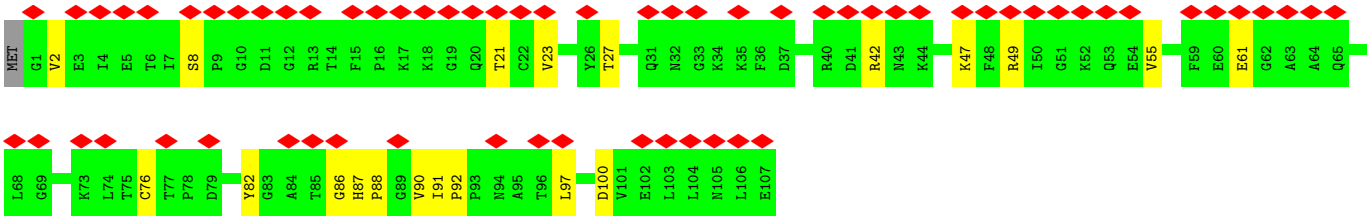
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



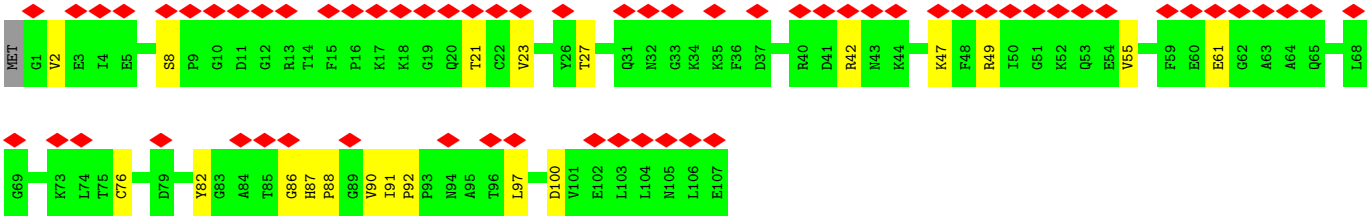
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



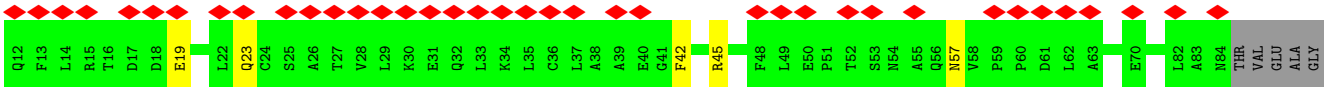
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

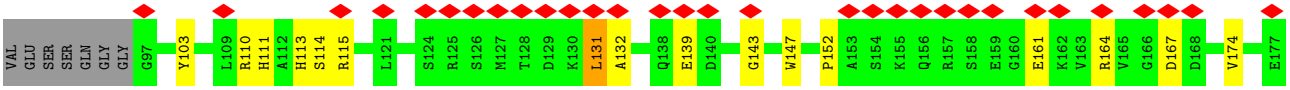
Chain J:

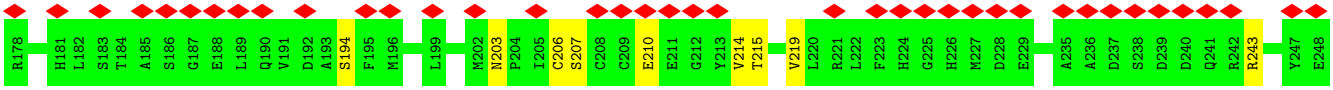


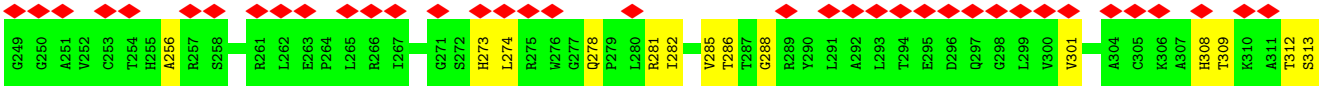
- Molecule 2: Ryanodine receptor 1

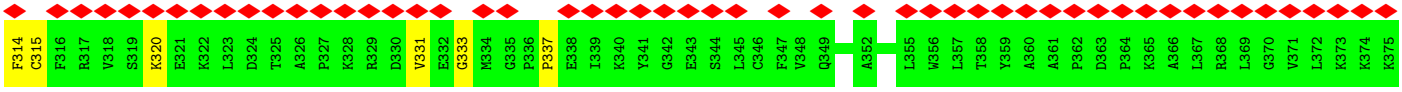
Chain B:

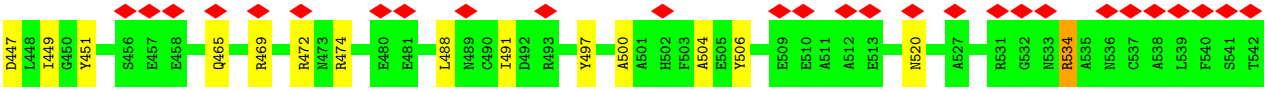


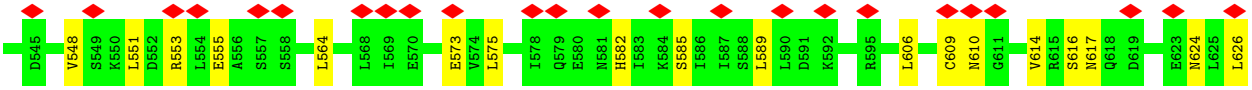


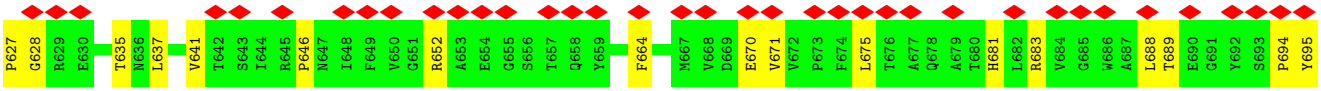


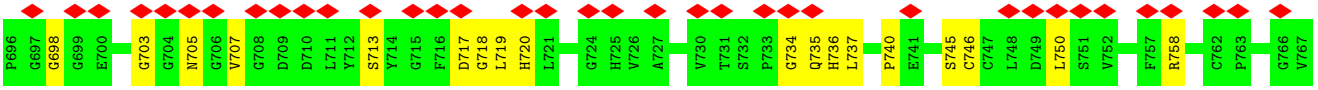


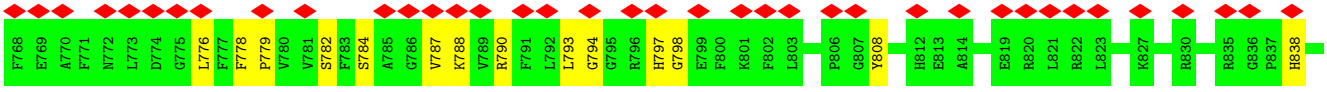












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K901 R902 L903 H904 P905 C906 L907 V908 N909 F910 H911 S912 L913 P914 E915 P916 E917 R918 N919 Y920 N921 L922 Q923 M924 S925 G926 E927 T928 L929 K930 T931 L932 L933 A934 L935 G936 C937 H938 V939 G940 M941 A942 D943 E944 K945 A946 E947 D948 N949 L950 K951 K952 T953 K954 L955 P956 K957 T958 Y959 M960

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GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 G1925 L1926 L1927 Q1928 L1931 P1932 K1936 L1937 Q1938 M1939 C1940 Q1949 L1958 A1959 A1960

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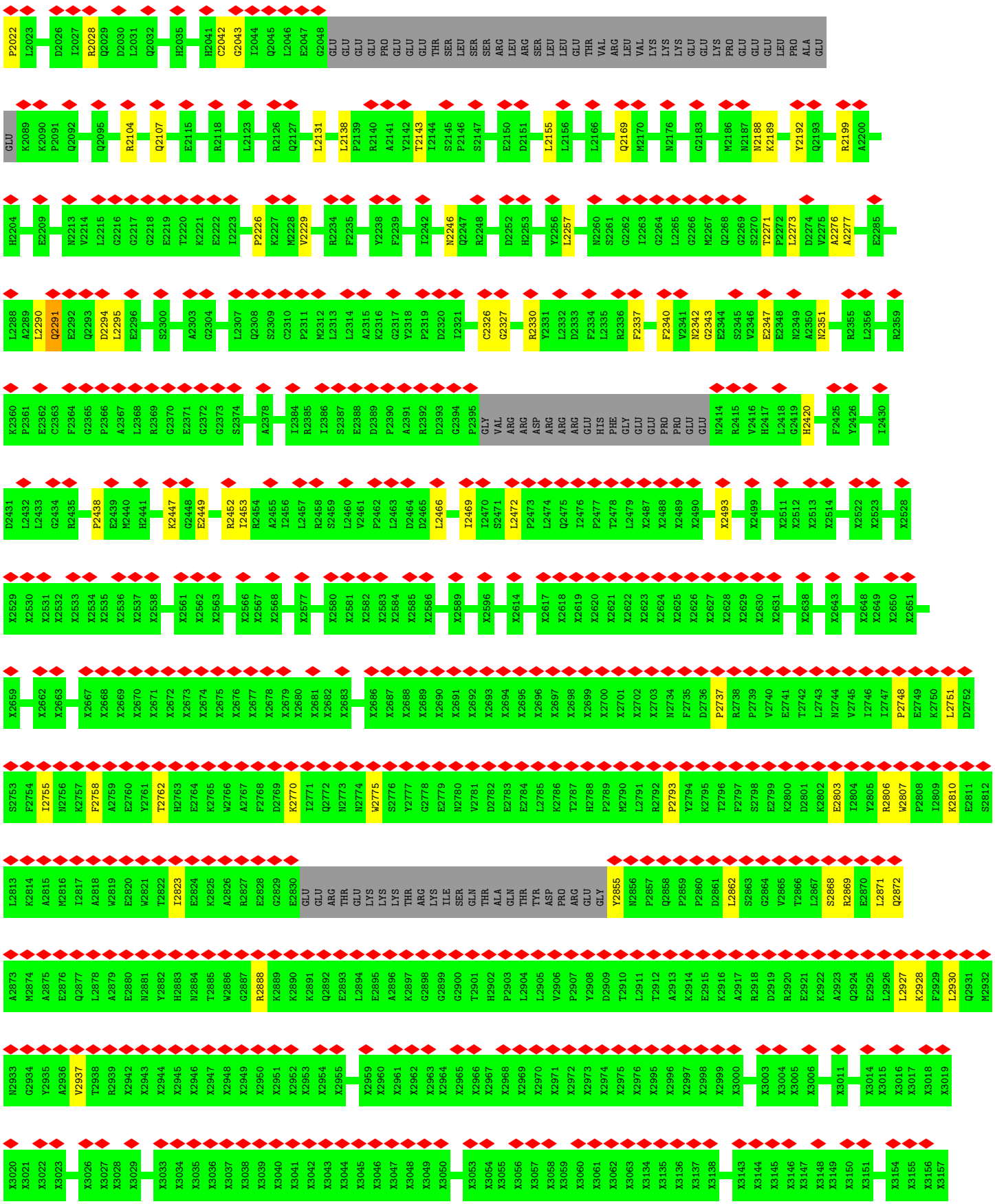
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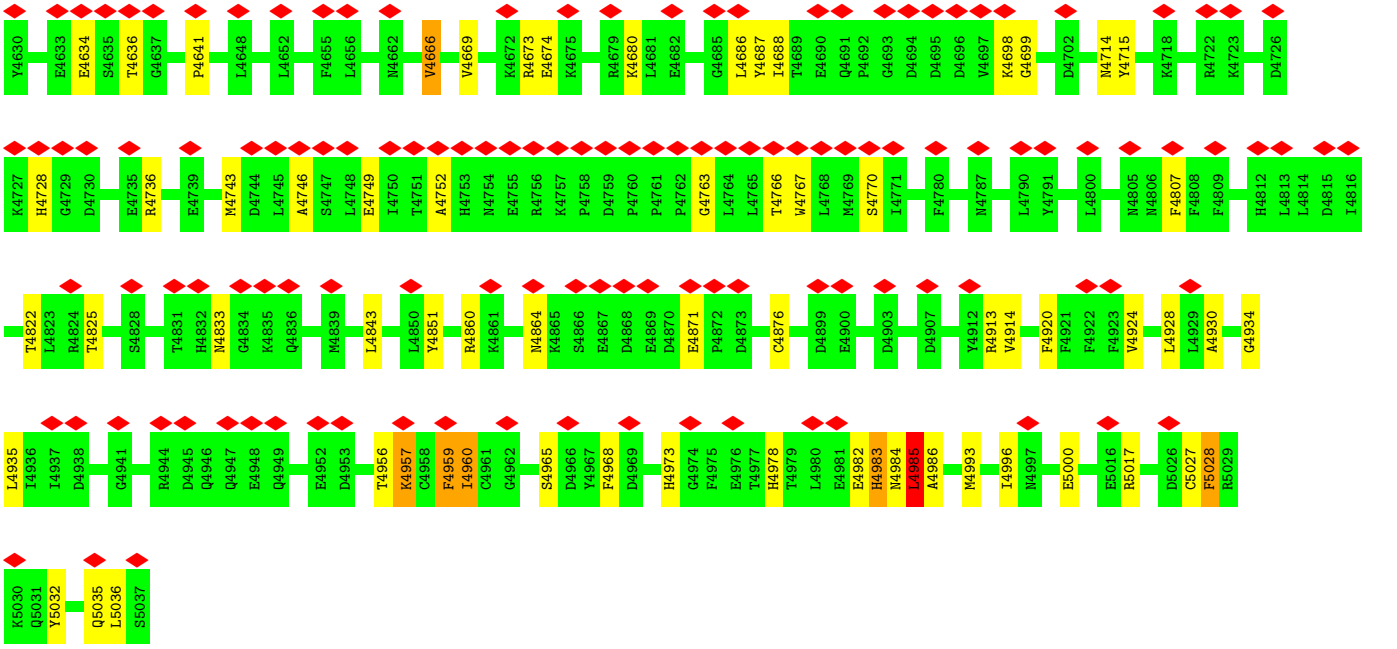

- Molecule 2: Ryanodine receptor 1

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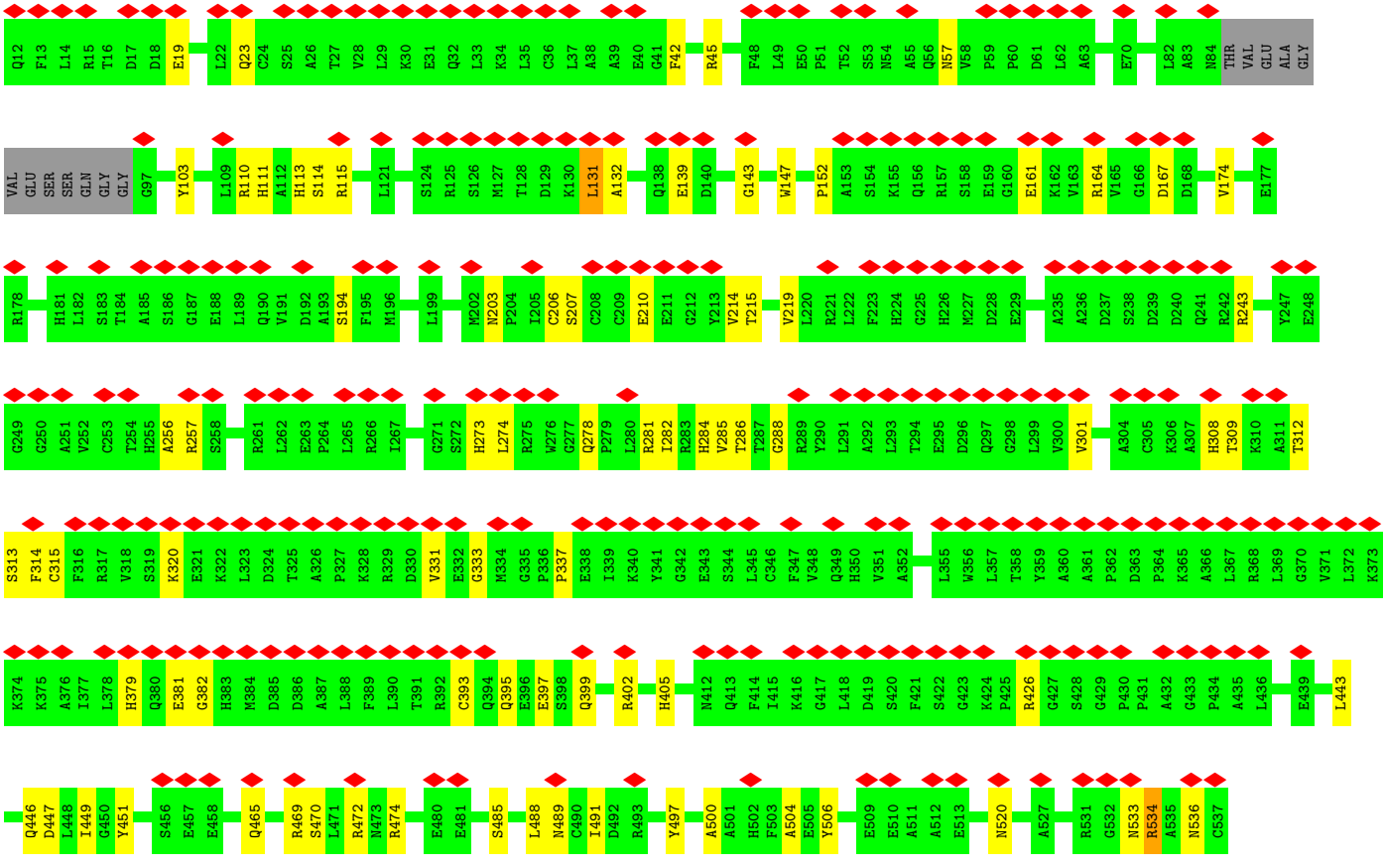

