wwPDB EM Validation Summary Report

Mar 6, 2026 – 10:10 AM UTC

PDB ID	:	8RRV / pdb_00008rrv
EMDB ID	:	EMD-19466
Title	:	Structure of RyR1 in detergent in close state in complex with FKBP and Nb9657.
Authors	:	Li, C.; Efremov, R.G.
Deposited on	:	2024-01-23
Resolution	:	3.20 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 ⓘ 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:

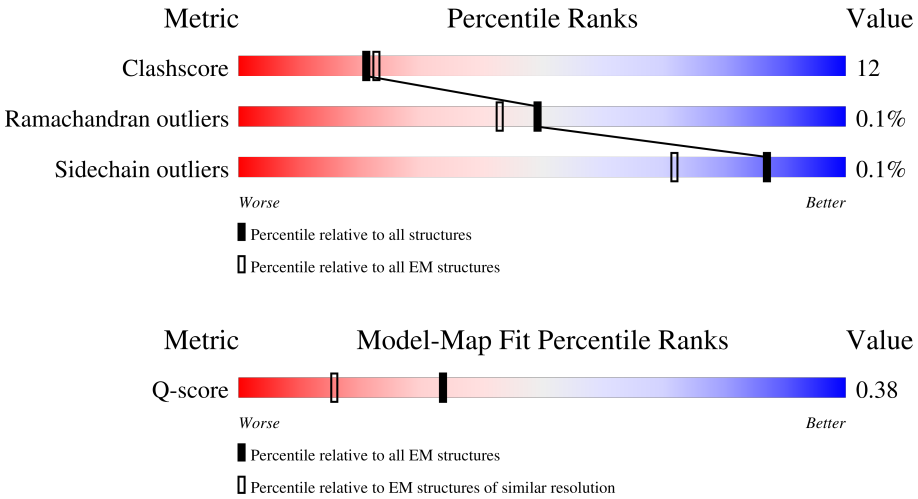
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	B	5037	63% 22% 15%
1	E	5037	63% 22% 15%
1	G	5037	63% 22% 15%
1	J	5037	63% 22% 15%

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Mol	Chain	Length	Quality of chain
2	A	107	77% 23%
2	D	107	77% 23%
2	H	107	75% 25%
2	I	107	75% 25%
3	C	137	18% 62% 30% 8%
3	F	137	18% 64% 28% 8%
3	K	137	18% 63% 29% 8%
3	M	137	17% 64% 28% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 142968 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	4290	Total	C	N	O	S	1	0
			33956	21639	5852	6236	229		
1	E	4290	Total	C	N	O	S	1	0
			33956	21639	5852	6236	229		
1	G	4290	Total	C	N	O	S	1	0
			33956	21639	5852	6236	229		
1	J	4290	Total	C	N	O	S	1	0
			33956	21639	5852	6236	229		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3221	SER	THR	conflict	UNP P11716
E	3221	SER	THR	conflict	UNP P11716
G	3221	SER	THR	conflict	UNP P11716
J	3221	SER	THR	conflict	UNP P11716

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	D	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	I	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ASP	GLY	conflict	UNP Q8HYX6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	100	ASP	GLY	conflict	UNP Q8HYX6
H	100	ASP	GLY	conflict	UNP Q8HYX6
I	100	ASP	GLY	conflict	UNP Q8HYX6

- Molecule 3 is a protein called nanobody9657.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
3	F	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
3	K	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
3	M	126	Total	C	N	O	S	0	0
			967	597	170	195	5		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

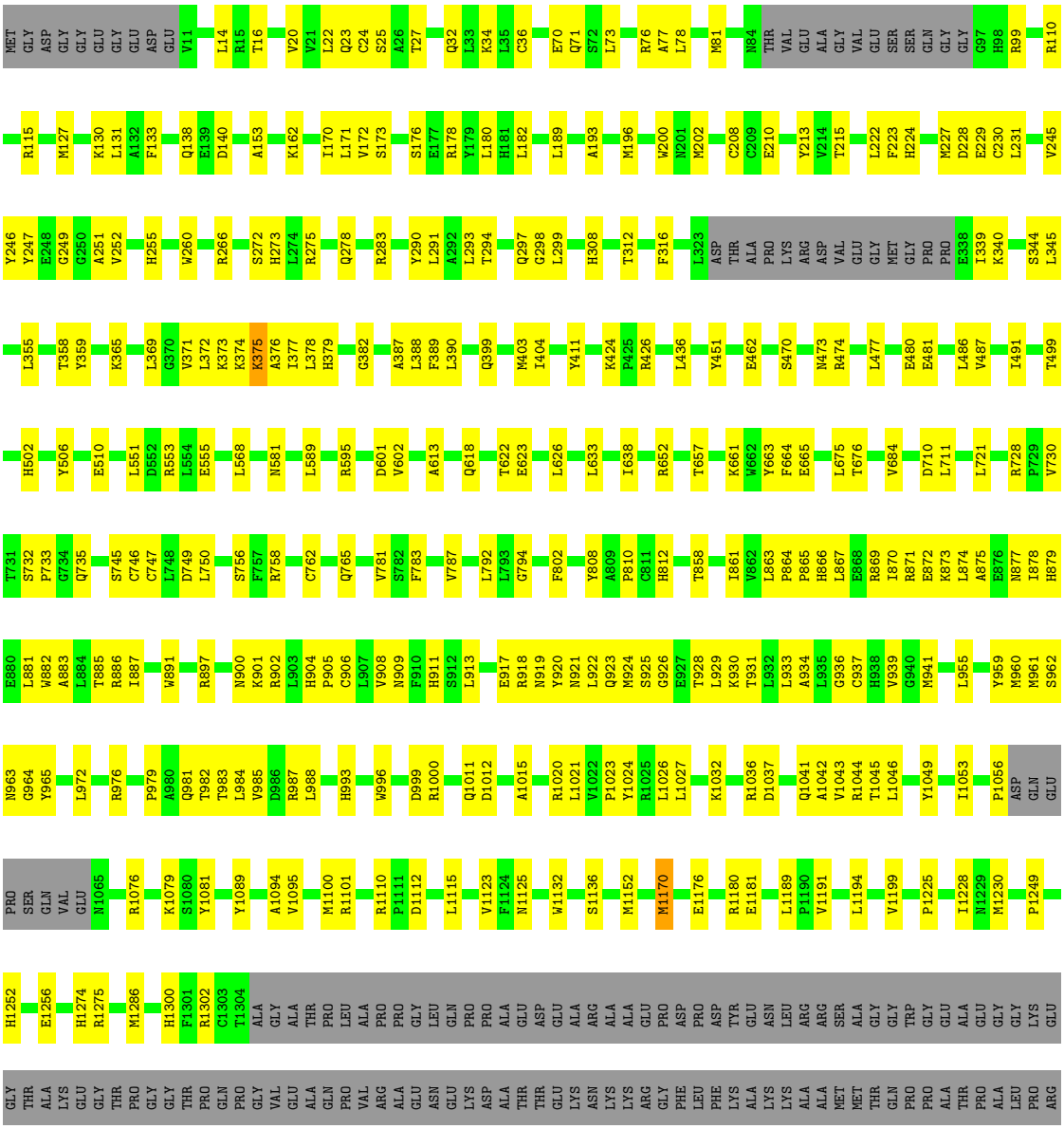
Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Zn	0
			1	1	
4	E	1	Total	Zn	0
			1	1	
4	G	1	Total	Zn	0
			1	1	
4	J	1	Total	Zn	0
			1	1	

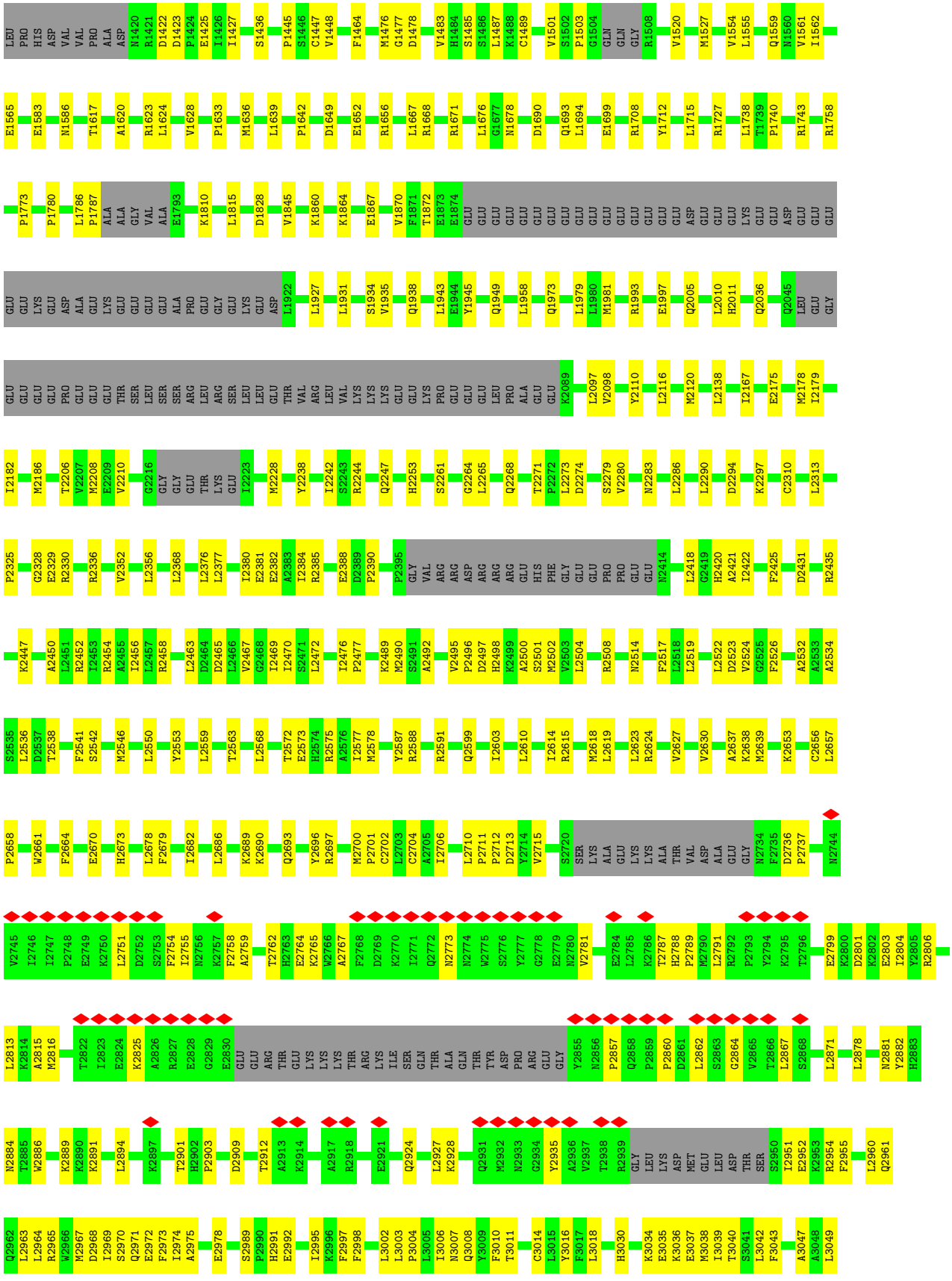
3 Residue-property plots (i)