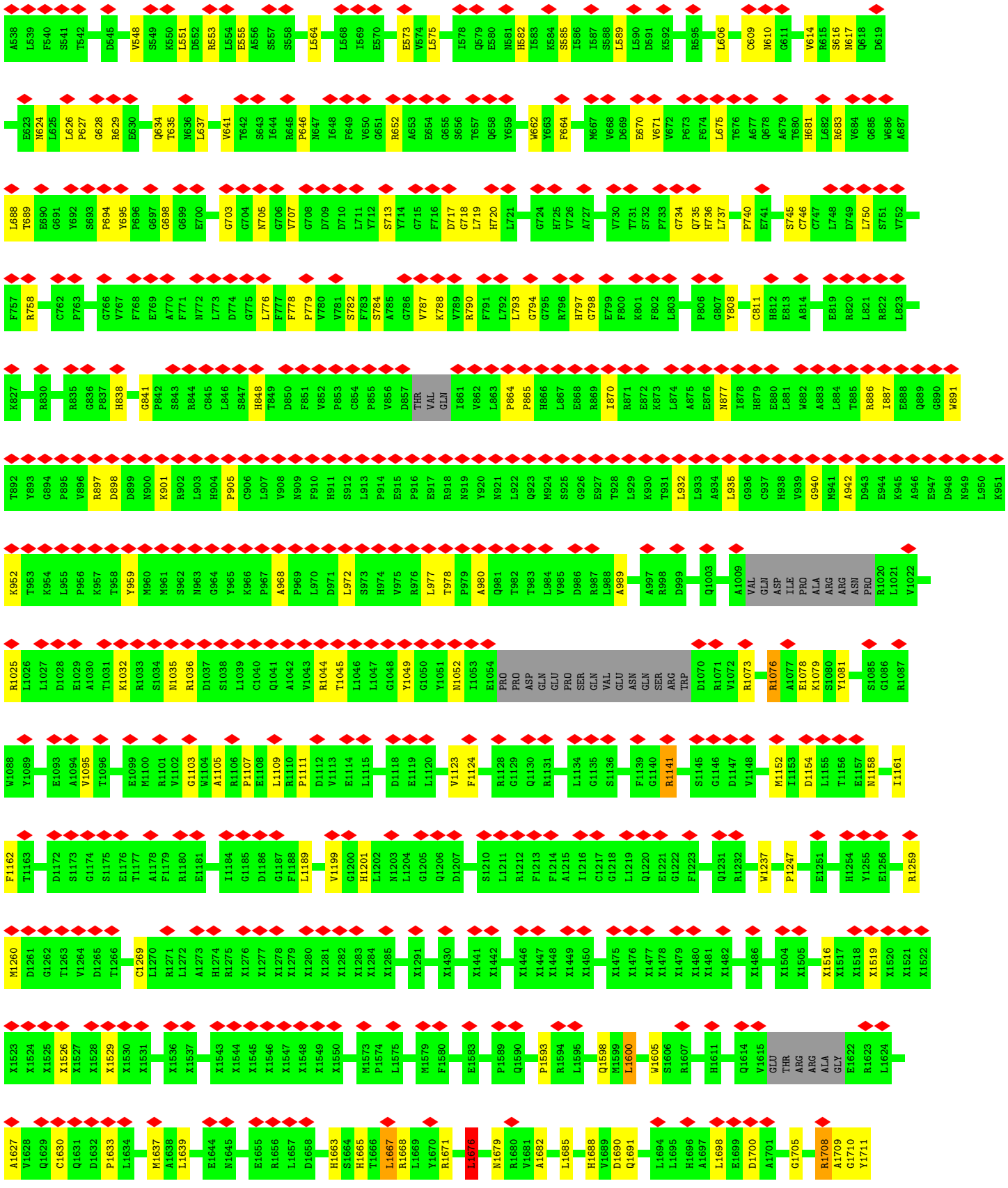
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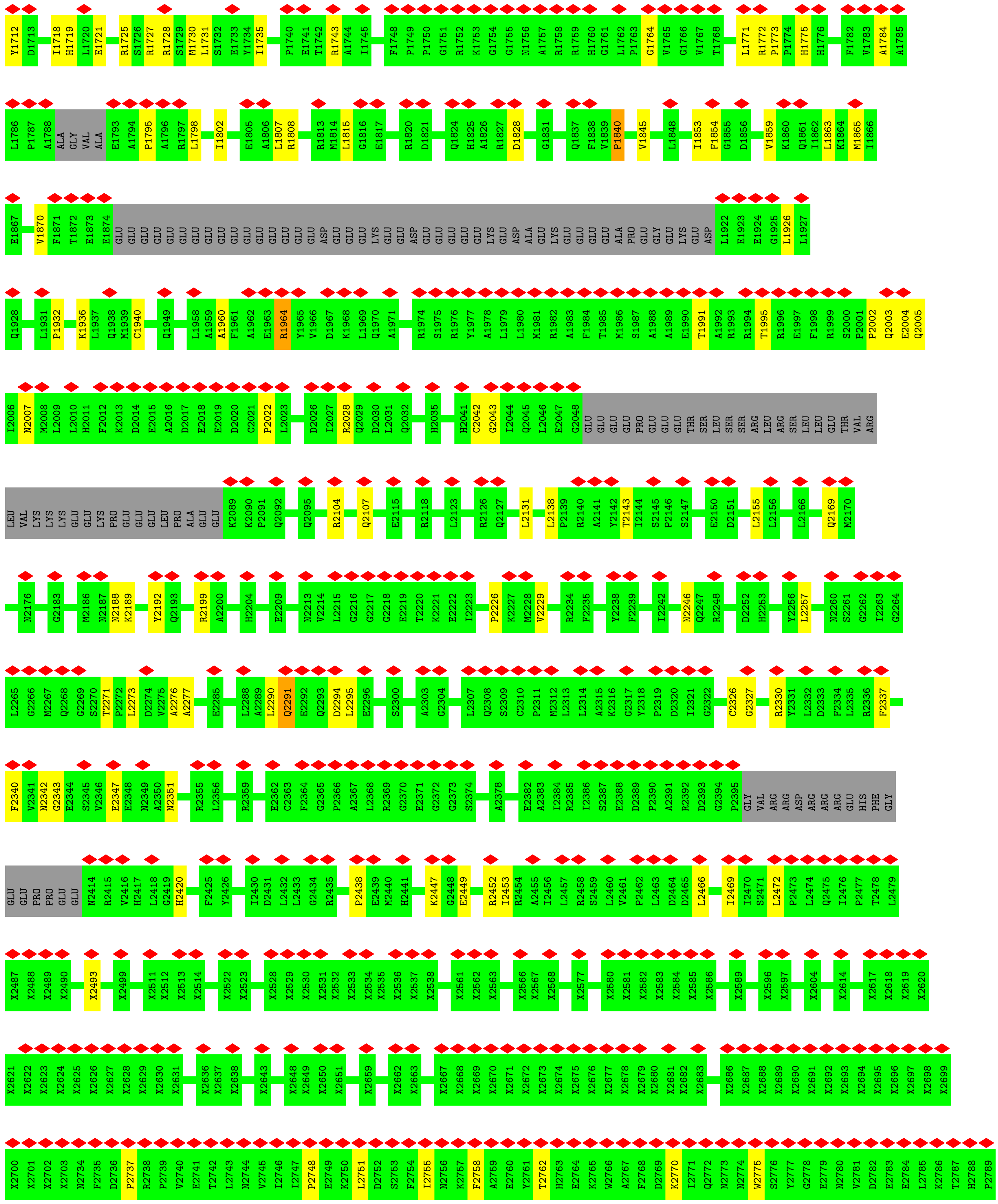
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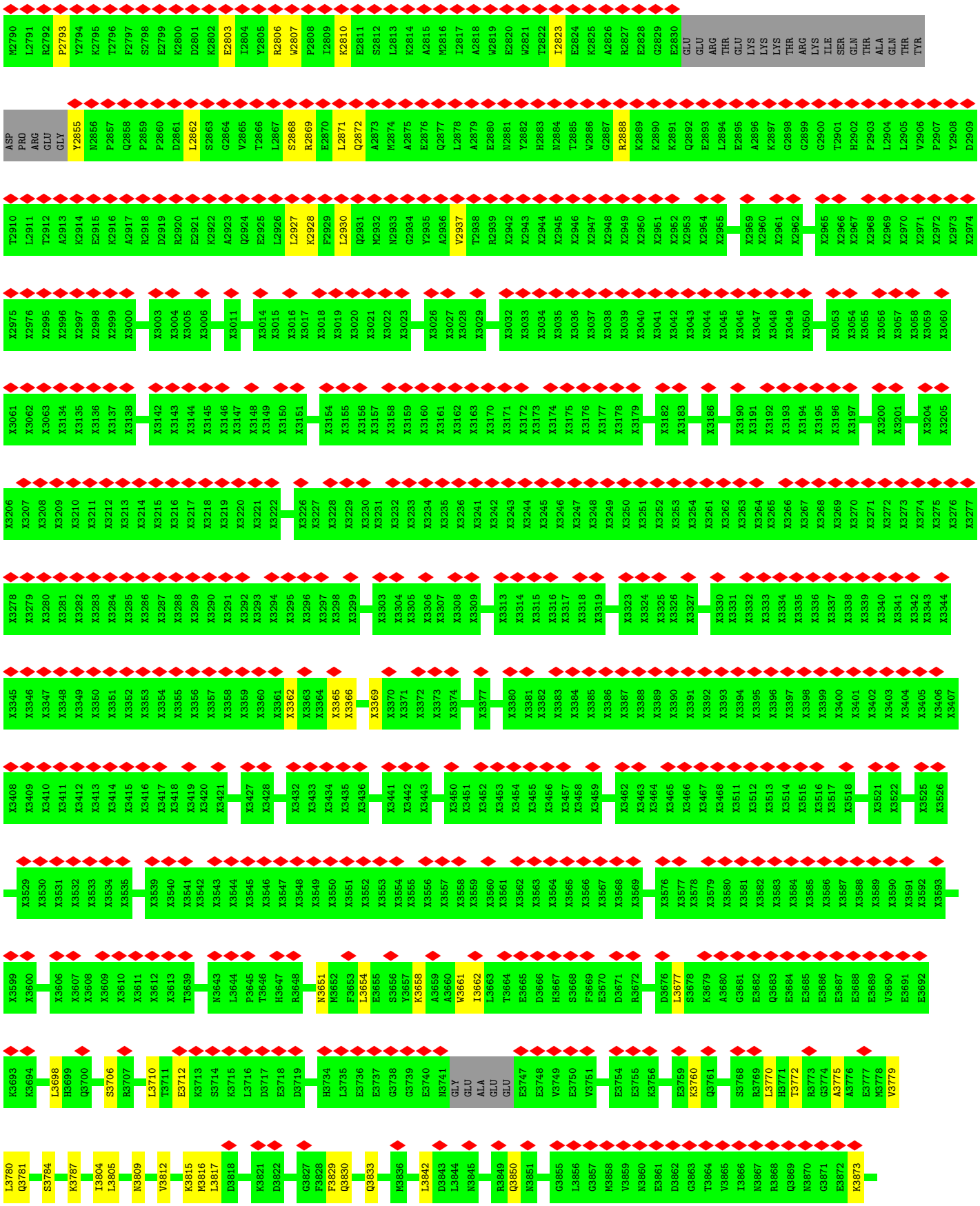
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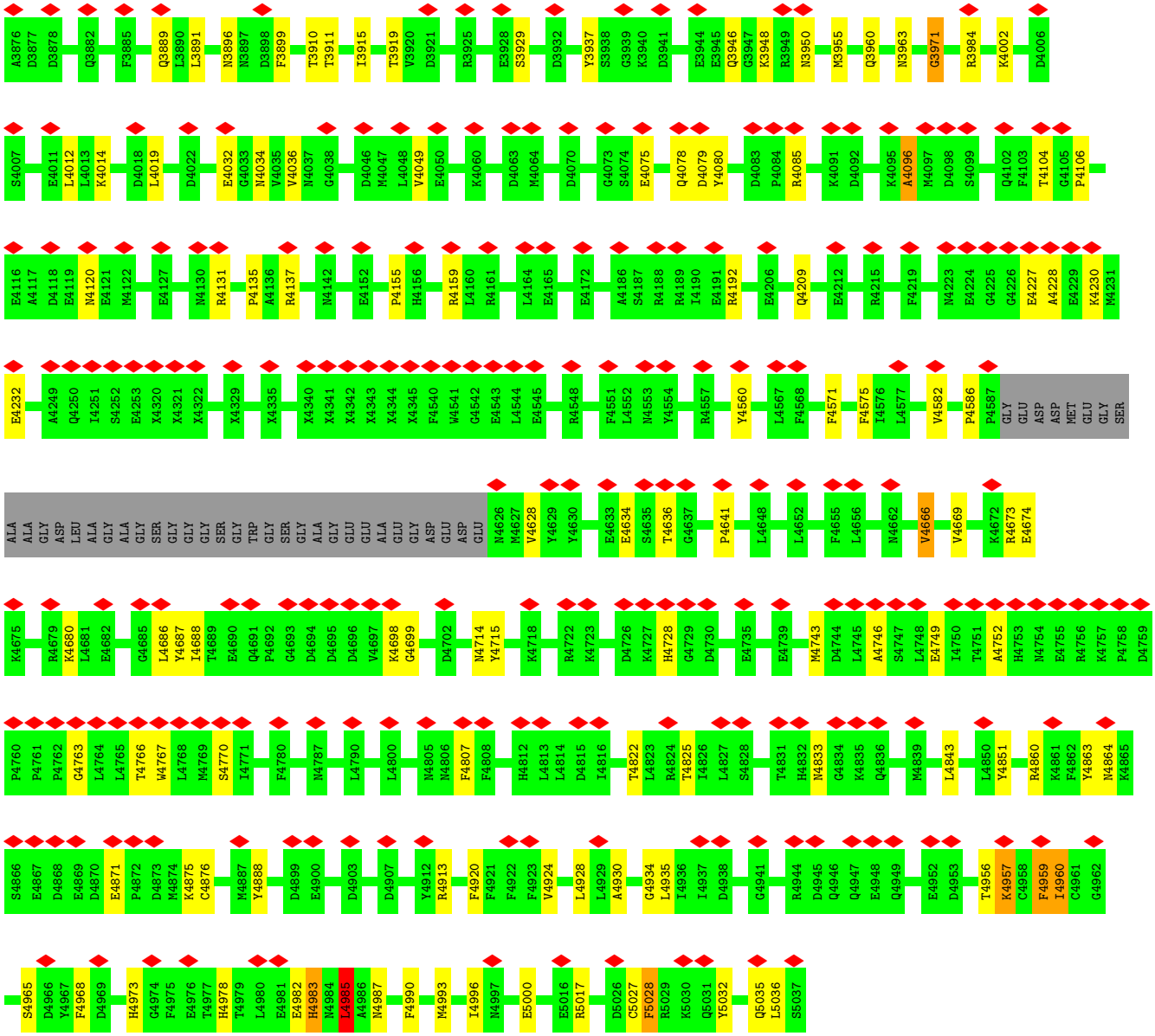

- Molecule 2: Ryanodine receptor 1

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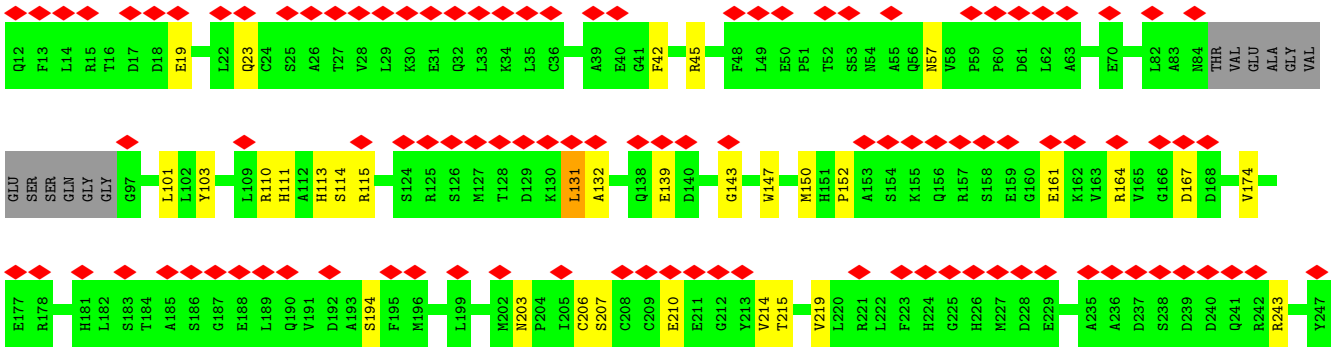

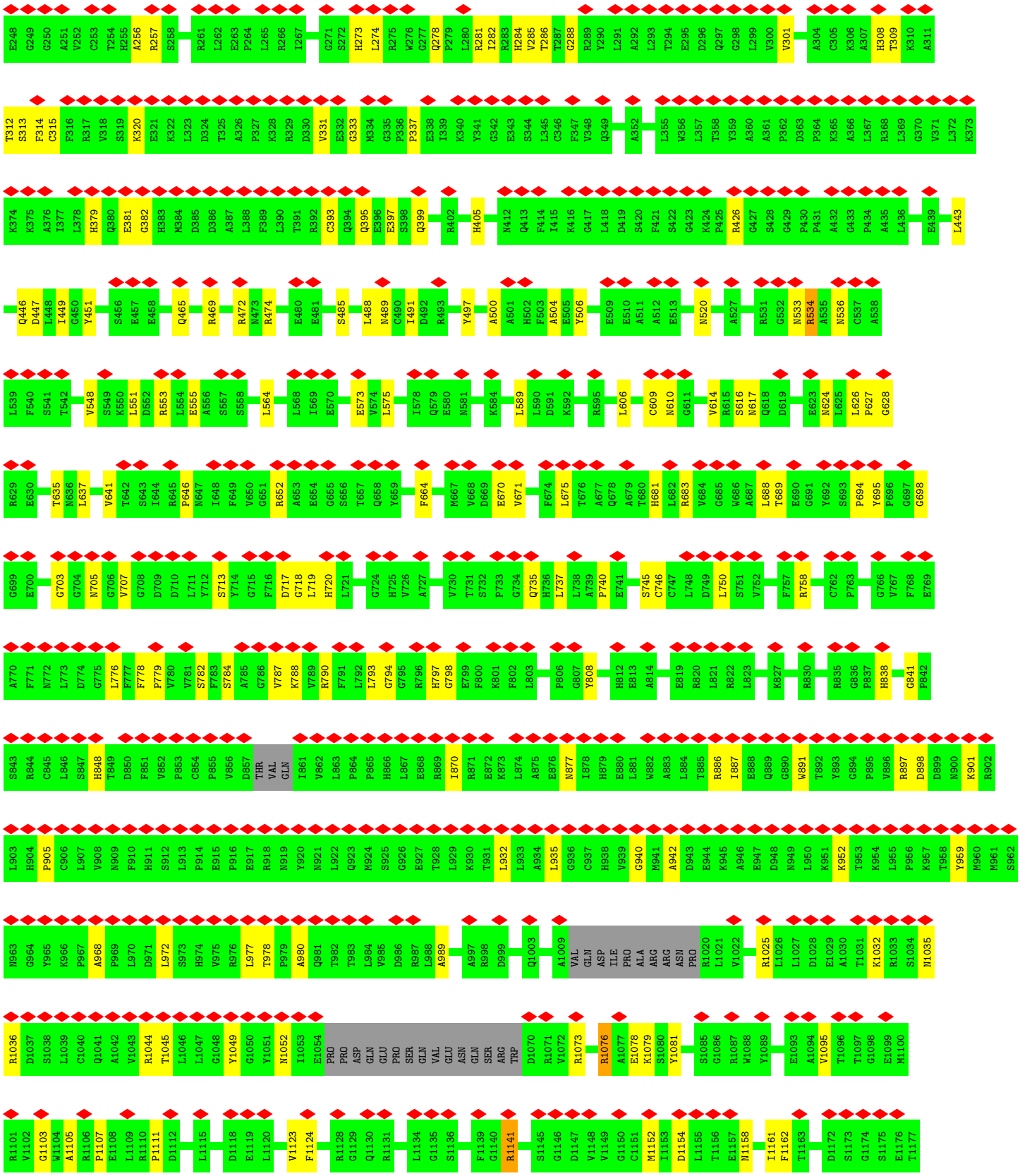
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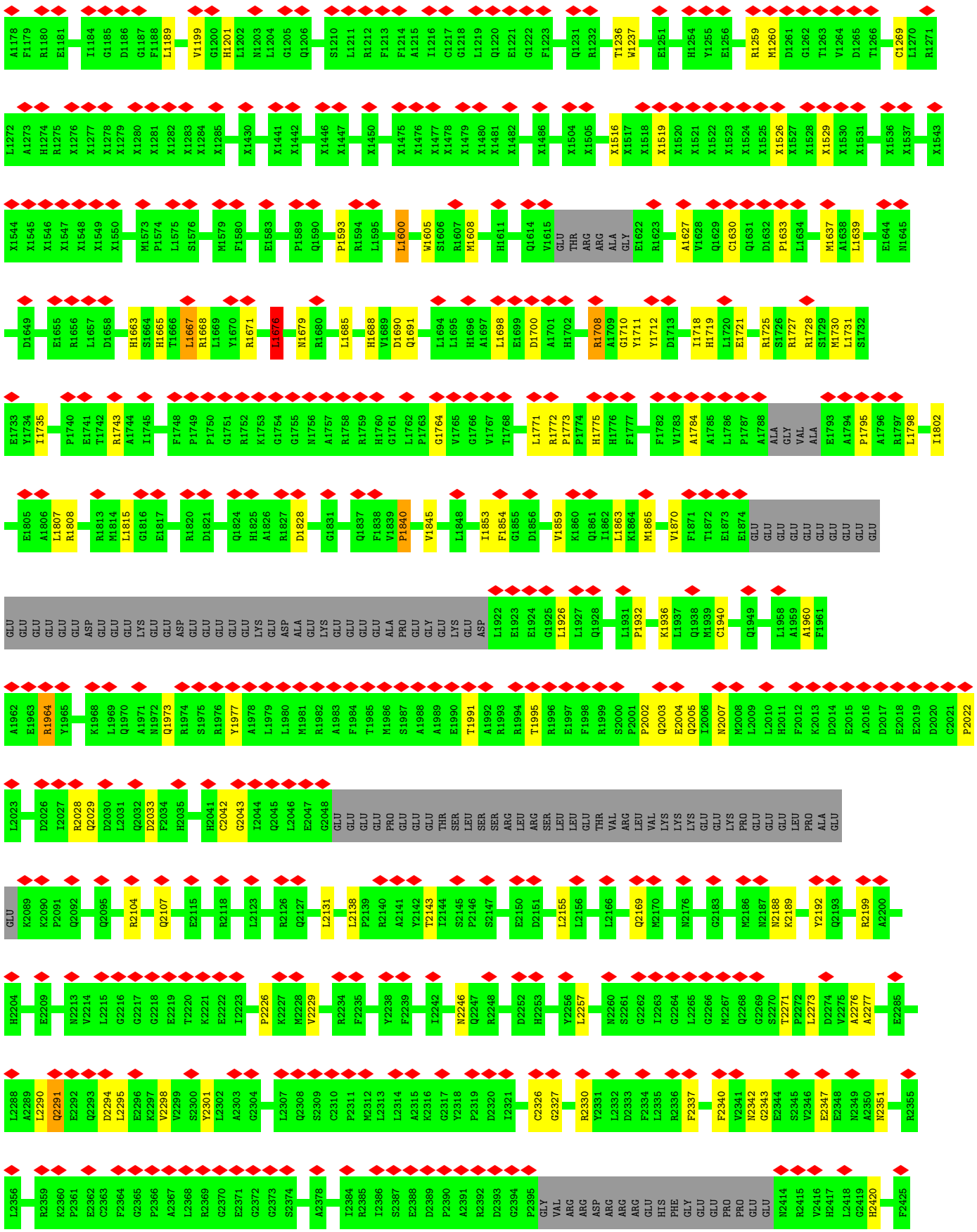
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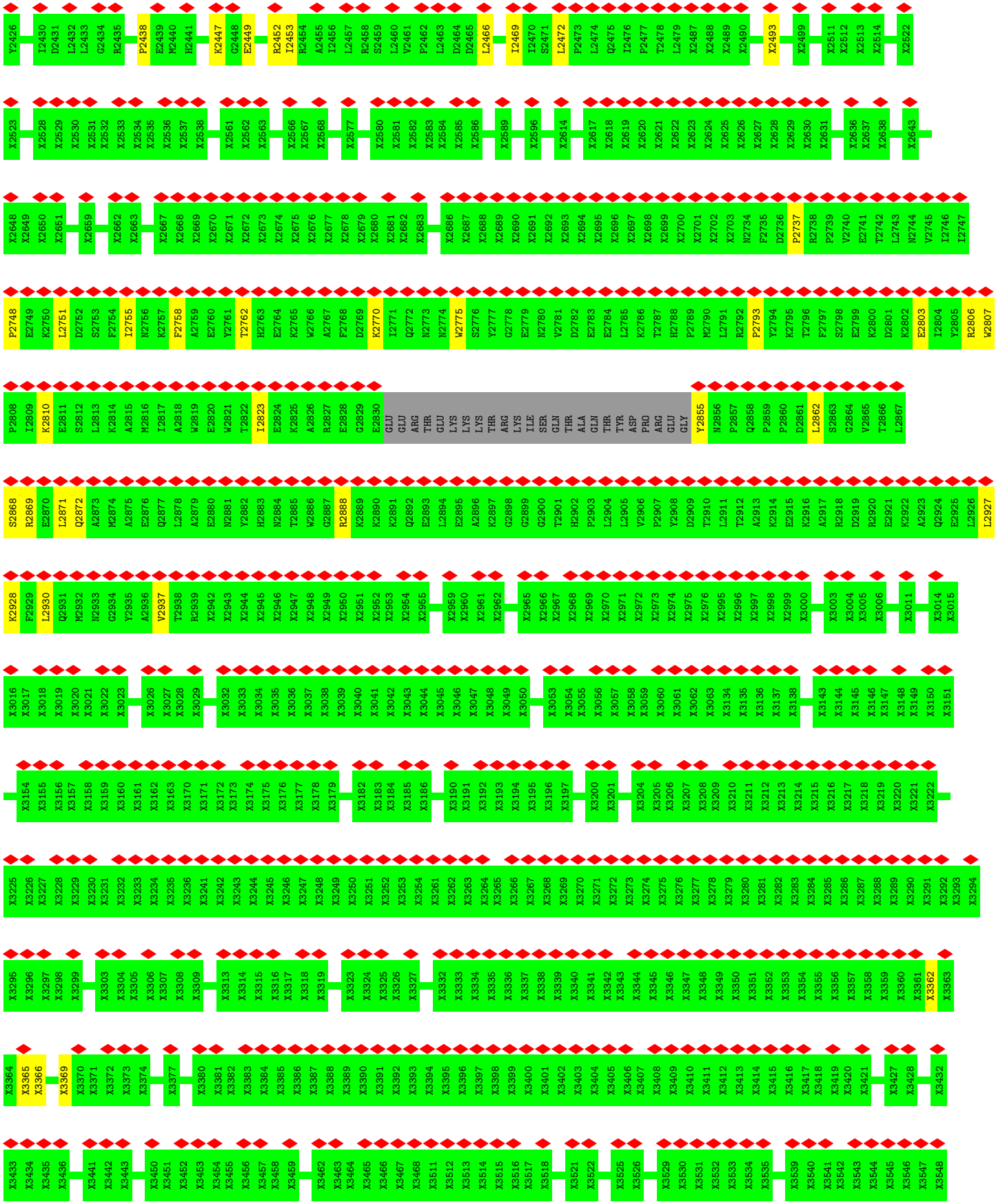
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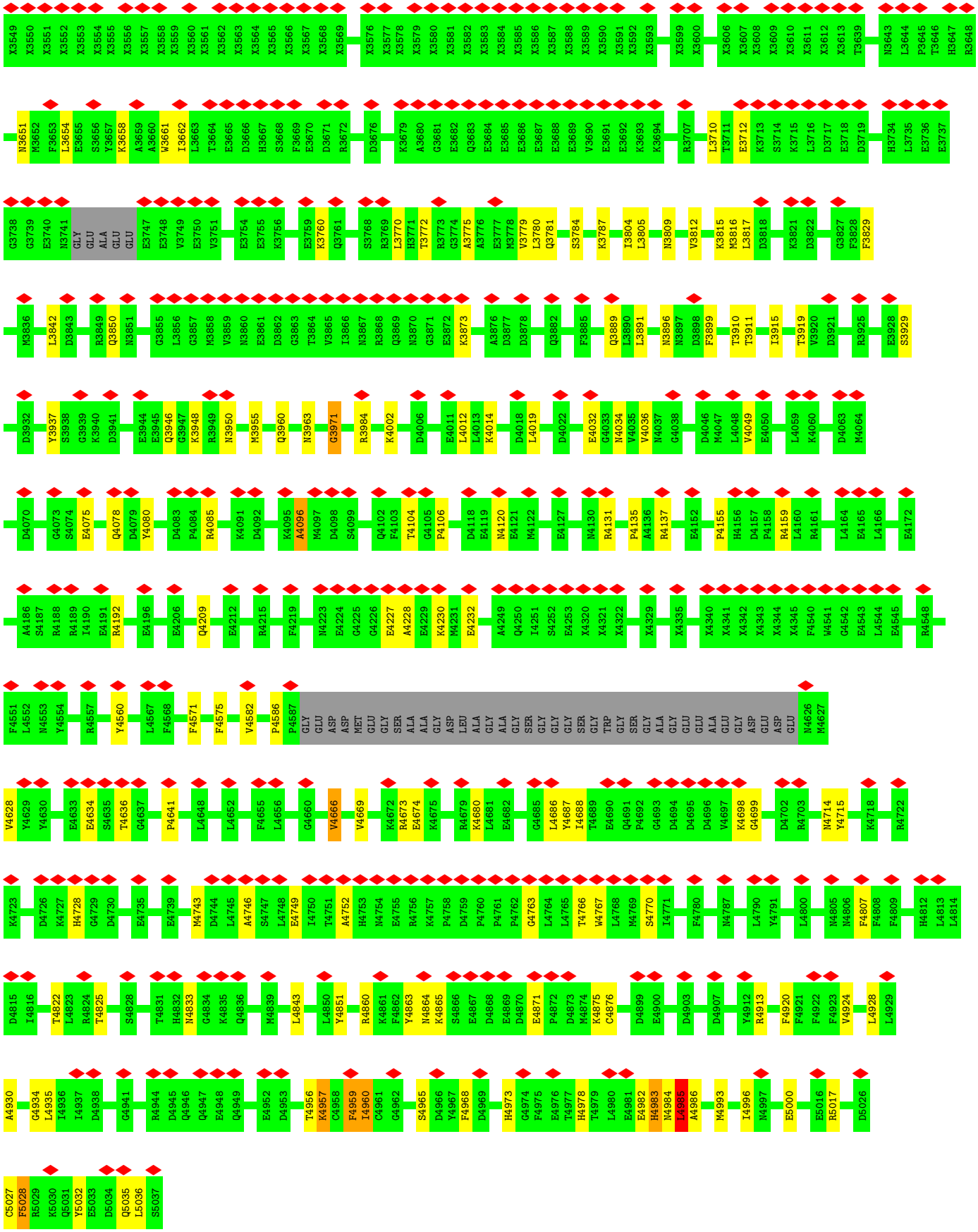
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- Molecule 2: Ryanodine receptor 1