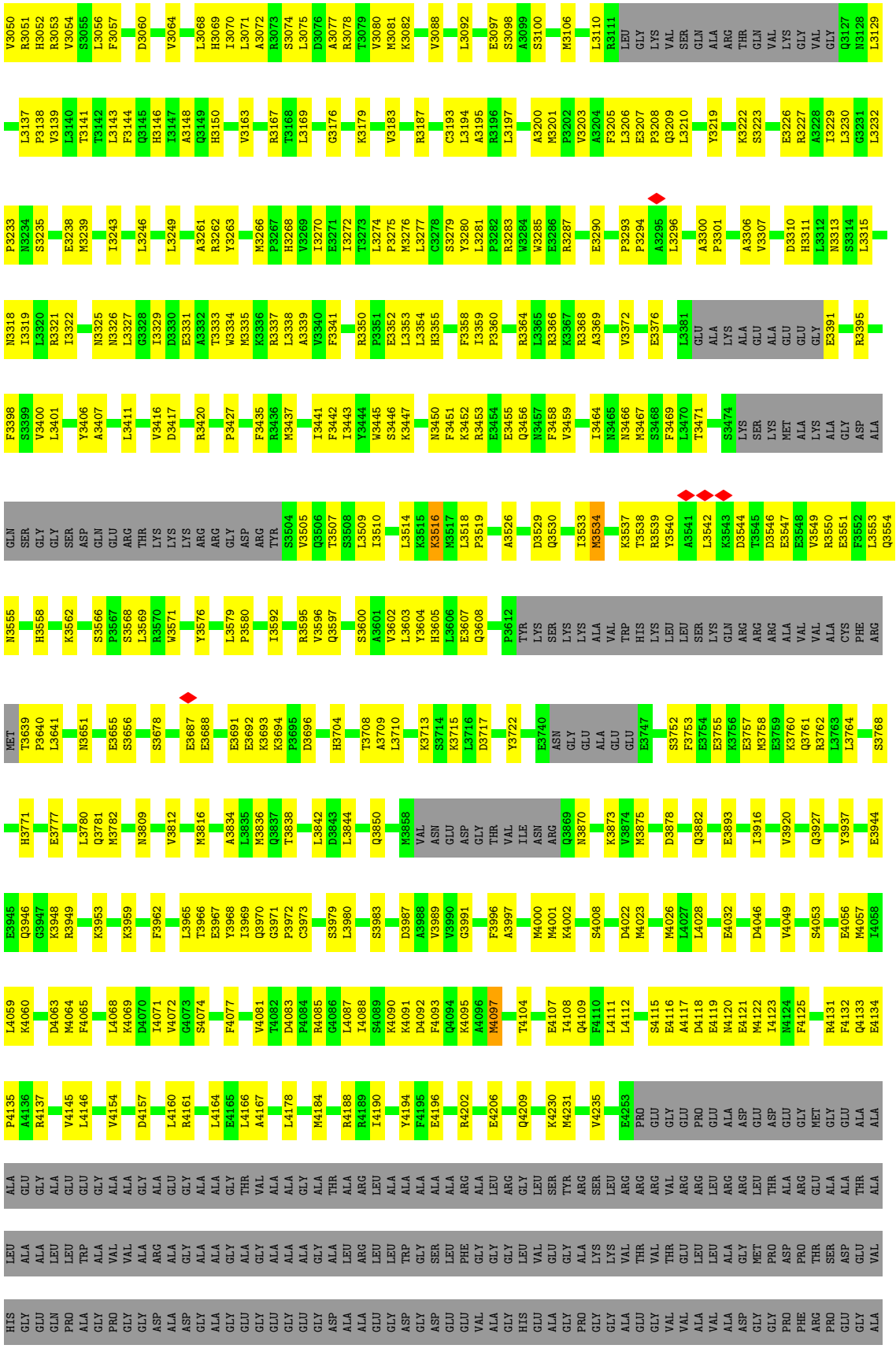
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

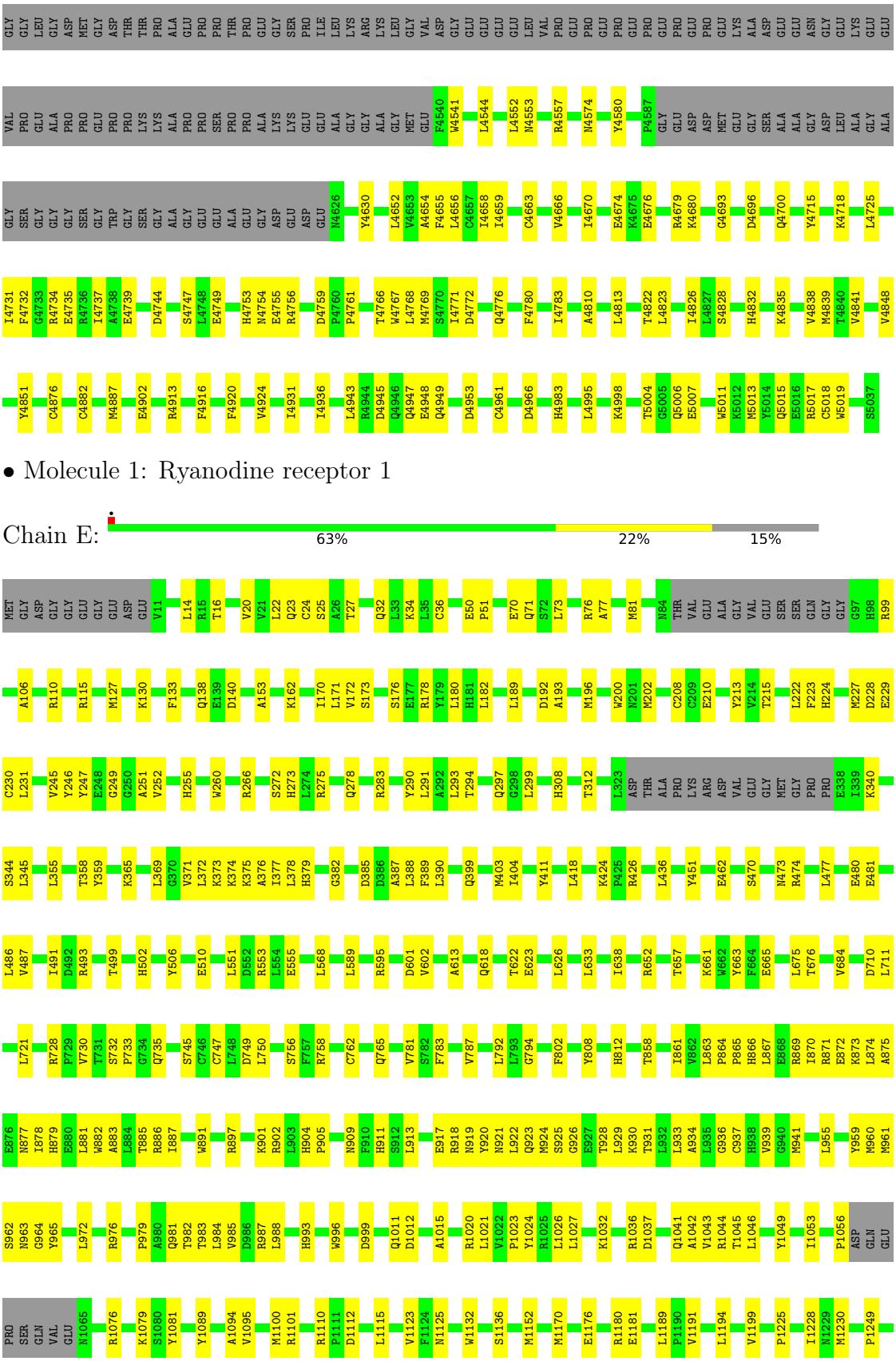
- Molecule 1: Ryanodine receptor 1

Chain B:



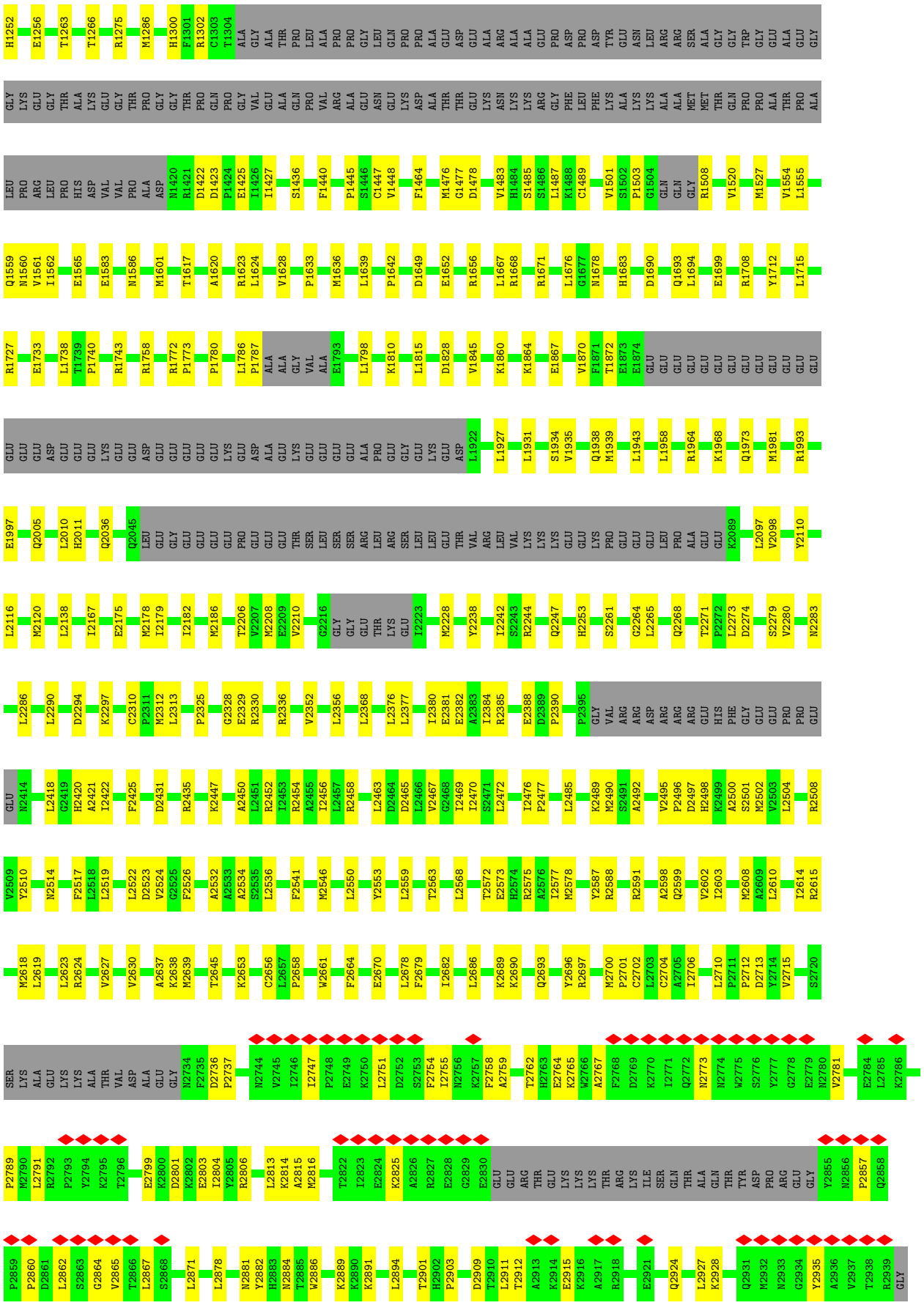


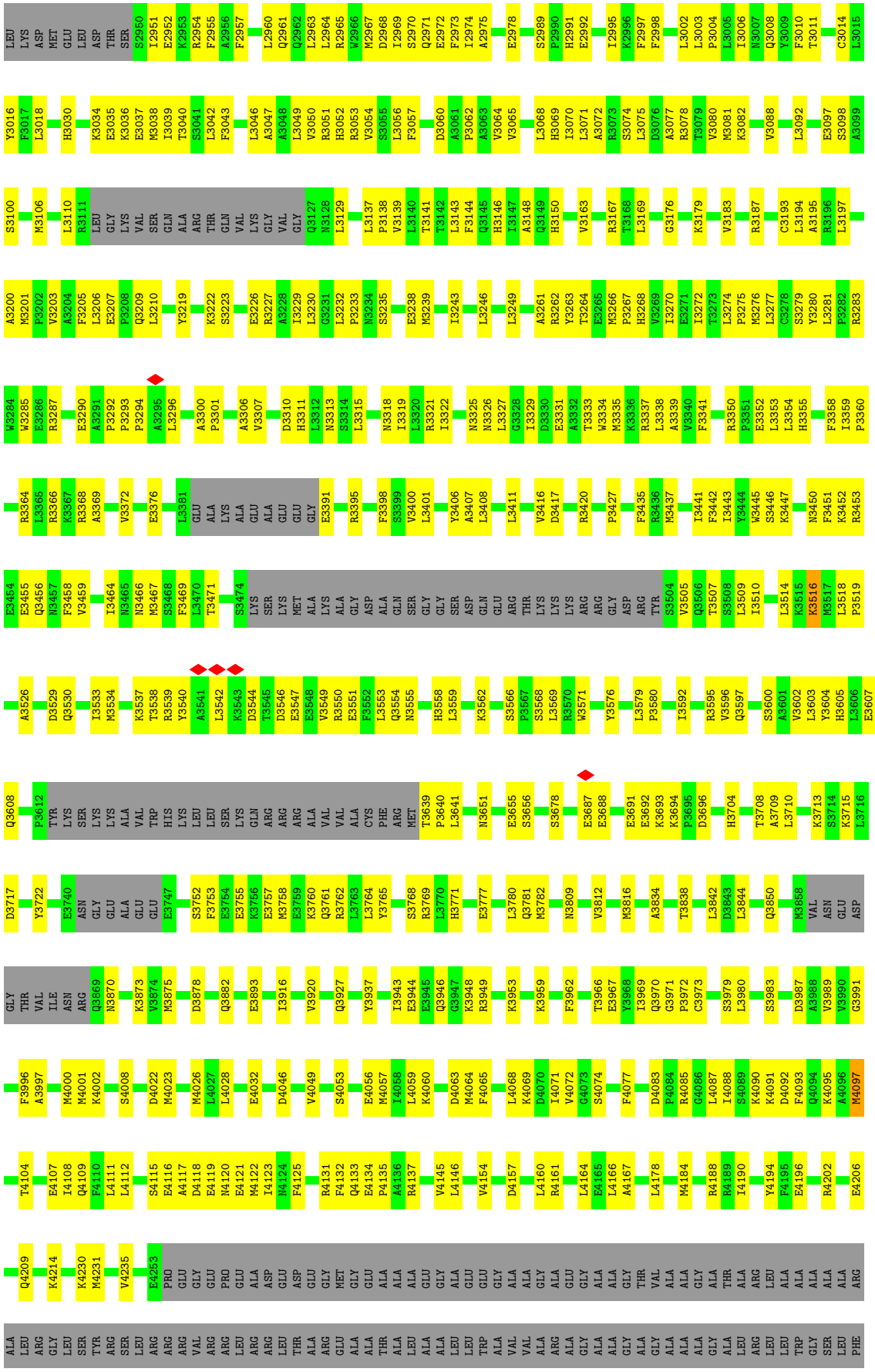


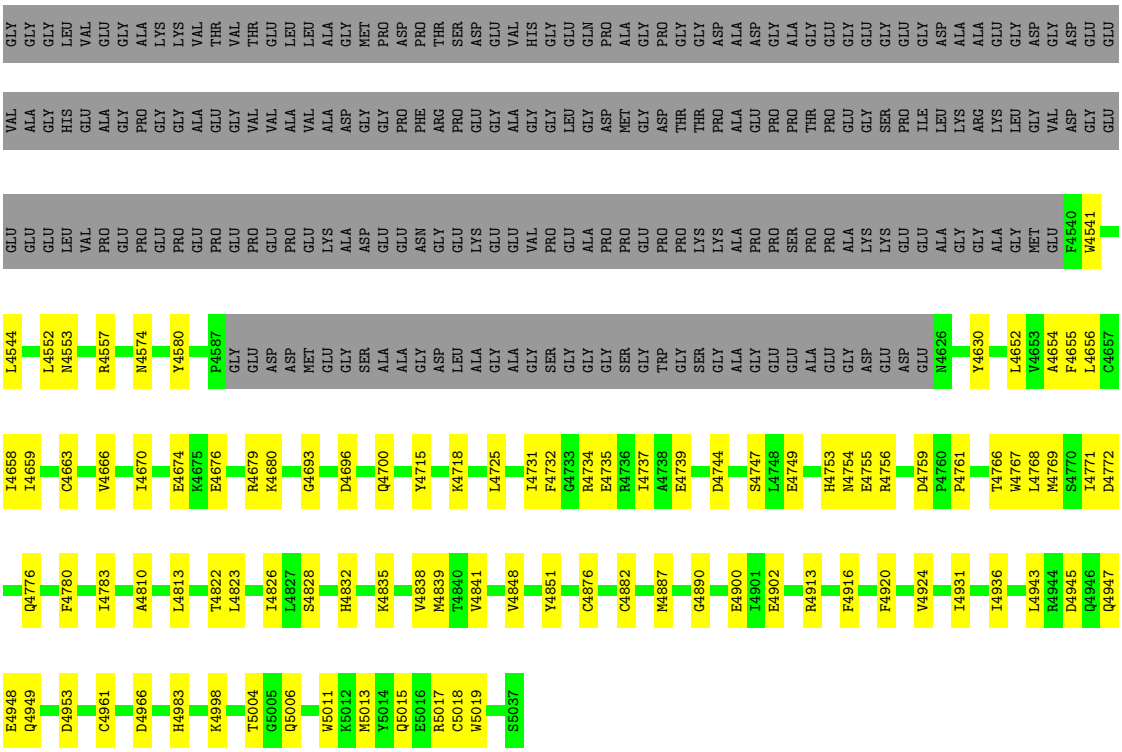


• Molecule 1: Ryanodine receptor 1

Chain E:

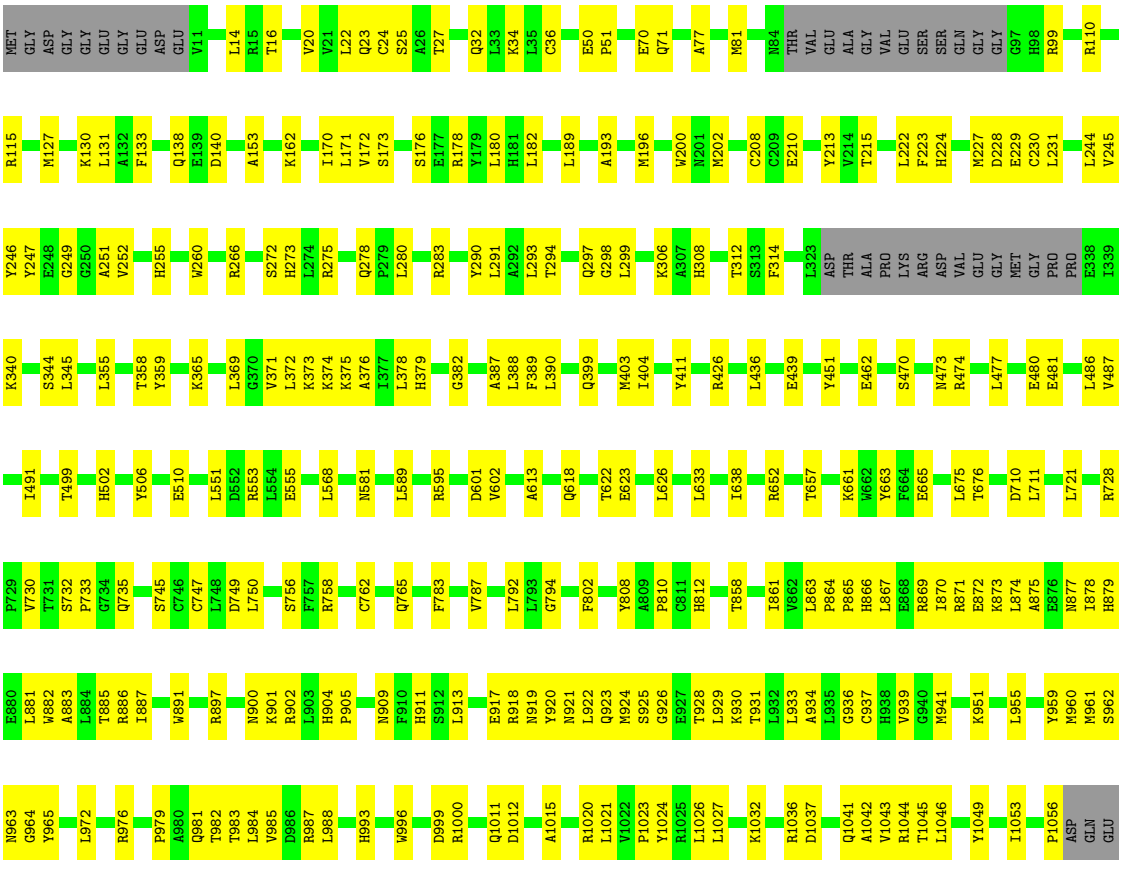


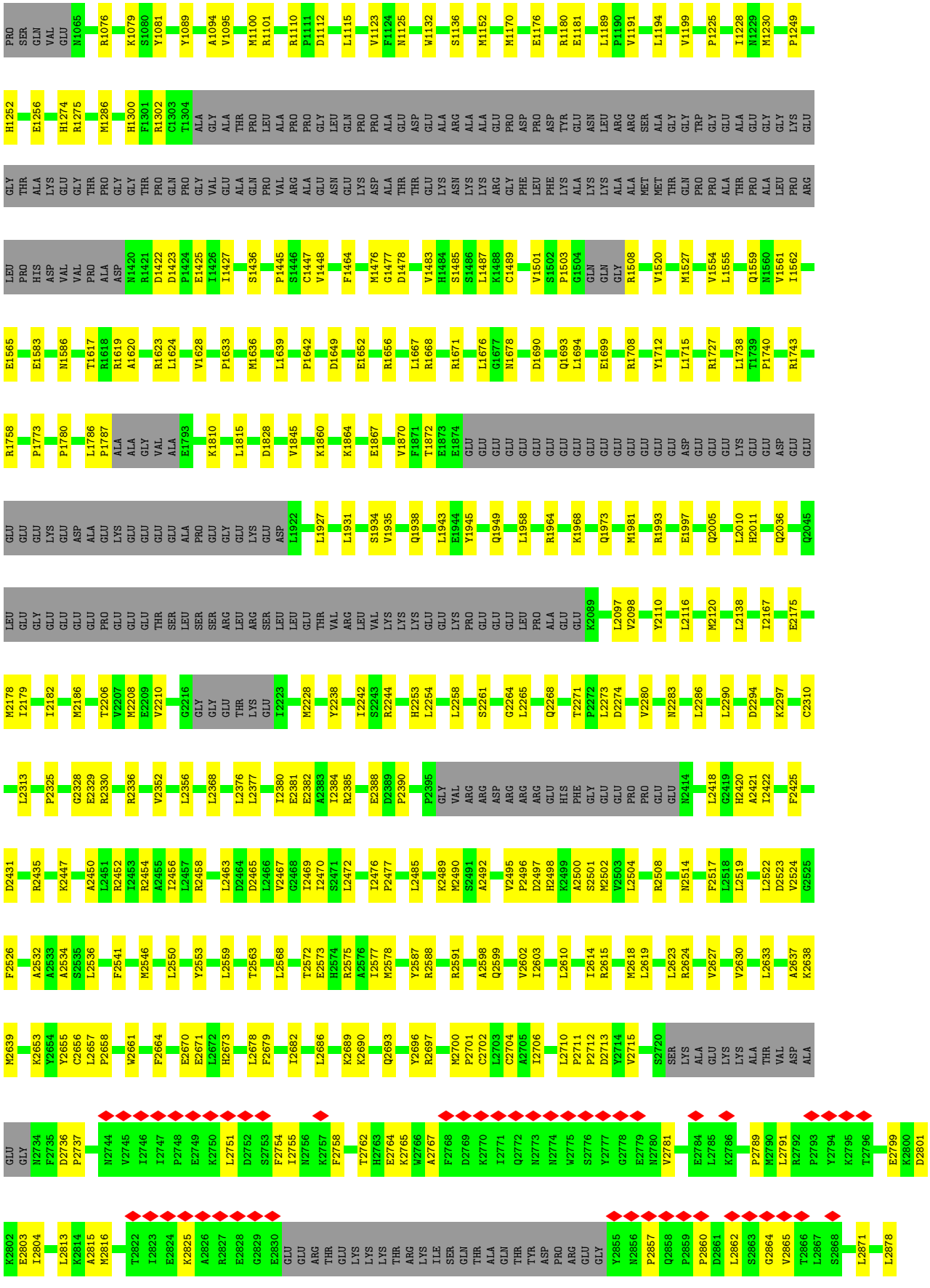




• Molecule 1: Ryanodine receptor 1

Chain G:

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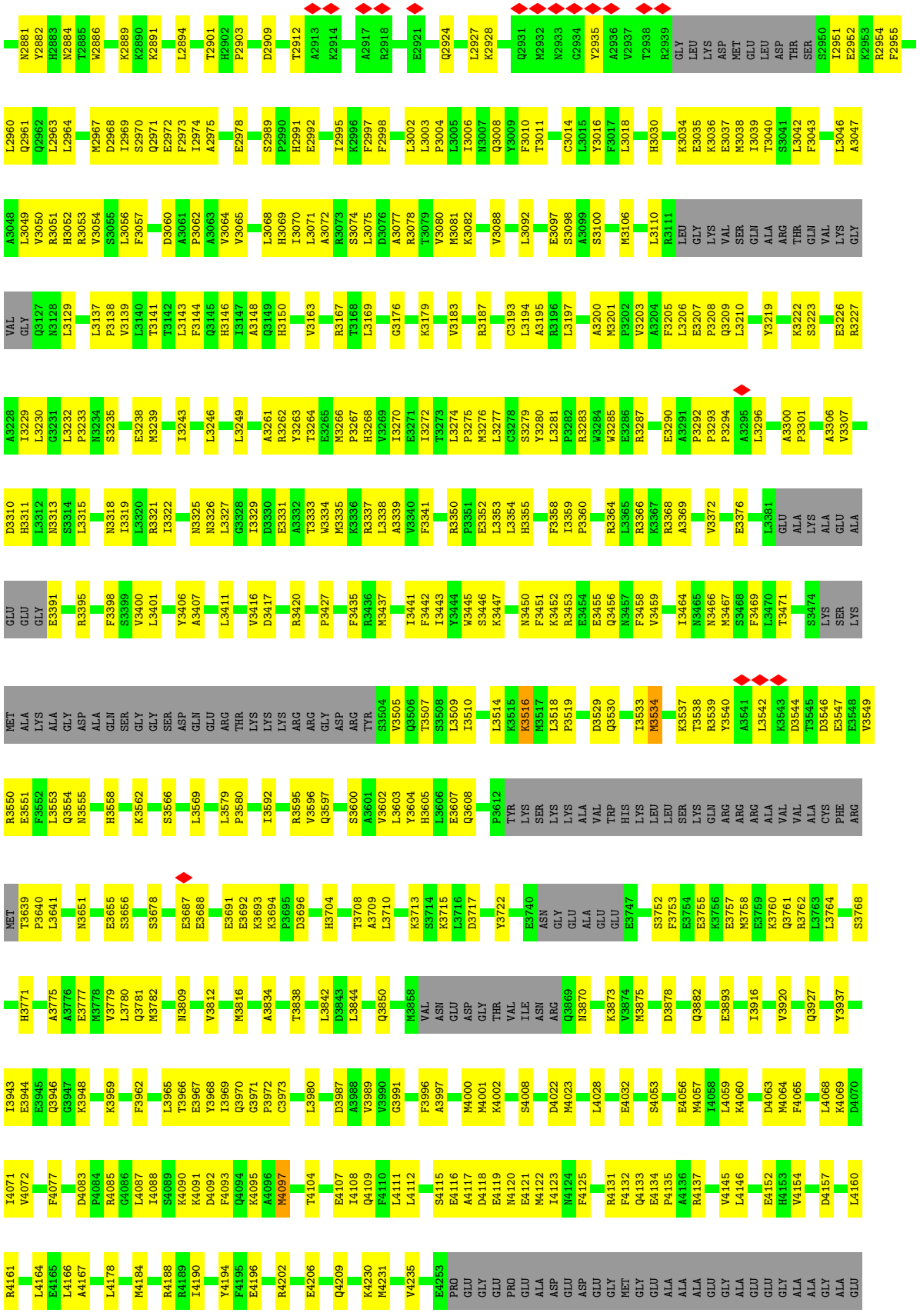
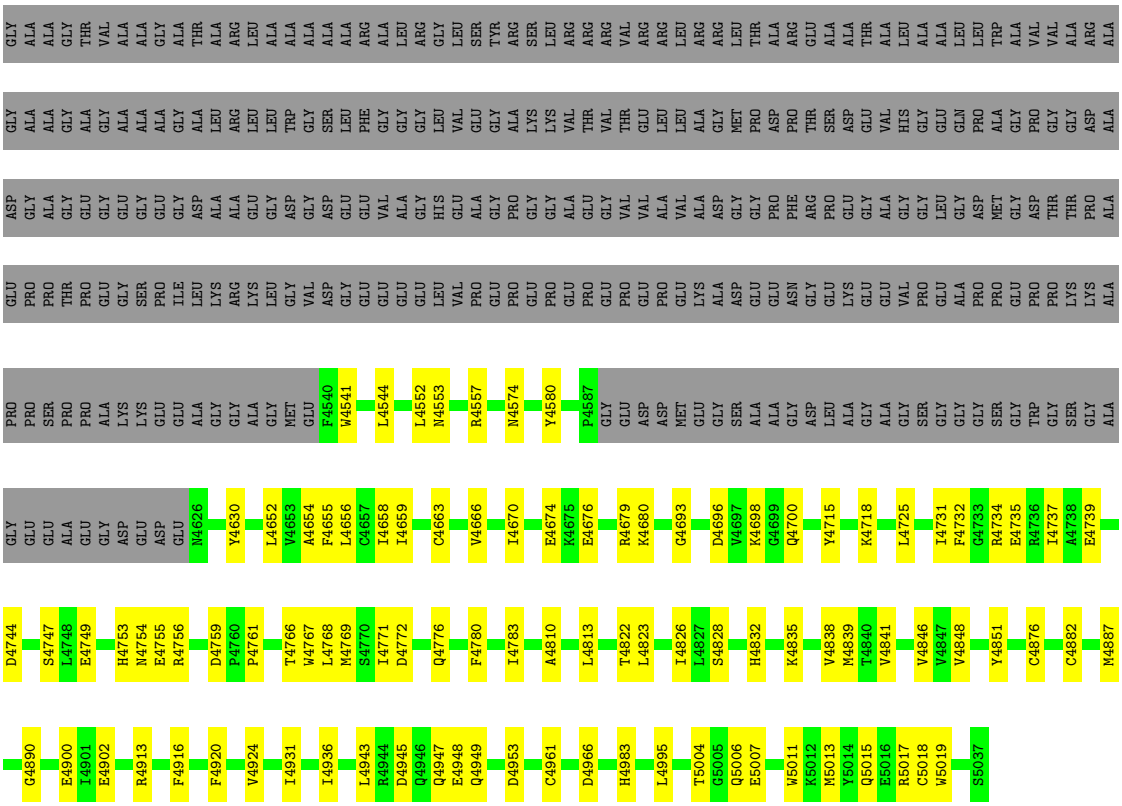
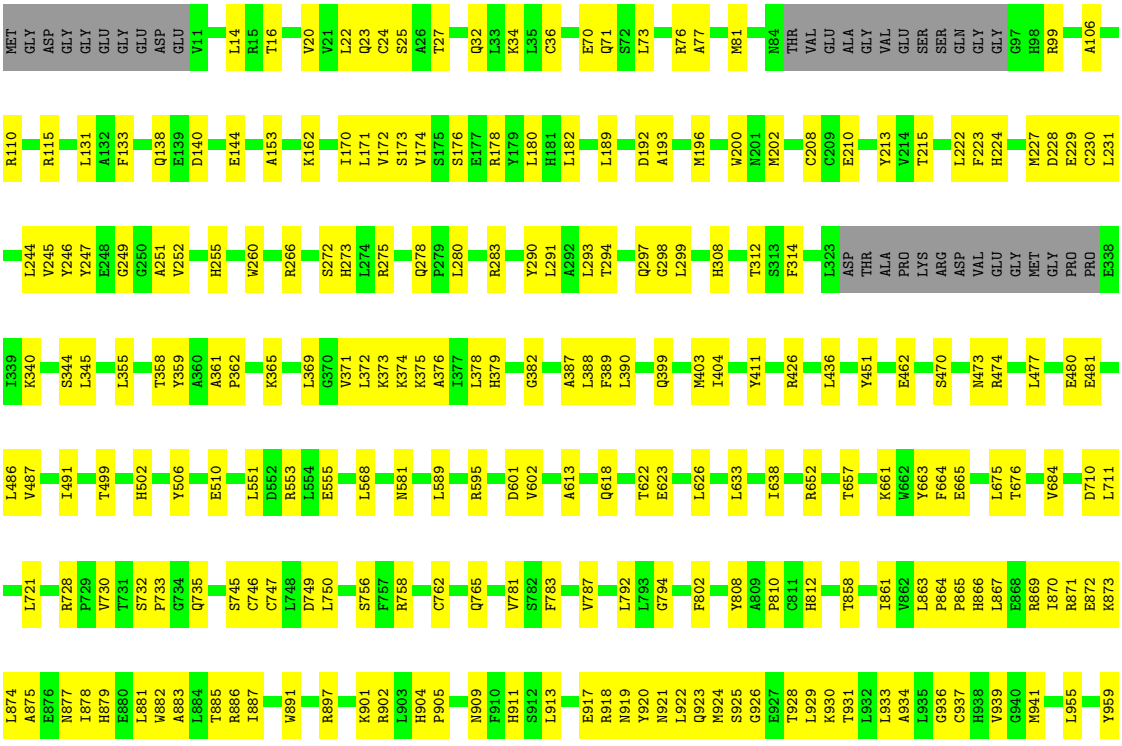
H1252 E1256 H1274 R1275 M1286 H1300 F1301 R1302 C1303 T1304 ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP PRO GLY GLU ALA GLU GLY LYS GLU
GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG
LEU PRO HIS ASP VAL VAL PRO ALA ASP N1420 R1421 D1422 D1423 P1424 E1425 I1426 I1427 S1436 P1445 S1446 C1447 V1448 F1464 M1476 G1477 D1478 V1483 H1484 S1485 S1486 L1487 K1488 C1489 V1501 S1502 P1503 G1504 GLN GLN GLY R1508 V1520 M1527 V1554 L1555 Q1559 N1560 V1561 I1562
E1565 E1583 N1586 T1617 R1618 R1619 A1620 R1623 L1624 V1628 P1633 M1636 L1639 P1642 D1649 E1652 R1656 L1667 R1668 R1671 L1676 G1677 N1678 D1690 Q1693 L1694 E1699 R1708 Y1712 L1715 R1727 L1738 T1739 P1740 R1743
R1758 P1773 P1780 L1786 P1787 ALA ALA GLY VAL ALA E1793 K1810 L1815 D1828 V1845 K1860 K1864 E1867 V1870 F1871 T1872 E1873 E1874 GLU GLU GLU