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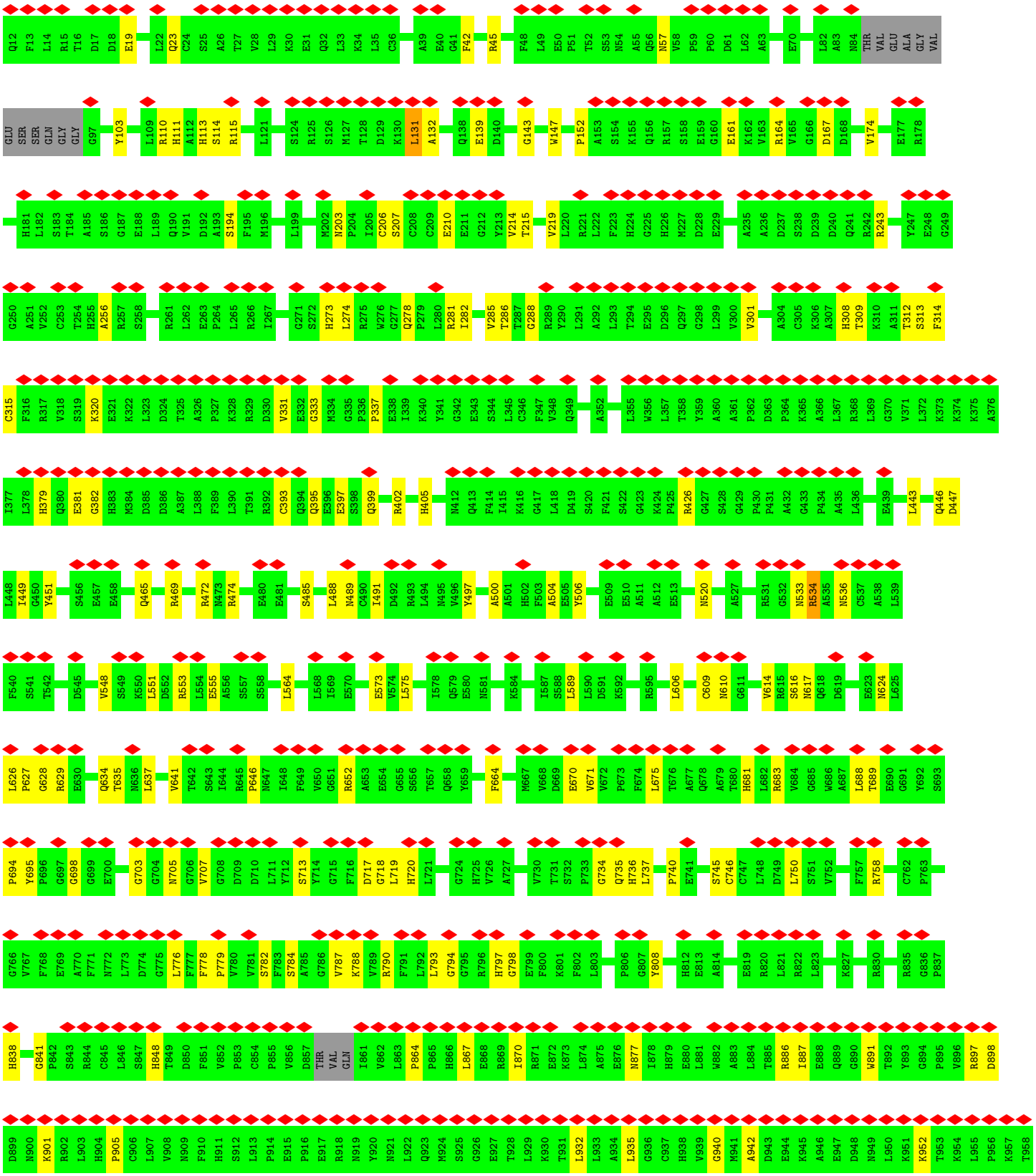

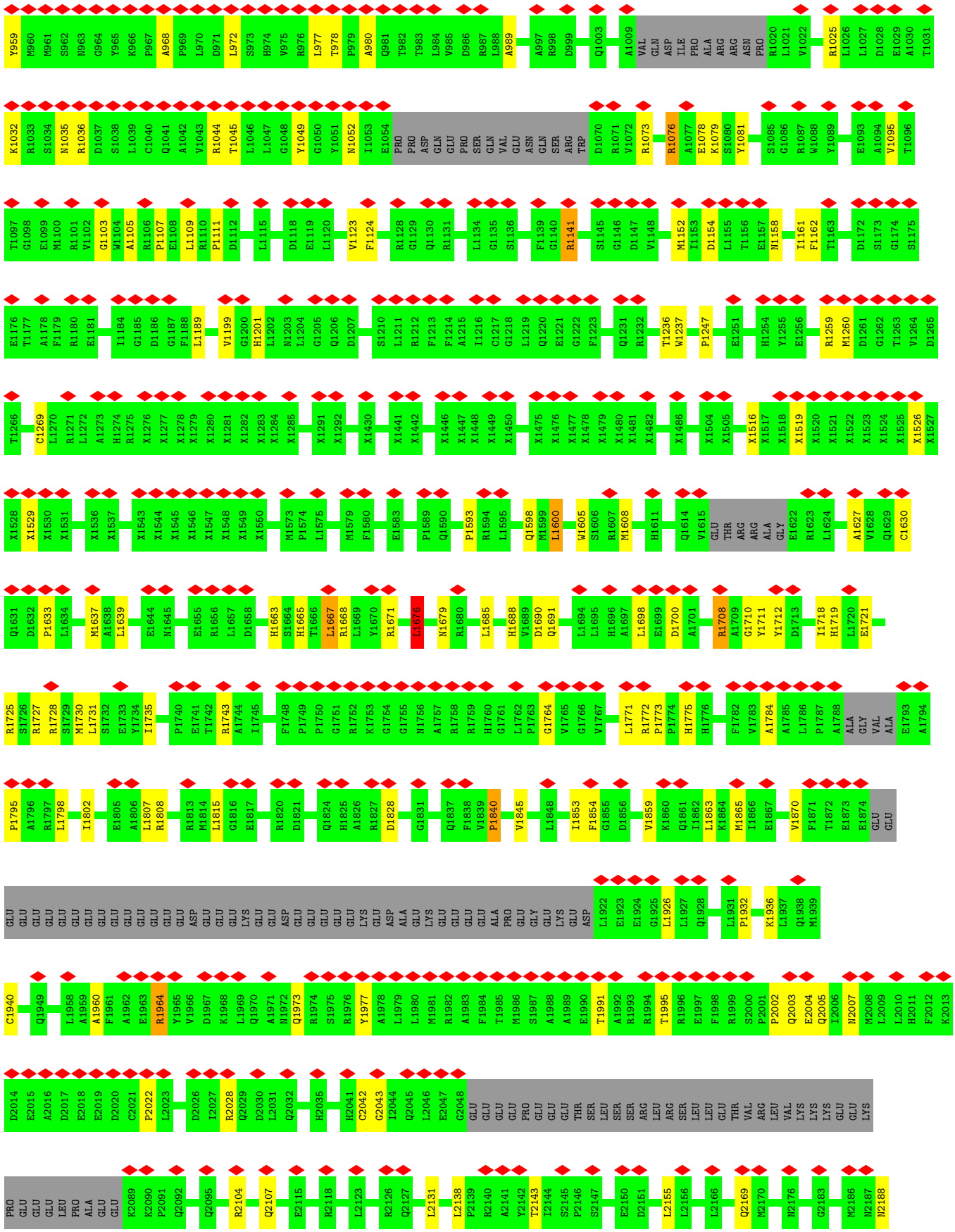
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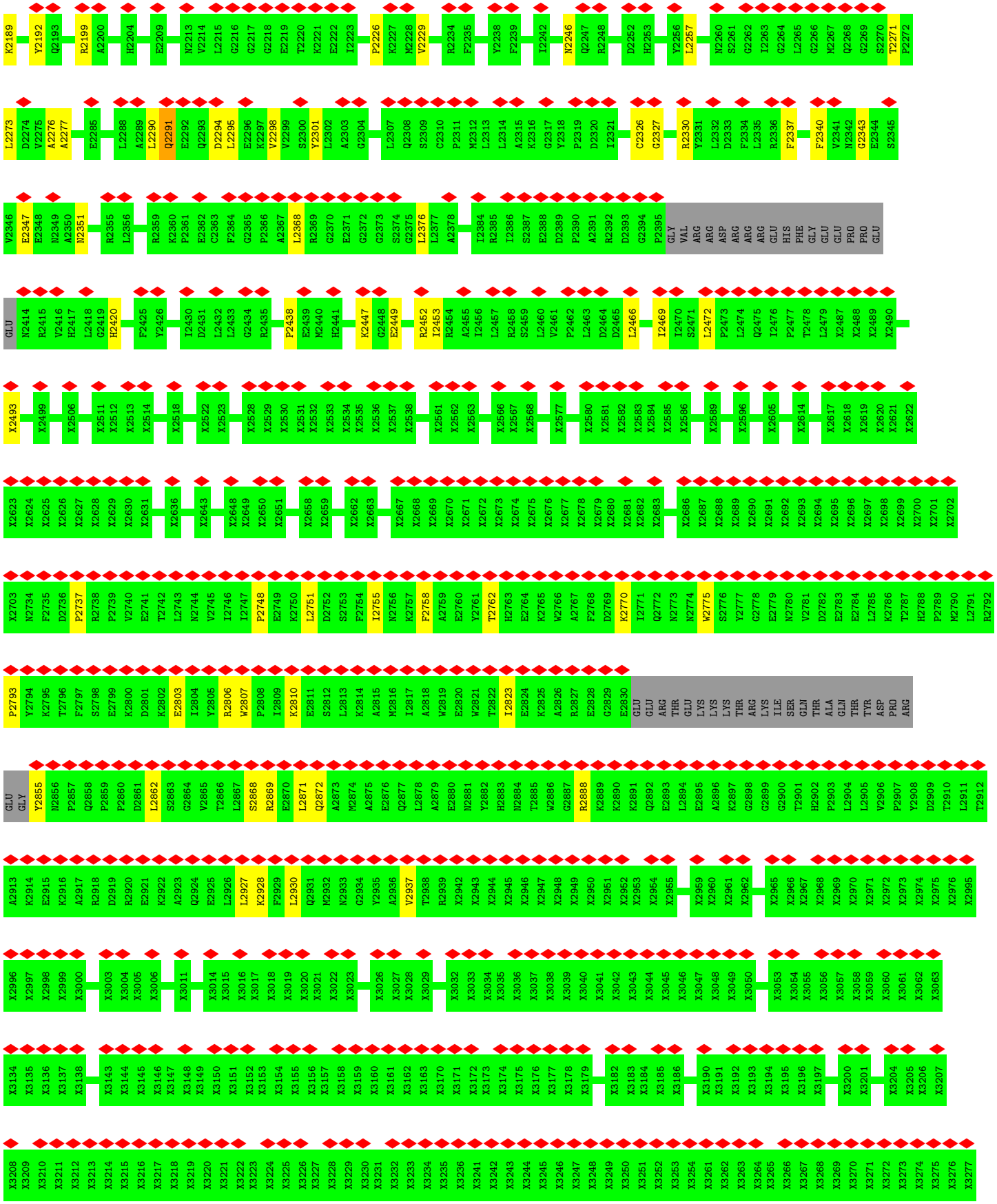
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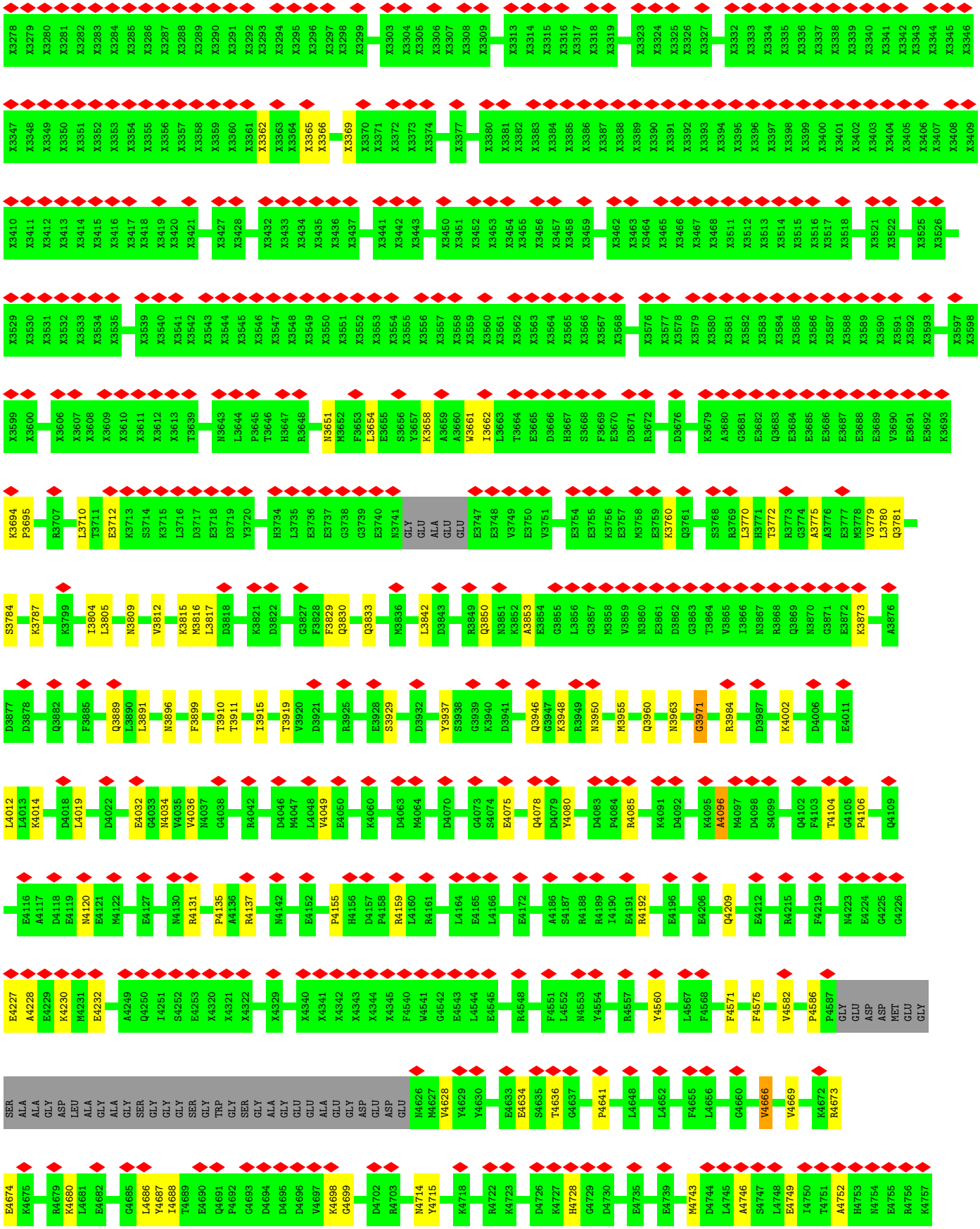
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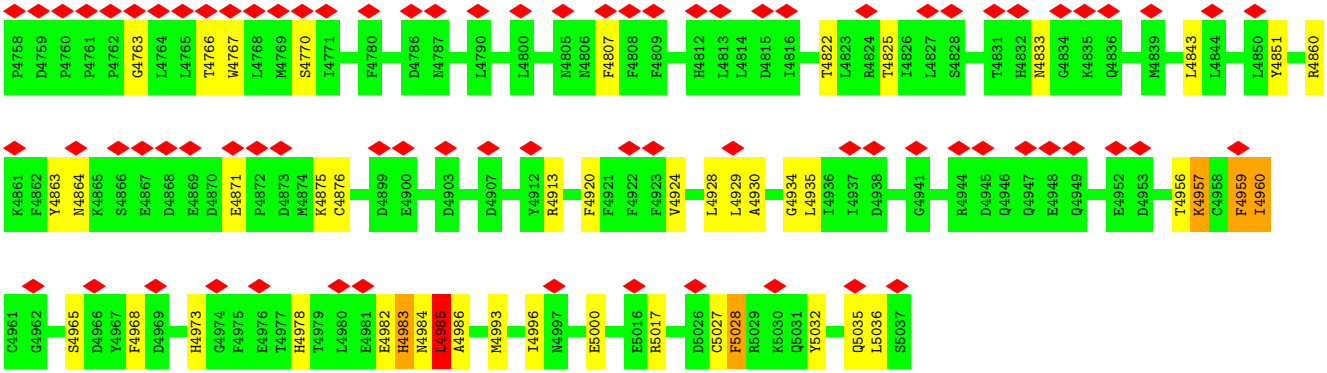
E4227 A4228 E4229 K4230 M4231 E4232 A4249 Q4250 I4251 S4252 E4253 X4320 X4321 X4322 X4329 X4340 X4341 X4342 X4343 X4344 X4345 F4540 W4541 G4542 E4543 L4544 E4545 R4548 F4551 L4552 N4553 Y4554 R4557 Y4560 L4567 F4568 F4571 F4575 V4582 P4586 P4587 GLY GLU ASP ASP MET GLU GLY
SER ALA ALA GLY ASP LEU ALA 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 P4641 L4648 L4652 F4655 L4656 G4660 V4666 V4669 K4672 R4673
E4674 K4675 R4679 K4680 L4681 E4682 G4685 L4686 Y4687 I4688 T4689 E4690 Q4691 P4692 G4693 D4694 D4695 D4696 V4697 K4698 G4699 D4702 R4703 N4714 Y4715 K4718 R4722 K4723 D4726 K4727 H4728 G4729 D4730 E4735 E4739 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
F4780
D4786 N4787
L4790
L4800
M4805 M4806 F4807 F4808 F4809
H4812 L4813 L4814 D4815 I4816
T4822 L4823 R4824 T4825 I4826 L4827 S4828
T4831 H4832 N4833 G4834 K4835 Q4836
M4839
L4843 L4844
L4850 Y4851
R4860
K4861 F4862 Y4863 N4864 K4865 S4866 E4867 D4868 E4869 D4870 E4871 P4872 D4873 M4874 K4875 C4876
D4899 E4900
D4903
D4907
Y4912 R4913
F4920 F4921 F4922 F4923 V4924
L4928 L4929 A4930
G4934 L4935 I4936 I4937 D4938
G4941
R4944 D4945 Q4946 Q4947 E4948 Q4949
E4952 D4953
T4956 K4957 C4958 F4959 I4960
C4961 G4962
S4965
D4966 Y4967 F4968 D4969
H4973 G4974 F4975 E4976 T4977 H4978 T4979 L4980 E4981 E4982 H4983 N4984 L4985 A4986
M4993
I4996 N4997
E5000
E5016 R5017
D5026 C5027 F5028 R5029 K5030 Q5031 Y5032
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	0.070	Depositor
Minimum map value	-0.034	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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.32	0/834	0.53	0/1123
1	F	0.32	0/834	0.53	0/1123
1	H	0.32	0/834	0.53	0/1123
1	J	0.32	0/834	0.53	0/1123
2	B	0.31	0/25428	0.55	8/34534 (0.0%)
2	E	0.31	0/25428	0.55	8/34534 (0.0%)
2	G	0.31	0/25428	0.55	8/34534 (0.0%)
2	I	0.31	0/25428	0.55	8/34534 (0.0%)
All	All	0.31	0/105048	0.55	32/142628 (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
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	18
2	E	0	18
2	G	0	18
2	I	0	18
All	All	0	76

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	131	LEU	CA-CB-CG	8.10	133.92	115.30
2	B	131	LEU	CA-CB-CG	8.09	133.90	115.30
2	E	131	LEU	CA-CB-CG	8.09	133.90	115.30
2	G	131	LEU	CA-CB-CG	8.09	133.90	115.30
2	I	4985	LEU	CA-CB-CG	6.89	131.16	115.30

There are no chirality outliers.

5 of 76 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
1	F	8	SER	Peptide
1	H	8	SER	Peptide
1	J	8	SER	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	12	0
1	F	818	0	824	12	0
1	H	818	0	824	12	0
1	J	818	0	824	12	0
2	B	29499	0	24753	296	0
2	E	29499	0	24753	305	0
2	G	29499	0	24753	299	0
2	I	29499	0	24753	295	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	1	0
4	E	14	0	10	1	0
4	G	14	0	10	1	0
4	I	14	0	10	1	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	1	0	0	0	0
5	I	1	0	0	0	0
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	102396	1213	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 1213 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:5028:PHE:CE1	2:E:5032:TYR:CD2	2.32	1.18
2:B:5028:PHE:CE1	2:B:5032:TYR:CD2	2.32	1.17
2:G:5028:PHE:CE1	2:G:5032:TYR:CD2	2.32	1.17
2:I:5028:PHE:CE1	2:I:5032:TYR:CD2	2.32	1.16
2:E:5028:PHE:HE1	2:E:5032:TYR:CE2	1.64	1.16

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%)	339 (10%)	6 (0%)	47 81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	3235/4416 (73%)	2894 (90%)	335 (10%)	6 (0%)	47	81
2	G	3235/4416 (73%)	2890 (89%)	339 (10%)	6 (0%)	47	81
2	I	3235/4416 (73%)	2891 (89%)	338 (10%)	6 (0%)	47	81
All	All	13360/18096 (74%)	11941 (89%)	1395 (10%)	24 (0%)	50	81

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE
2	E	5028	PHE
2	I	5028	PHE
2	G	5028	PHE
2	B	1708	ARG

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%)	2473 (99%)	20 (1%)	81	89
2	E	2493/3022 (82%)	2473 (99%)	20 (1%)	81	89
2	G	2493/3022 (82%)	2473 (99%)	20 (1%)	81	89
2	I	2493/3022 (82%)	2473 (99%)	20 (1%)	81	89
All	All	10324/12444 (83%)	10244 (99%)	80 (1%)	82	89

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	4959	PHE

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Mol	Chain	Res	Type
2	G	4085	ARG
2	I	4983	HIS
2	G	1600	LEU
2	G	4913	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 149 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	111	HIS
2	G	4120	ASN
2	G	383	HIS
2	G	1719	HIS
2	E	379	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	G	5101	-	26,33,33	0.84	1 (3%)	31,52,52	1.56	6 (19%)
3	ATP	E	5101	-	26,33,33	0.85	1 (3%)	31,52,52	1.55	6 (19%)
4	CFF	I	5102	-	8,15,15	2.48	3 (37%)	8,23,23	1.23	1 (12%)
4	CFF	G	5102	-	8,15,15	2.49	3 (37%)	8,23,23	1.24	1 (12%)
3	ATP	I	5101	-	26,33,33	0.84	1 (3%)	31,52,52	1.55	6 (19%)
4	CFF	B	5102	-	8,15,15	2.49	3 (37%)	8,23,23	1.24	1 (12%)
4	CFF	E	5102	-	8,15,15	2.50	3 (37%)	8,23,23	1.23	1 (12%)
3	ATP	B	5101	-	26,33,33	0.84	1 (3%)	31,52,52	1.55	6 (19%)

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	G	5101	-	-	4/18/38/38	0/3/3/3
3	ATP	E	5101	-	-	4/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	-	0/2/2/2
4	CFF	G	5102	-	-	-	0/2/2/2
3	ATP	I	5101	-	-	4/18/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
4	CFF	E	5102	-	-	-	0/2/2/2
3	ATP	B	5101	-	-	4/18/38/38	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5102	CFF	C5-C4	-4.67	1.33	1.39
4	B	5102	CFF	C5-C4	-4.60	1.33	1.39
4	I	5102	CFF	C5-C4	-4.60	1.33	1.39
4	G	5102	CFF	C5-C4	-4.60	1.33	1.39
4	E	5102	CFF	C6-N1	-3.99	1.32	1.38

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	5101	ATP	PB-O3B-PG	-3.60	120.46	132.83
3	E	5101	ATP	PB-O3B-PG	-3.60	120.47	132.83
3	G	5101	ATP	PB-O3B-PG	-3.60	120.48	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	5101	ATP	PB-O3B-PG	-3.60	120.48	132.83
3	G	5101	ATP	N3-C2-N1	-3.48	123.24	128.68

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

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

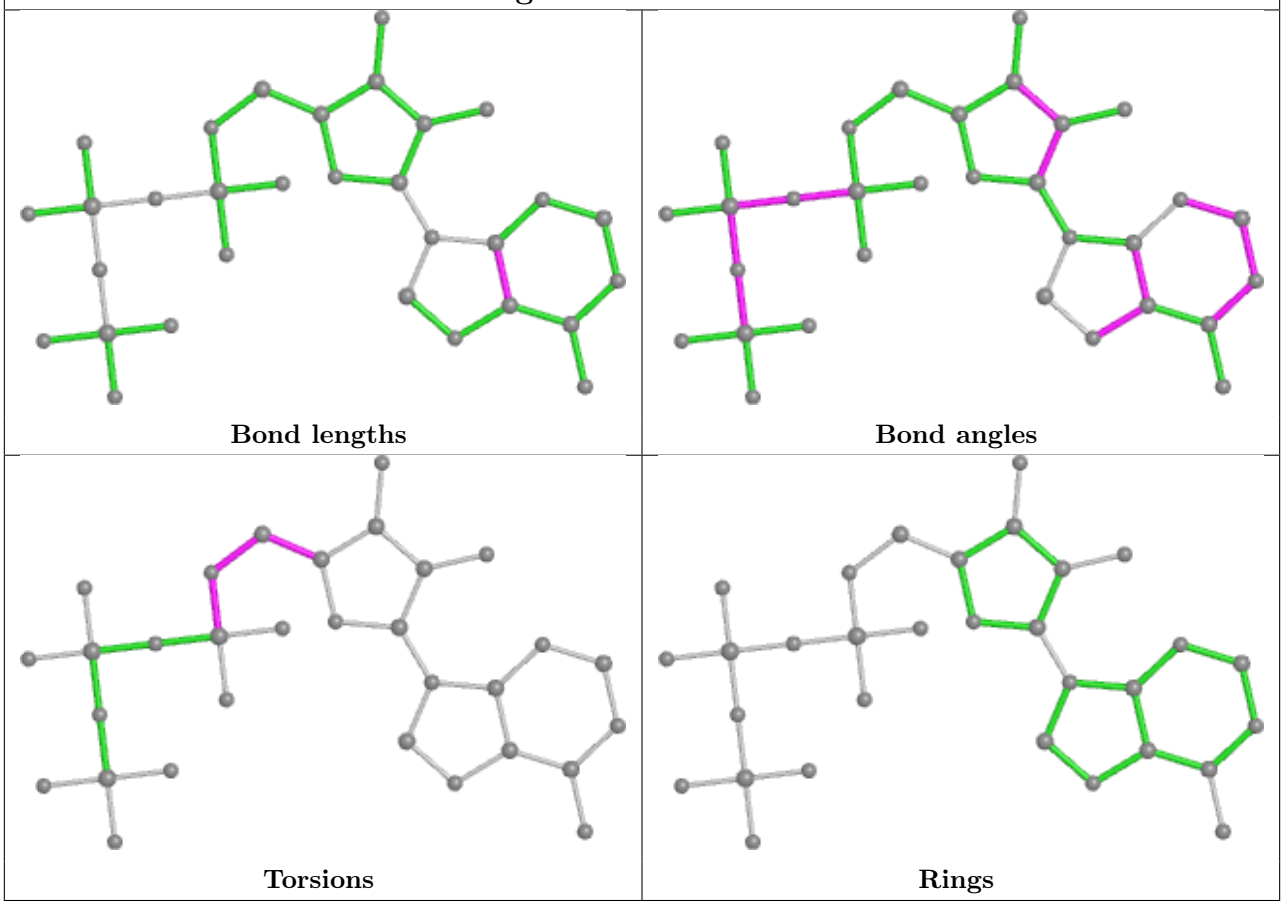
There are no ring outliers.

8 monomers are involved in 8 short contacts:

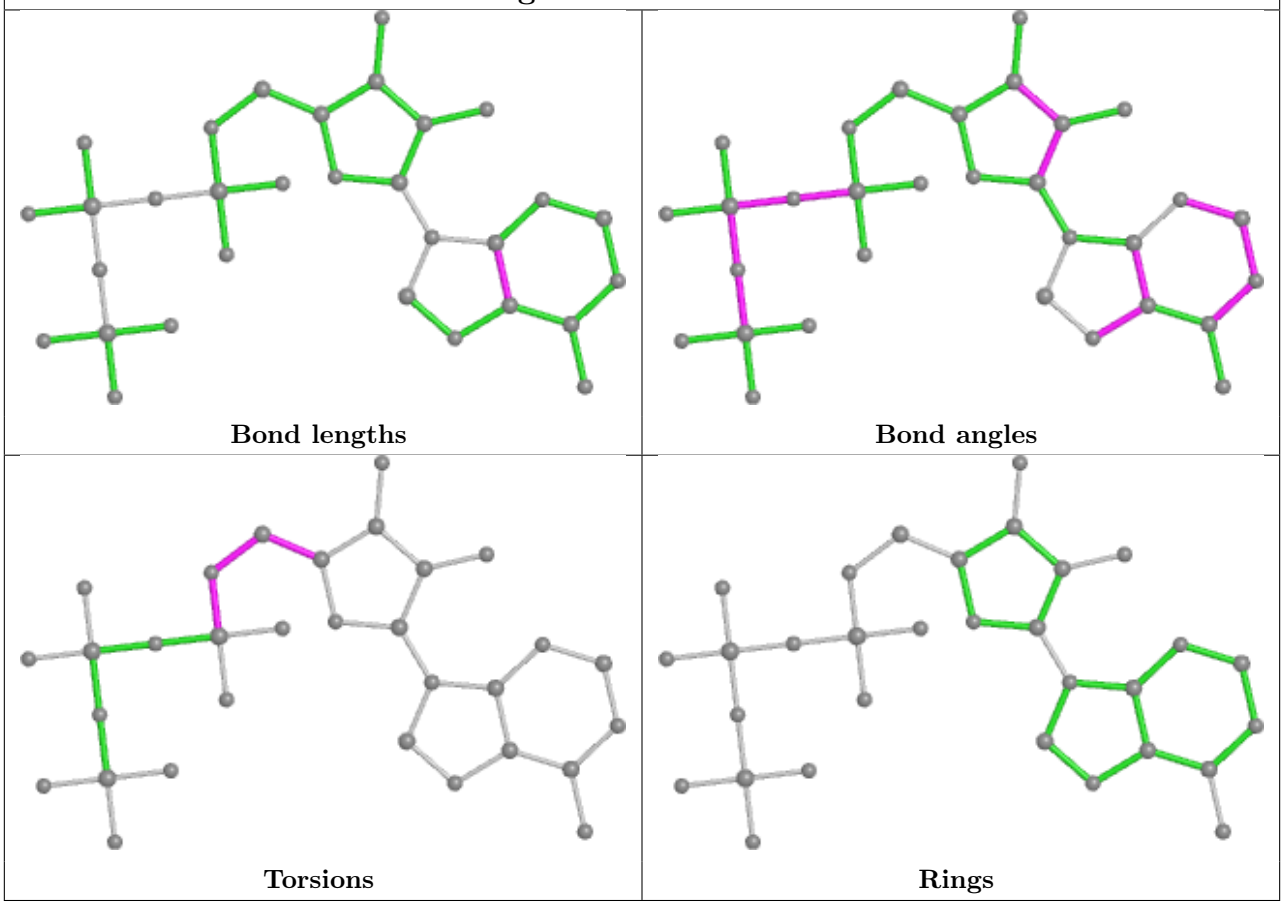
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	5101	ATP	1	0
3	E	5101	ATP	1	0
4	I	5102	CFF	1	0
4	G	5102	CFF	1	0
3	I	5101	ATP	1	0
4	B	5102	CFF	1	0
4	E	5102	CFF	1	0
3	B	5101	ATP	1	0

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.

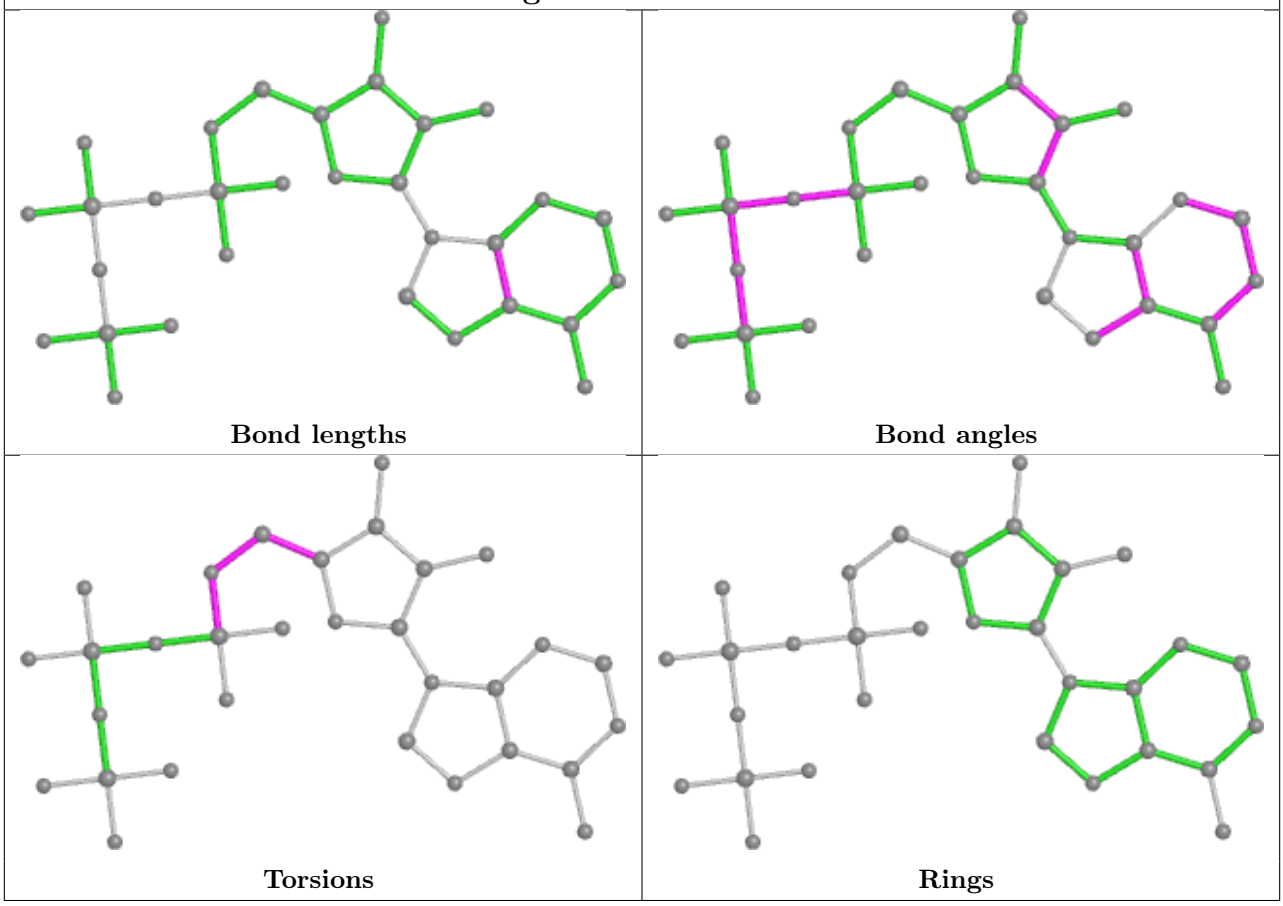
Ligand ATP G 5101



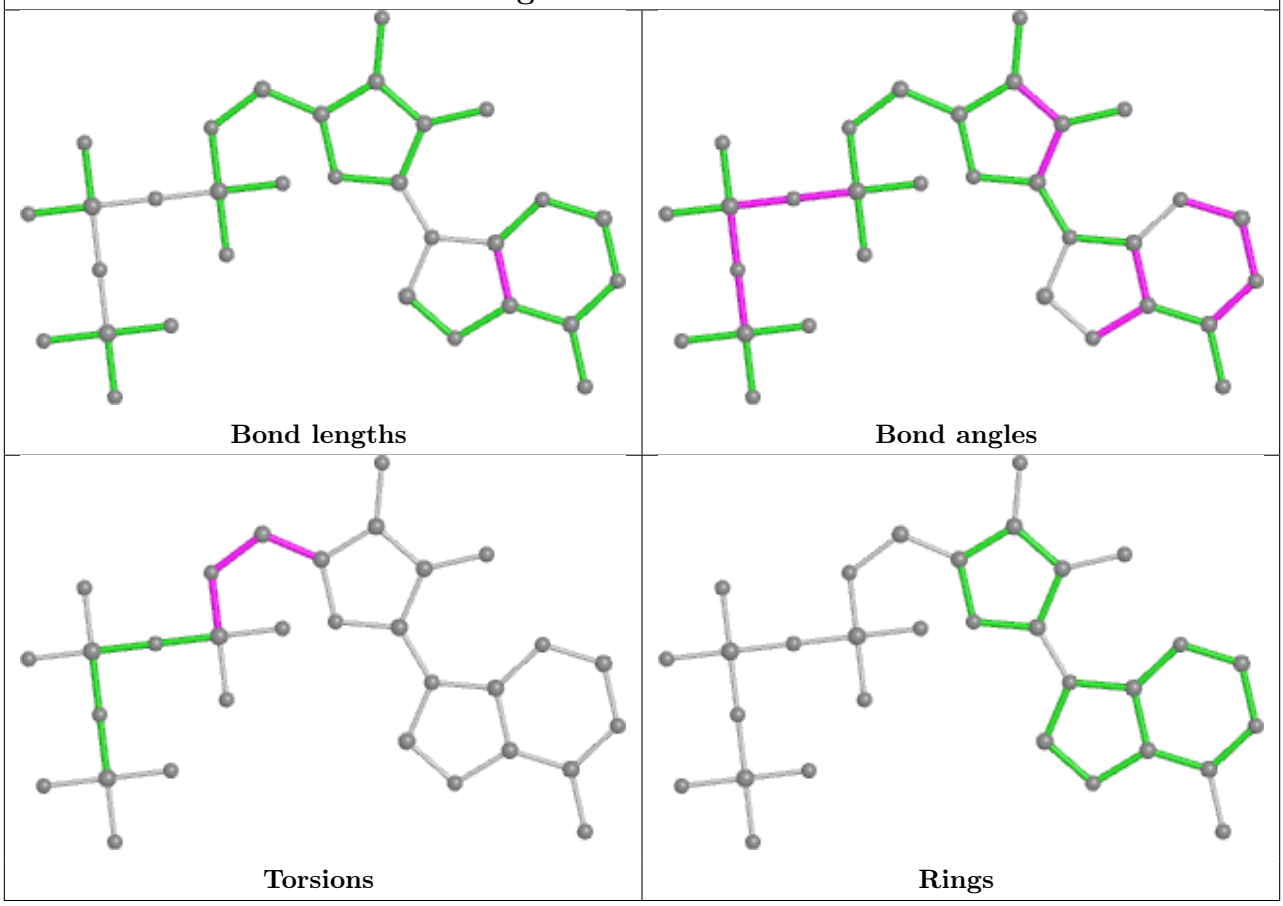
Ligand ATP E 5101



Ligand ATP I 5101



Ligand ATP B 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	E	14
2	I	14
2	G	14

The worst 5 of 56 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	72.44
1	E	4345:UNK	C	4540:PHE	N	72.44

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	72.44
1	G	4345:UNK	C	4540:PHE	N	72.44
1	B	3613:UNK	C	3639:THR	N	42.93

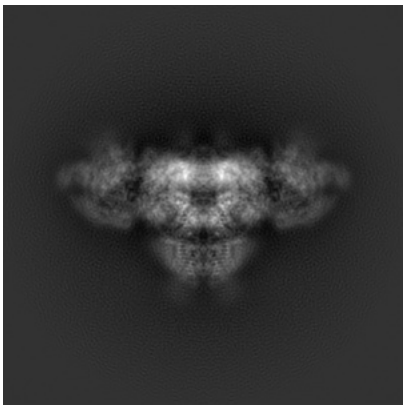
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8380. These allow visual inspection of the internal detail of the map and identification of artifacts.

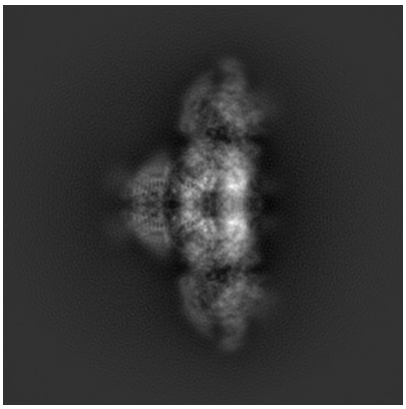
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



X



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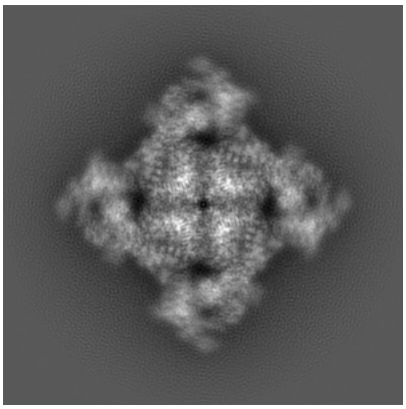
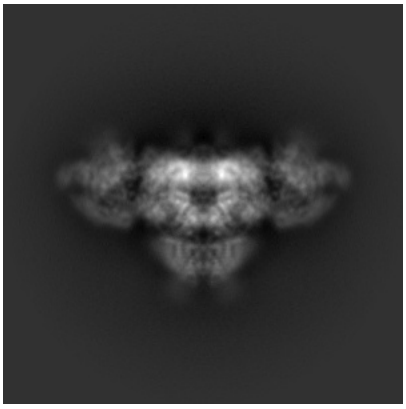


Z

6.1.2 Raw map



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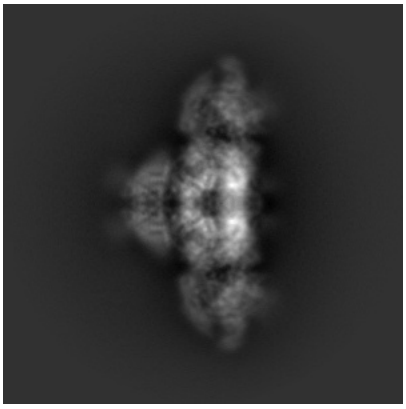
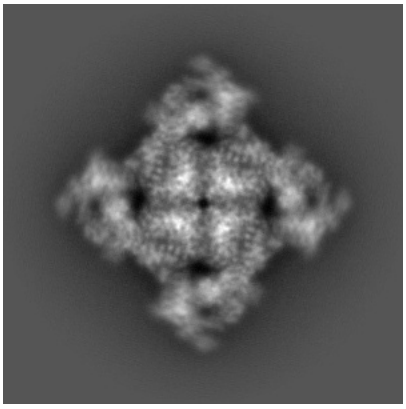


Y

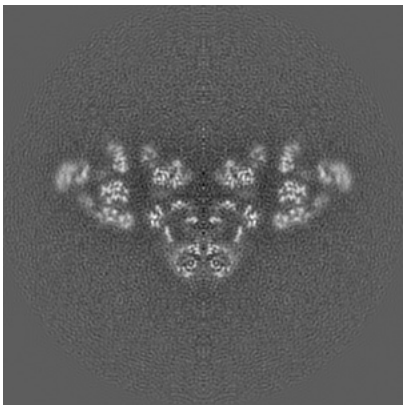


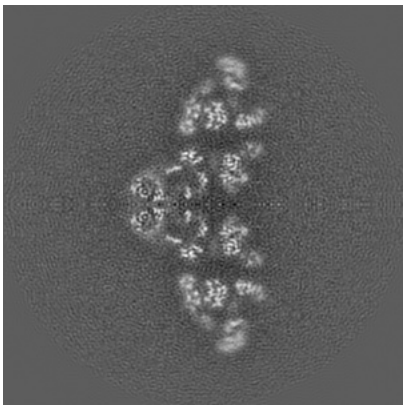
Z

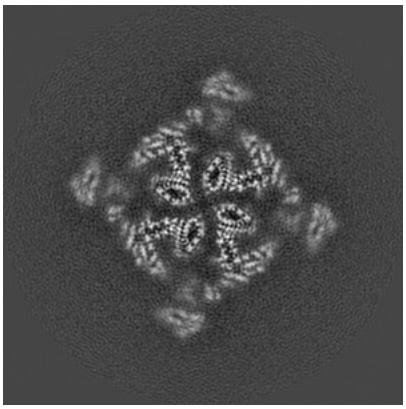
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

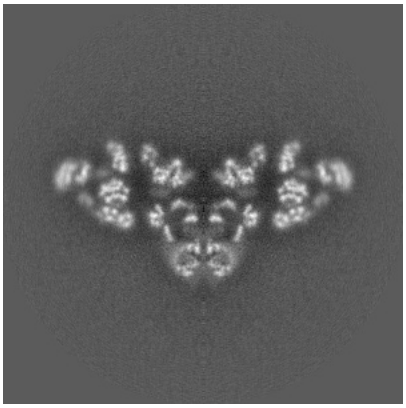
6.2.1 Primary map

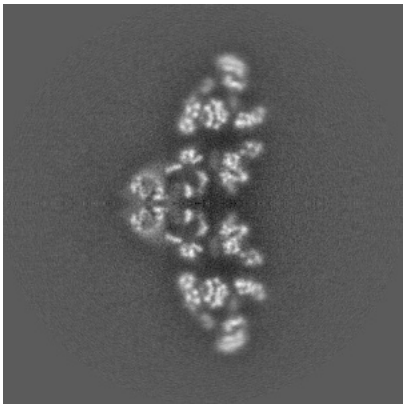

X Index: 200

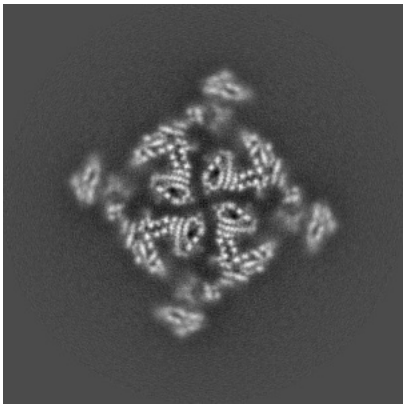

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

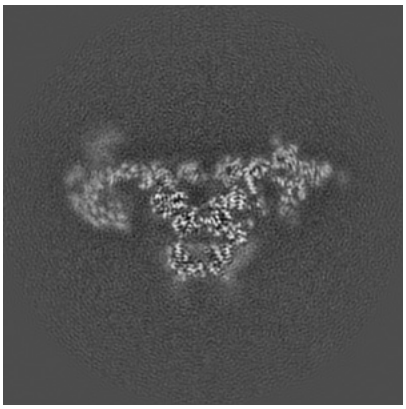

Y Index: 200


Z Index: 200

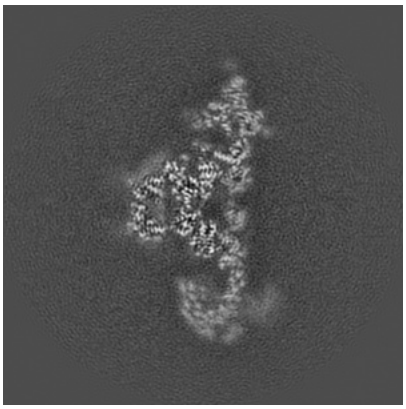
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

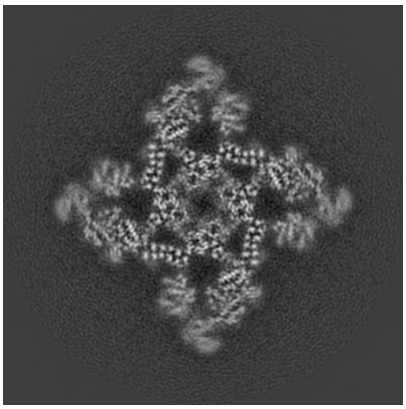
6.3.1 Primary map



X Index: 183

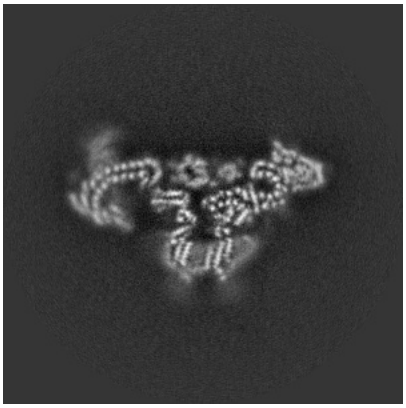


Y Index: 217

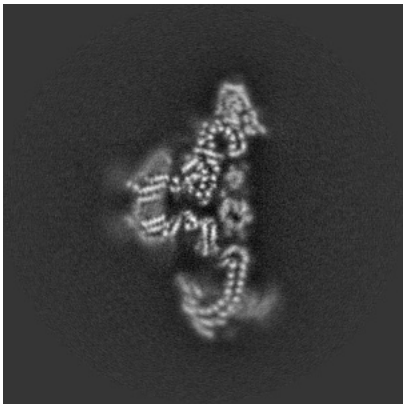


Z Index: 226

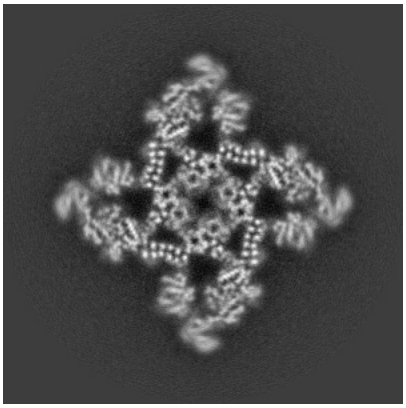
6.3.2 Raw map



X Index: 176



Y Index: 224

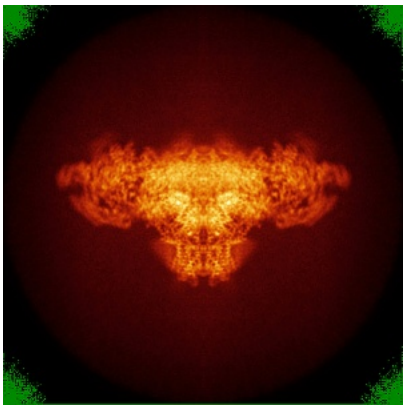


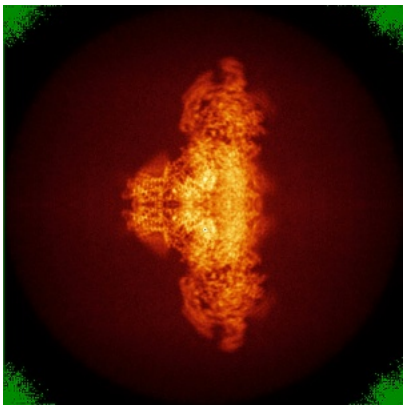
Z Index: 226

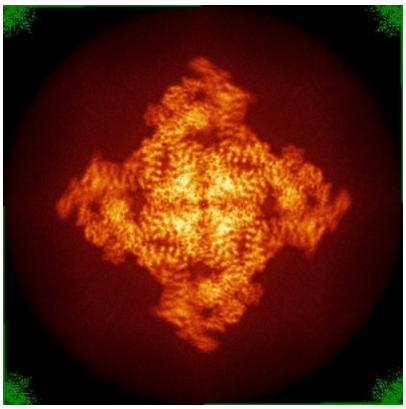
The images above show the largest variance slices of the map in three orthogonal directions.

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

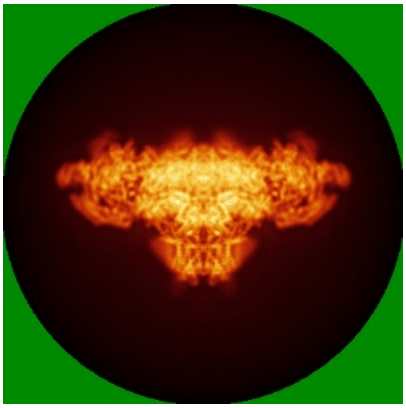
6.4.1 Primary map

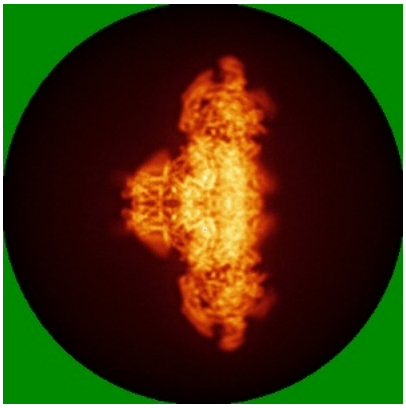

X

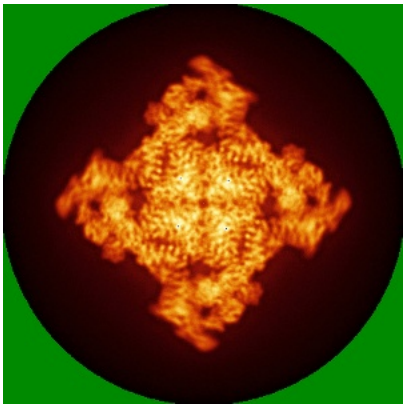

Y


Z

6.4.2 Raw map


X

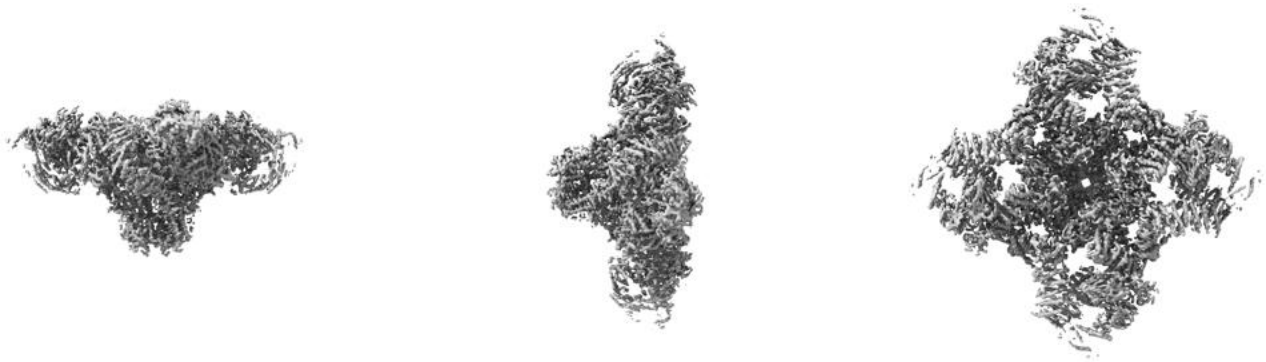

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

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

6.5.2 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.

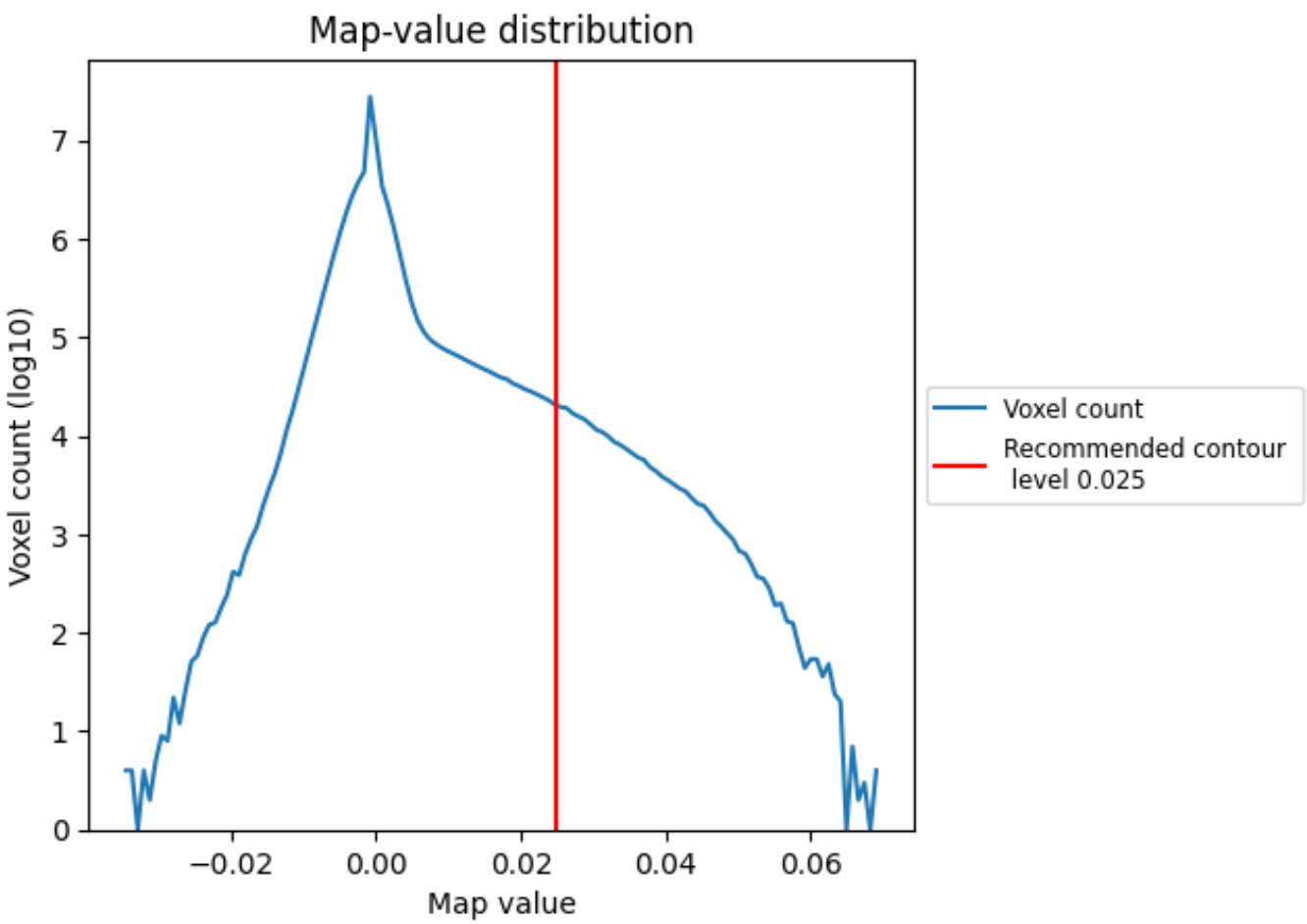
6.6 Mask visualisation (i)

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

7 Map analysis (i)

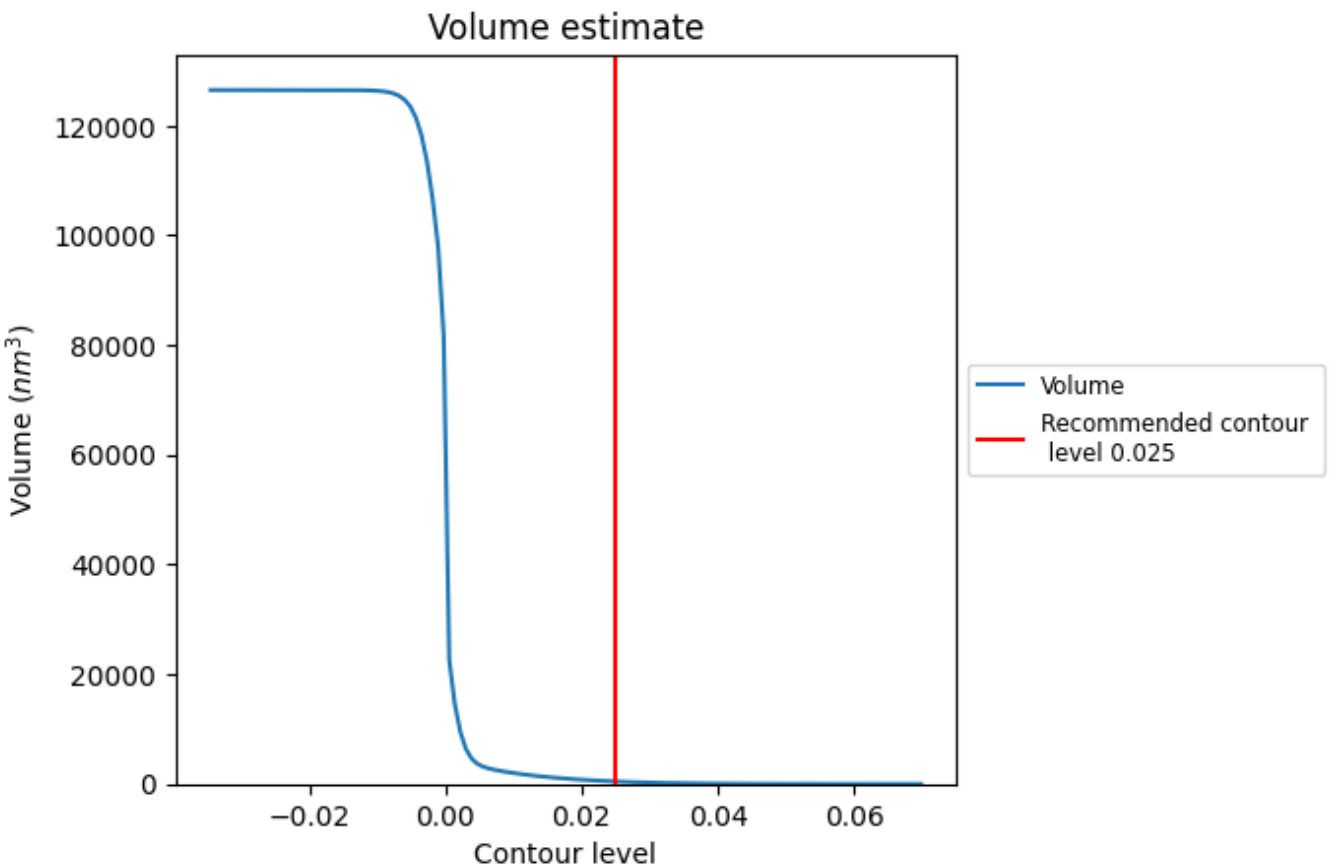
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

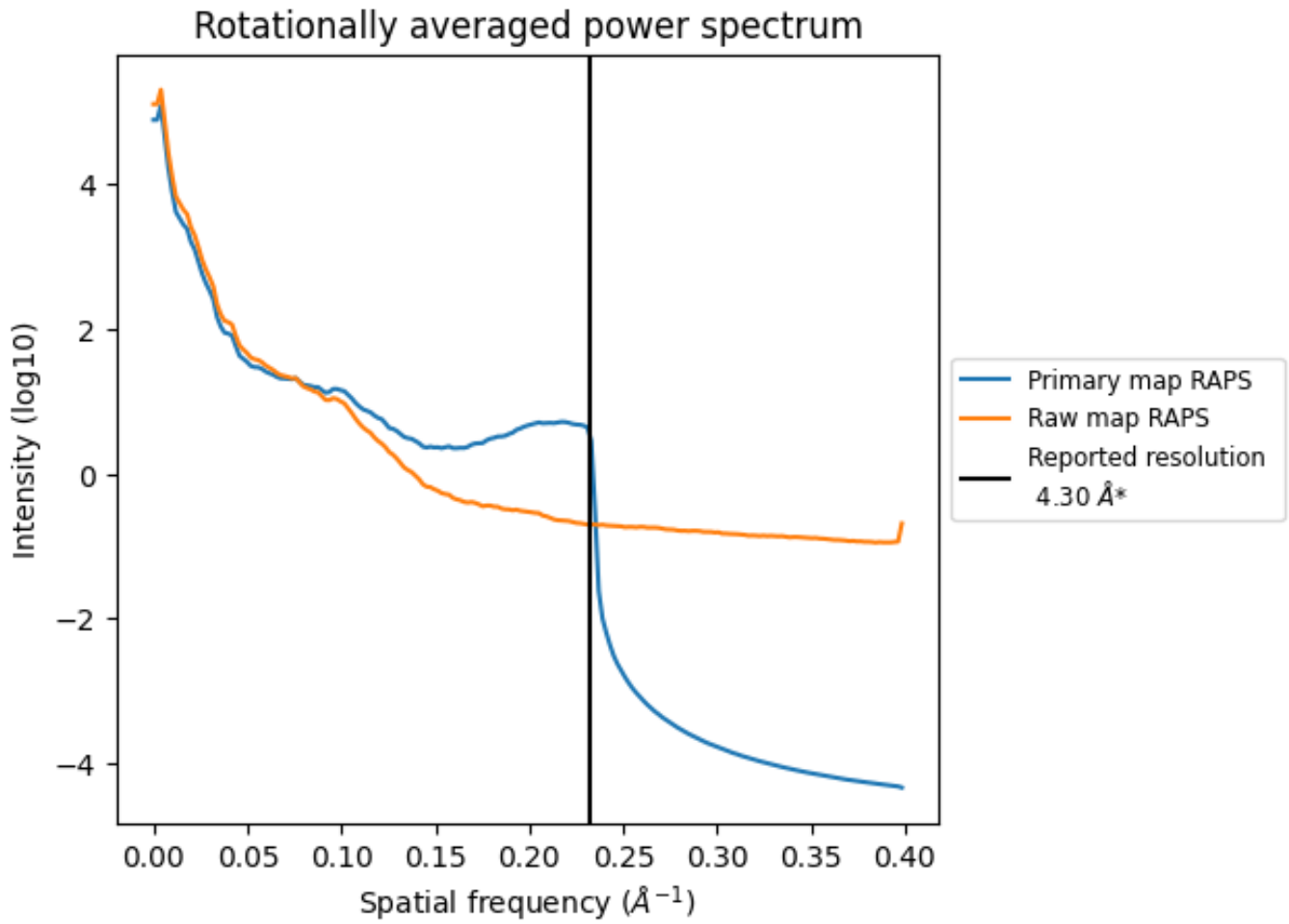
7.2 Volume estimate (i)



The volume at the recommended contour level is 452 nm^3; this corresponds to an approximate mass of 408 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)

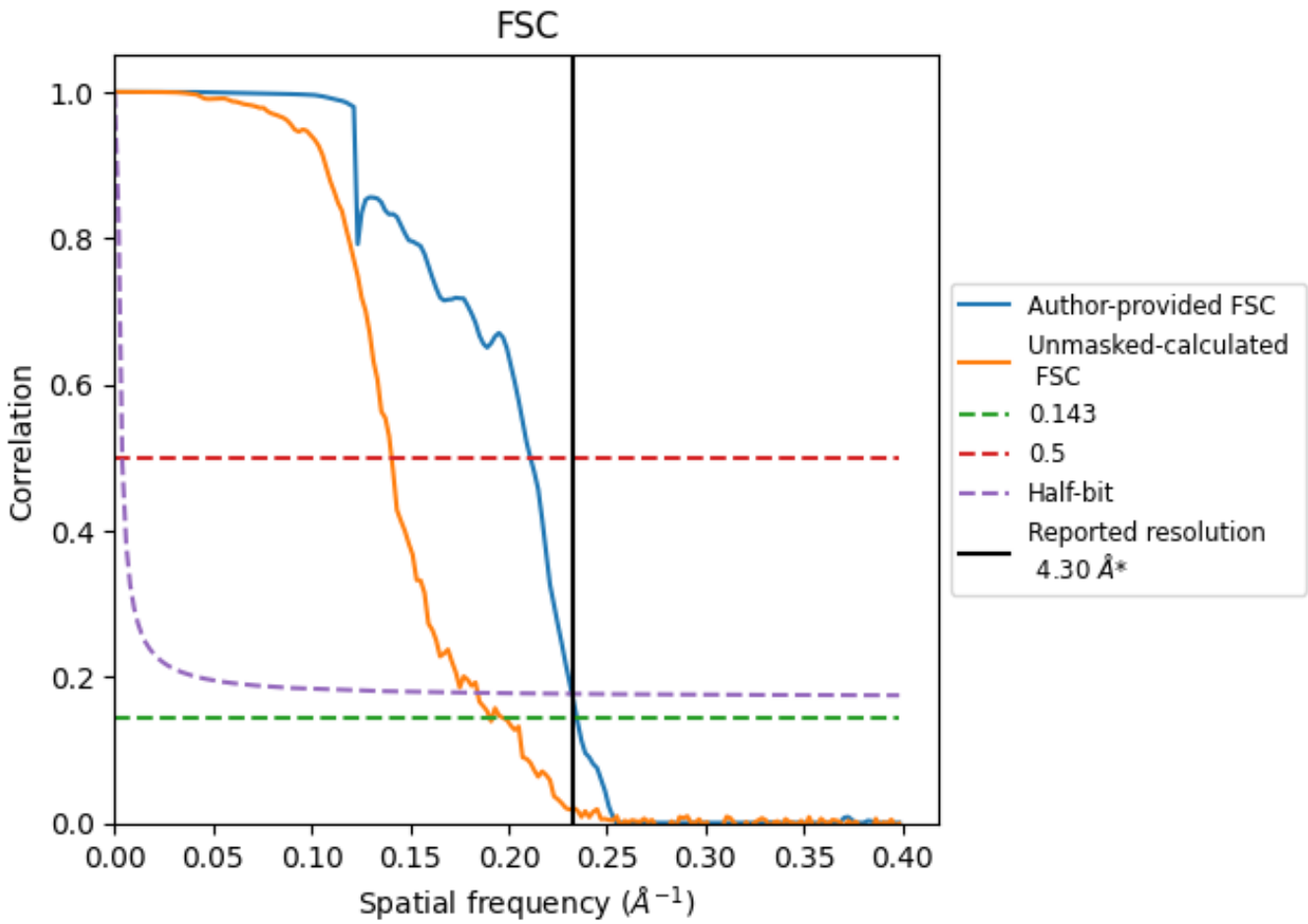


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8.2 Resolution estimates (i)

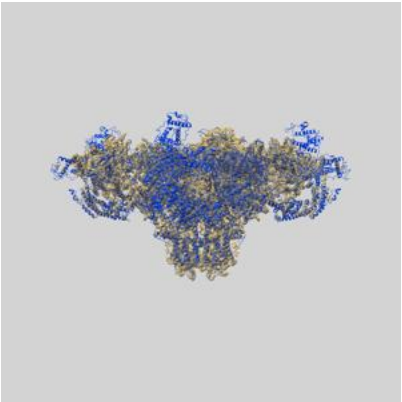
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.26	4.74	4.31
Unmasked-calculated*	5.24	7.11	5.43

*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 5.24 differs from the reported value 4.3 by more than 10 %

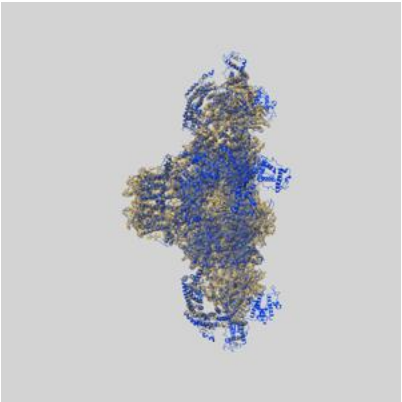
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8380 and PDB model 5TAN. Per-residue inclusion information can be found in section 3 on page 6.

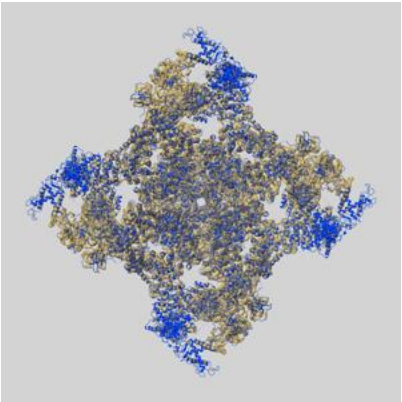
9.1 Map-model overlay (i)



X



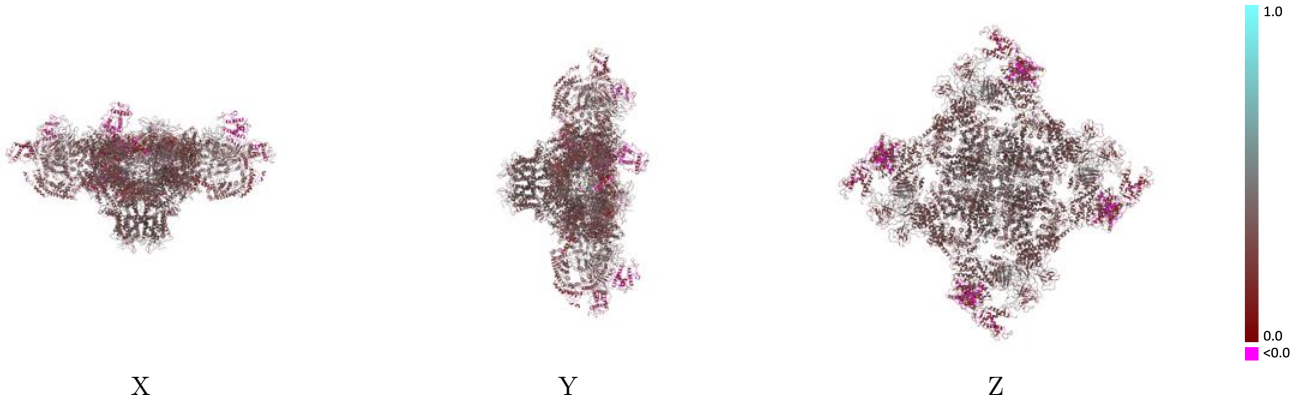
Y



Z

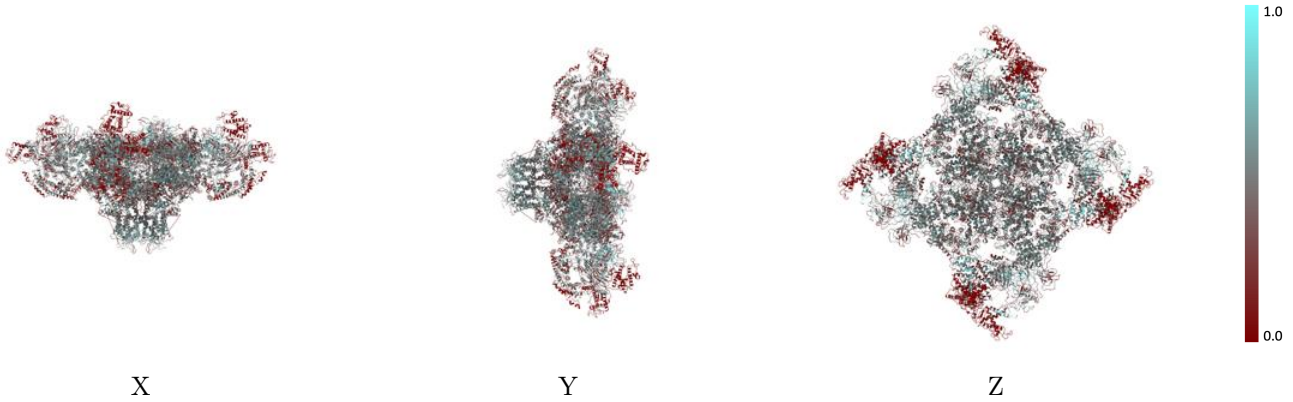
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



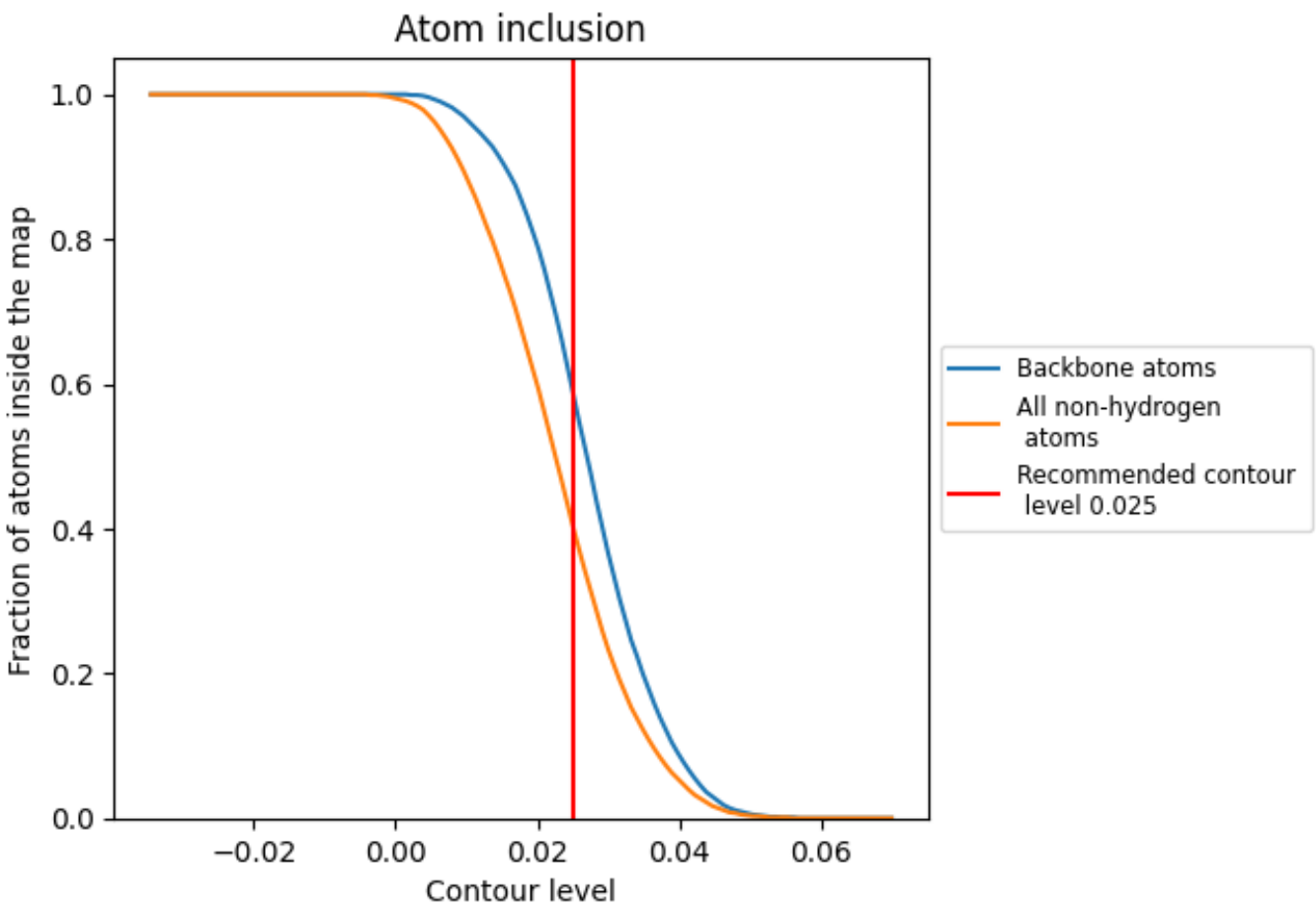
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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, 59% of all backbone atoms, 40% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4020	0.3150
A	0.3500	0.3180
B	0.4040	0.3140
E	0.4030	0.3140
F	0.3450	0.3230
G	0.4030	0.3140
H	0.3470	0.3230
I	0.4040	0.3140
J	0.3500	0.3190