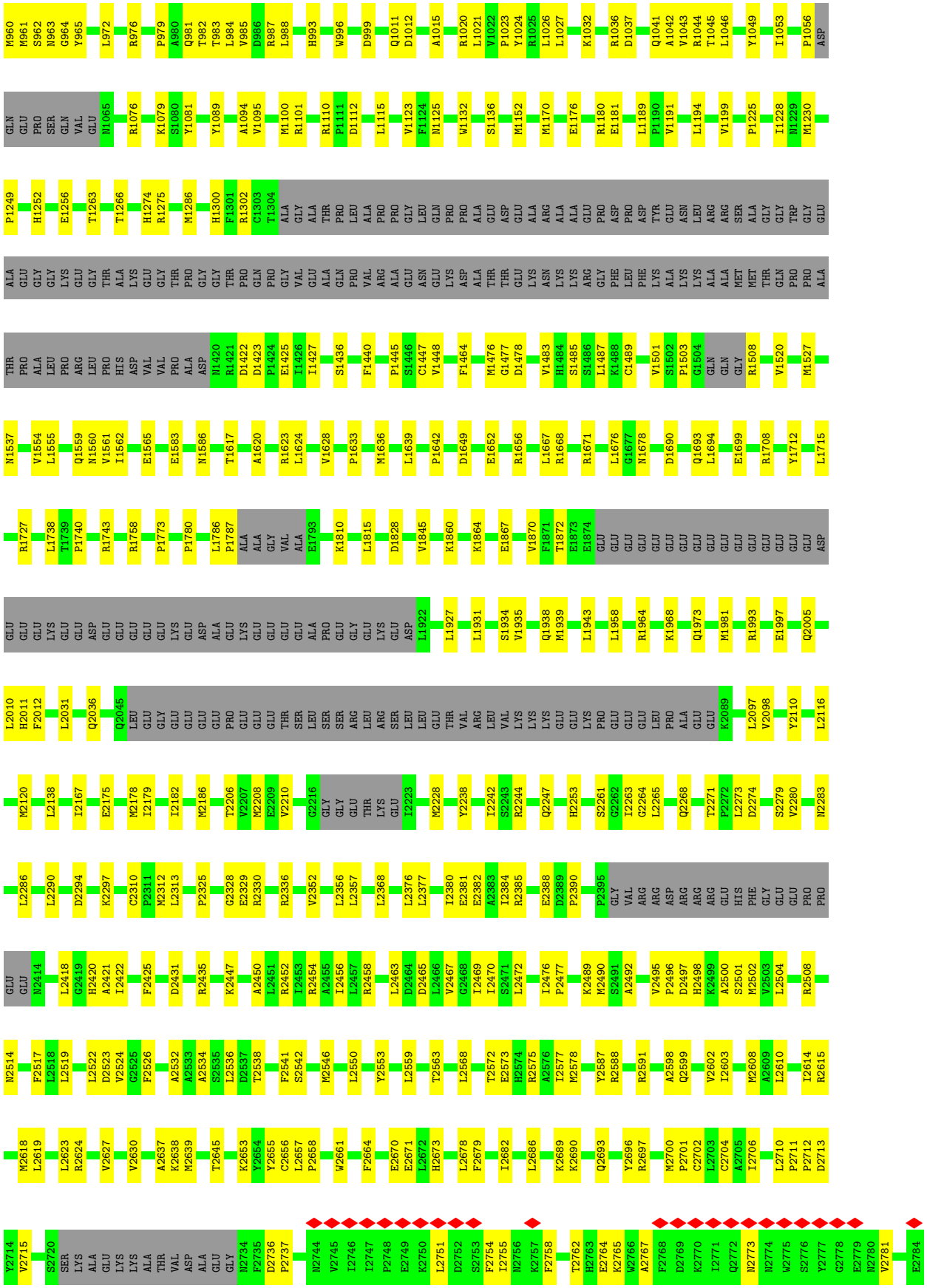




• Molecule 1: Ryanodine receptor 1

Chain J:

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GLN GLU PRO SER GLN VAL GLU N1065 R1076 K1079 S1080 Y1081 Y1089 A1094 V1095 M1100 R1101 R1110 P1111 D1112 L1115 V1123 F1124 N1125 W1132 S1136 M1152 M1170 E1176 R1180 E1181 L1189 P1190 V1191 L1194 V1199 P1225 I1228 N1229 M1230
P1249 H1252 E1256 T1263 T1266 H1274 R1275 M1286 H1300 F1301 R1302 C1303 T1304 ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU
ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA
THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP N1420 R1421 D1422 D1423 P1424 E1425 I1426 I1427 S1436 F1440 P1445 S1446 C1447 V1448 F1464 M1476 G1477 D1478 V1483 H1484 S1485 S1486 L1487 K1488 C1489 V1501 S1502 P1503 G1504 GLN GLN GLY R1508 V1520 M1527
N1537 V1554 L1555 Q1559 N1560 V1561 I1562 E1565 E1583 N1586 T1617 A1620 R1623 L1624 V1628 P1633 M1636 L1639 P1642 D1649 F1652 R1656 L1667 R1668 R1671 L1676 G1677 N1678 D1690 Q1693 L1694 E1699 R1708 Y1712 L1715
R1727 L1738 T1739 P1740 R1743 R1758 P1773 P1780 L1786 P1787 ALA ALA GLY VAL ALA E1793 K1810 L1815 D1828 V1845 K1860 K1864 E1867 V1870 F1871 T1872 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP
GLU GLU GLU LYS GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU ASP ALA LEU PRO GLU GLY GLU LYS GLU ASP L1922 L1927 L1931 S1934 V1935 Q1938 M1939 L1943 L1958 R1964 K1968 Q1973 M1981 R1993 E1997 Q2005
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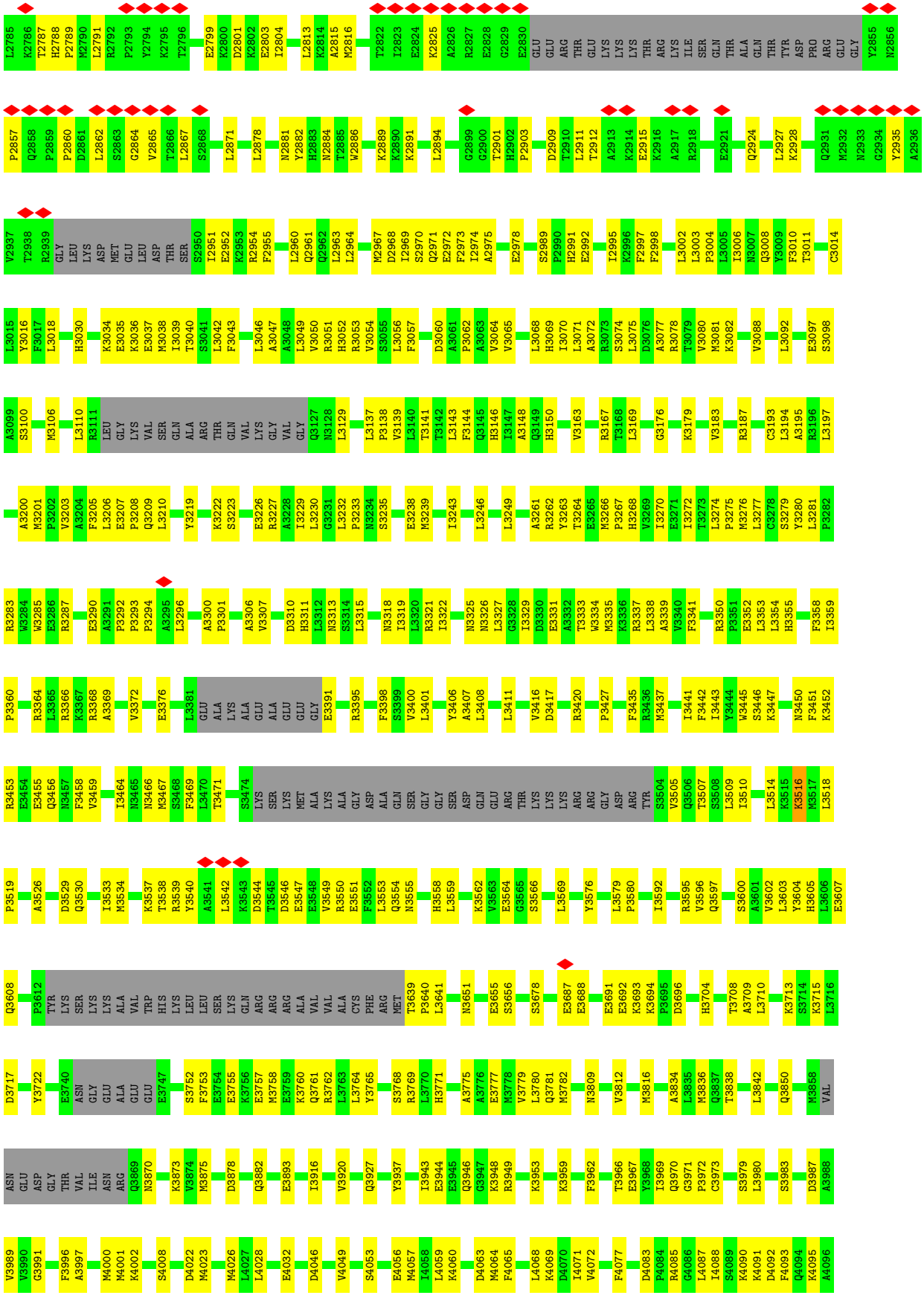
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P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 L2871 L2878 N2881 Y2882 H2883 N2884 T2885 W2886 K2889 K2890 K2891 L2894 G2899 G2900 T2901 H2902 P2903 D2909 T2910 L2911 T2912 A2913 K2914 E2915 K2916 A2917 R2918 E2921 Q2924 L2927 K2928 Q2931 M2932 N2933 G2934 Y2935 A2936
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L3015 Y3016 F3017 L3018 H3030 K3034 E3035 K3036 E3037 M3038 I3039 T3040 S3041 L3042 F3043 L3046 A3047 A3048 L3049 V3050 R3051 H3052 R3053 V3054 S3055 L3056 F3057 D3060 A3061 P3062 A3063 V3064 V3065 L3068 H3069 I3070 L3071 A3072 R3073 S3074 L3075 D3076 A3077 R3078 T3079 V3080 M3081 K3082 V3088 L3092 E3097 S3098
A3099 S3100 M3106 L3110 R3111 LEU GLY LYS VAL SER GLN ALA ARG THR GLN VAL LYS GLY VAL GLY Q3127 N3128 L3129 L3137 P3138 V3139 L3140 T3141 T3142 L3143 F3144 Q3145 H3146 I3147 A3148 Q3149 H3150 V3163 R3167 T3168 L3169 G3176 K3179 V3183 R3187 C3193 L3194 A3195 R3196 L3197
A3200 M3201 P3202 V3203 A3204 F3205 L3206 E3207 P3208 Q3209 L3210 Y3219 K3222 S3223 E3226 R3227 A3228 I3229 L3230 G3231 L3232 P3233 N3234 S3235 E3238 M3239 I3243 L3246 L3249 A3261 R3262 Y3263 T3264 E3265 M3266 P3267 H3268 V3269 I3270 E3271 I3272 T3273 L3274 P3275 M3276 L3277 C3278 S3279 Y3280 L3281 P3282
R3283 W3284 W3285 E3286 R3287 E3290 A3291 P3292 P3293 P3294 A3295 L3296 A3300 P3301 A3306 V3307 D3310 H3311 L3312 N3313 S3314 L3315 N3318 I3319 L3320 R3321 I3322 N3325 N3326 L3327 G3328 I3329 D3330 E3331 A3332 T3333 W3334 M3335 K3336 R3337 L3338 A3339 V3340 F3341 R3350 P3351 E3352 L3353 L3354 H3355 F3358 I3359
P3360 R3364 L3365 R3366 K3367 R3368 A3369 V3372 E3376 L3381 GLU ALA LYS ALA GLU ALA GLU GLU GLY E3391 R3395 F3398 S3399 V3400 L3401 Y3406 A3407 L3408 L3411 V3416 D3417 R3420 P3427 F3435 R3436 M3437 I3441 F3442 I3443 Y3444 W3445 S3446 K3447 N3450 F3451 K3452
R3453 E3454 E3455 Q3456 N3457 F3458 V3459 I3464 N3465 N3466 M3467 S3468 F3469 L3470 T3471 S3474 LYS SER LYS MET ALA LYS ALA GLY ASP ALA GLN SER GLY GLY SER ASP GLN GLU ARG THR LYS LYS LYS ARG ARG GLY ASP ARG TYR S3504 V3505 Q3506 T3507 S3508 L3509 I3510 L3514 K3515 K3516 M3517 L3518
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Q3608 P3612 TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL ALA CYS PHE ARG MET T3639 P3640 L3641 N3651 E3655 S3656 S3678 E3687 E3688 E3691 E3692 K3693 K3694 P3695 D3696 H3704 T3708 A3709 L3710 K3713 S3714 K3715 L3716
D3717 Y3722 E3740 ASN GLY GLU ALA GLU GLU E3747 S3752 F3753 E3754 E3755 K3756 E3757 M3758 E3759 K3760 Q3761 R3762 L3763 L3764 Y3765 S3768 R3769 L3770 H3771 A3775 A3776 E3777 M3778 V3779 L3780 Q3781 M3782 N3809 V3812 M3816 A3834 L3835 M3836 Q3837 T3838 L3842 Q3850 M3858 VAL
ASN GLU ASP GLY THR VAL ILE ASN ARG Q3869 N3870 K3873 V3874 M3875 D3878 Q3882 E3883 I3916 V3920 Q3927 Y3937 I3943 E3944 E3945 Q3946 G3947 K3948 R3949 K3953 K3959 F3962 T3966 E3967 Y3968 I3969 Q3970 G3971 P3972 C3973 S3979 L3980 S3983 D3987 A3988
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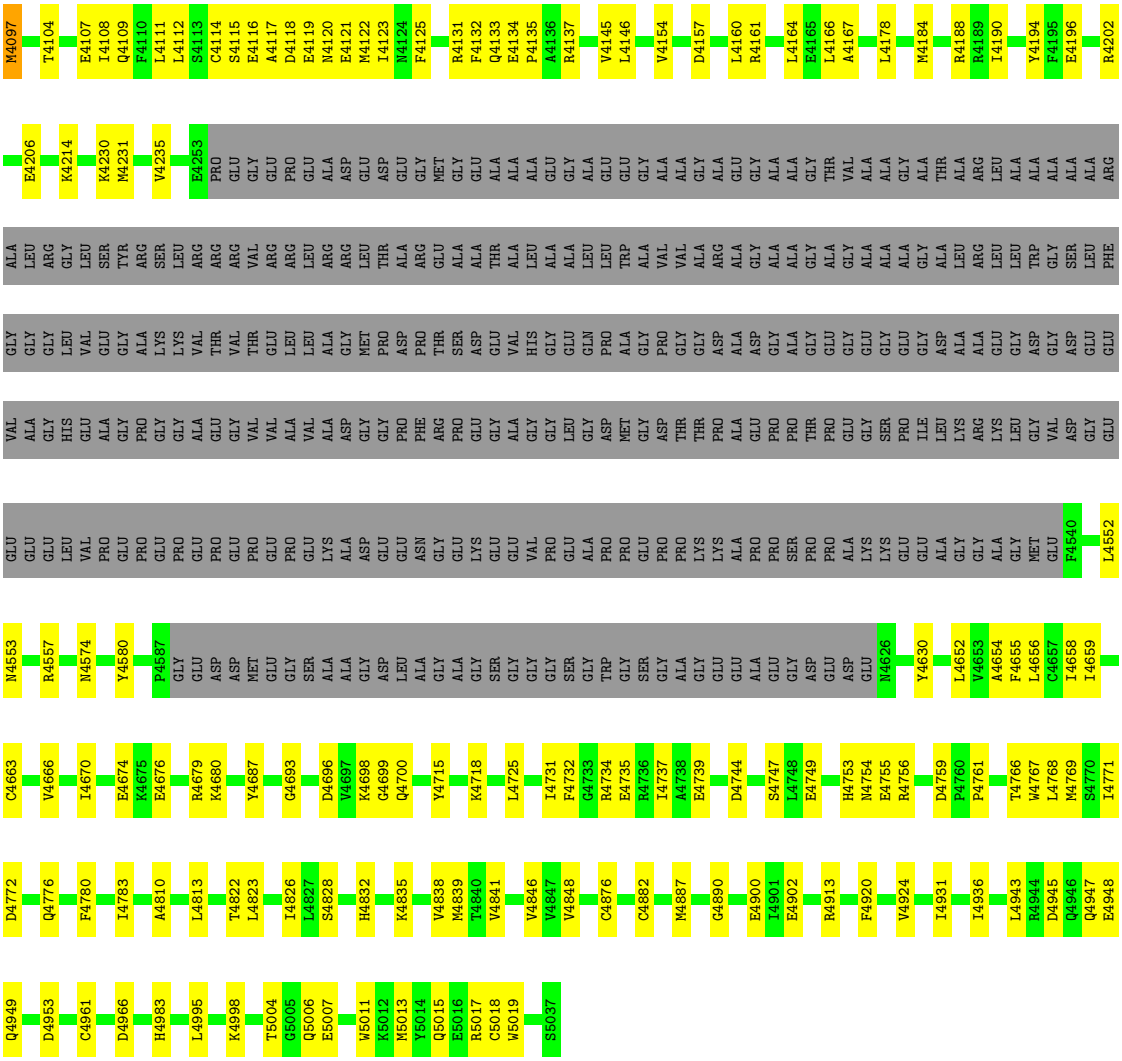
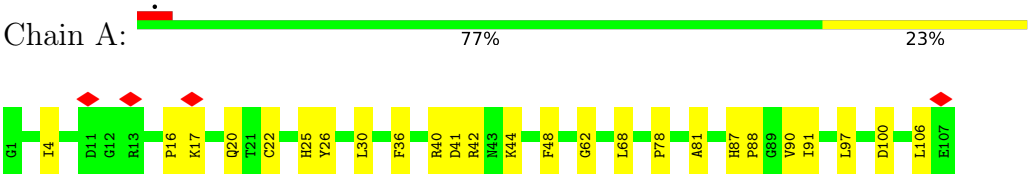


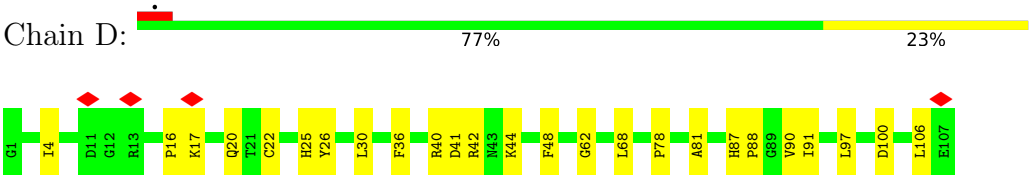
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



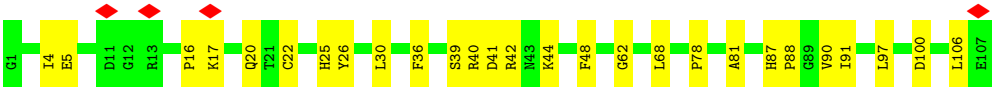
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain D:

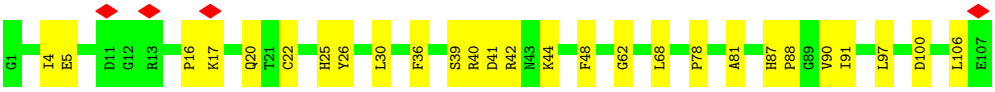


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

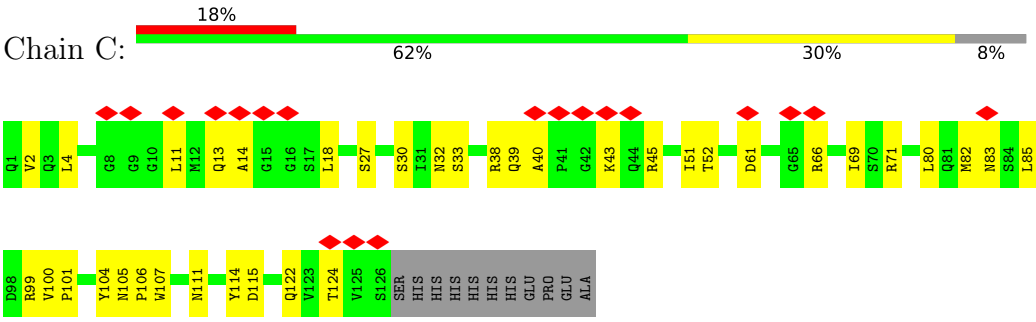
Chain H:



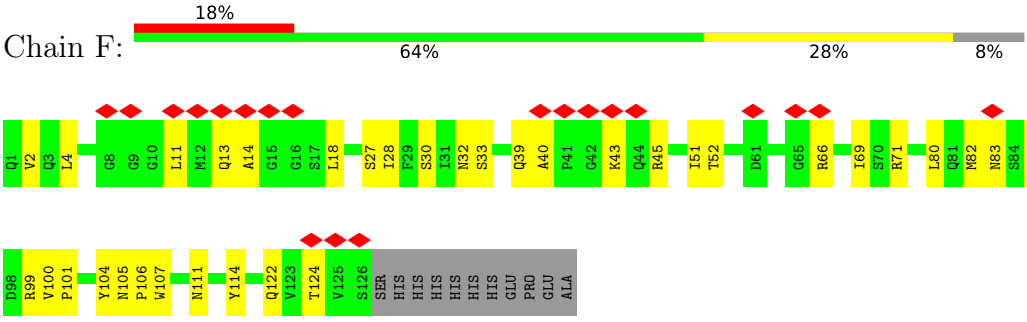
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



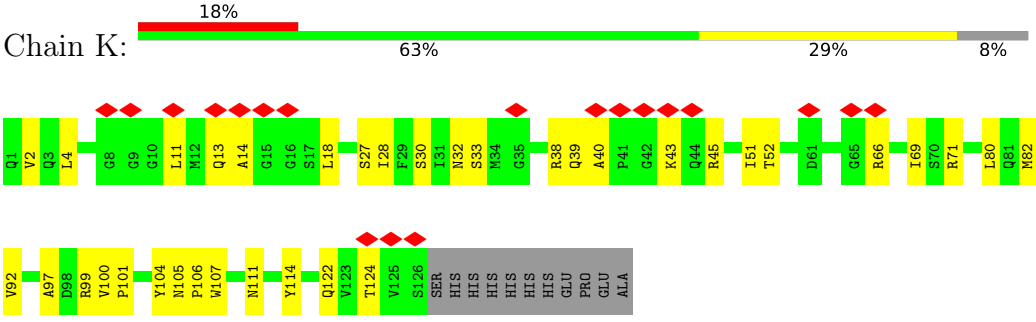
• Molecule 3: nanobody9657



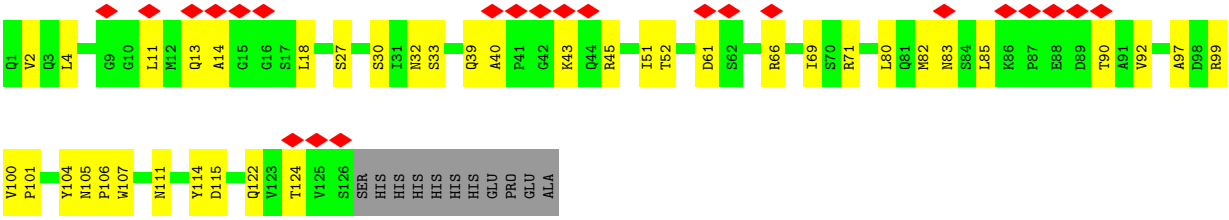
• Molecule 3: nanobody9657



• Molecule 3: nanobody9657



• Molecule 3: nanobody9657


Q1 V2 Q3 L4 G9 G10 L11 M12 Q13 A14 G15 G16 S17 L18 S27 S30 I31 N32 S33 Q39 A40 P41 G42 K43 Q44 R45 I51 T52 D61 S62 R66 I69 S70 R71 L80 Q81 M82 N83 S84 L85 K86 P87 E88 D89 T90 A91 V92 A97 D98 R99
V100 P101 Y104 N105 P106 W107 N111 Y114 D115 Q122 V123 T124 V125 S126 SER HIS HIS HIS HIS HIS HIS GLU PRO GLU ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171023	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.350	Depositor
Minimum map value	-0.105	Depositor
Average map value	0.076	Depositor
Map value standard deviation	0.164	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	499.96802, 499.96802, 499.96802	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.488, 1.488, 1.488	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	B	0.12	0/34727	0.32	2/47063 (0.0%)
1	E	0.13	0/34727	0.32	2/47063 (0.0%)
1	G	0.13	0/34727	0.32	2/47063 (0.0%)
1	J	0.13	0/34727	0.32	2/47063 (0.0%)
2	A	0.10	0/834	0.30	0/1123
2	D	0.10	0/834	0.30	0/1123
2	H	0.10	0/834	0.30	0/1123
2	I	0.10	0/834	0.30	0/1123
3	C	0.16	0/987	0.44	0/1340
3	F	0.15	0/987	0.44	0/1340
3	K	0.15	0/987	0.44	0/1340
3	M	0.15	0/987	0.44	0/1340
All	All	0.13	0/146192	0.32	8/198104 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1503	PRO	N-CA-CB	6.96	110.19	103.51
1	E	1503	PRO	N-CA-CB	6.96	110.19	103.51
1	G	1503	PRO	N-CA-CB	6.91	110.14	103.51
1	J	1503	PRO	N-CA-CB	6.91	110.14	103.51
1	E	4097	MET	CB-CG-SD	-5.25	96.94	112.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	33956	0	33378	793	0
1	E	33956	0	33378	807	0
1	G	33956	0	33378	788	0
1	J	33956	0	33378	814	0
2	A	818	0	824	17	0
2	D	818	0	824	17	0
2	H	818	0	824	19	0
2	I	818	0	824	19	0
3	C	967	0	916	39	0
3	F	967	0	916	37	0
3	K	967	0	916	38	0
3	M	967	0	916	40	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
All	All	142968	0	140472	3373	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 12.

The worst 5 of 3373 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4961:CYS:SG	1:J:4983:HIS:CE1	2.58	0.97
1:B:4961:CYS:SG	1:B:4983:HIS:CE1	2.58	0.96
1:E:4961:CYS:SG	1:E:4983:HIS:CE1	2.58	0.96
1:G:4961:CYS:SG	1:G:4983:HIS:CE1	2.58	0.95
1:B:870:ILE:HA	1:B:873:LYS:HE2	1.57	0.86

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	B	4247/5037 (84%)	4148 (98%)	96 (2%)	3 (0%)	48 79
1	E	4247/5037 (84%)	4149 (98%)	96 (2%)	2 (0%)	100 100
1	G	4247/5037 (84%)	4148 (98%)	97 (2%)	2 (0%)	100 100
1	J	4247/5037 (84%)	4148 (98%)	97 (2%)	2 (0%)	100 100
2	A	105/107 (98%)	102 (97%)	3 (3%)	0	100 100
2	D	105/107 (98%)	102 (97%)	3 (3%)	0	100 100
2	H	105/107 (98%)	102 (97%)	3 (3%)	0	100 100
2	I	105/107 (98%)	102 (97%)	3 (3%)	0	100 100
3	C	124/137 (90%)	118 (95%)	6 (5%)	0	100 100
3	F	124/137 (90%)	118 (95%)	6 (5%)	0	100 100
3	K	124/137 (90%)	118 (95%)	6 (5%)	0	100 100
3	M	124/137 (90%)	117 (94%)	7 (6%)	0	100 100
All	All	17904/21124 (85%)	17472 (98%)	423 (2%)	9 (0%)	49 79

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4117	ALA
1	E	4117	ALA
1	G	4117	ALA
1	J	4117	ALA
1	B	375	LYS

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	B	3658/4276 (86%)	3653 (100%)	5 (0%)	88	91
1	E	3658/4276 (86%)	3656 (100%)	2 (0%)	88	91
1	G	3658/4276 (86%)	3655 (100%)	3 (0%)	88	91
1	J	3658/4276 (86%)	3656 (100%)	2 (0%)	88	91
2	A	88/88 (100%)	88 (100%)	0	100	100
2	D	88/88 (100%)	88 (100%)	0	100	100
2	H	88/88 (100%)	88 (100%)	0	100	100
2	I	88/88 (100%)	88 (100%)	0	100	100
3	C	104/114 (91%)	104 (100%)	0	100	100
3	F	104/114 (91%)	104 (100%)	0	100	100
3	K	104/114 (91%)	104 (100%)	0	100	100
3	M	104/114 (91%)	104 (100%)	0	100	100
All	All	15400/17912 (86%)	15388 (100%)	12 (0%)	87	91

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	3069	HIS
1	G	3516	LYS
1	J	3516	LYS
1	G	3534	MET
1	B	3516	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 137 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	3734	HIS
1	J	3970	GLN
3	C	3	GLN
1	E	3069	HIS
1	E	3033	ASN

5.3.3 RNA

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

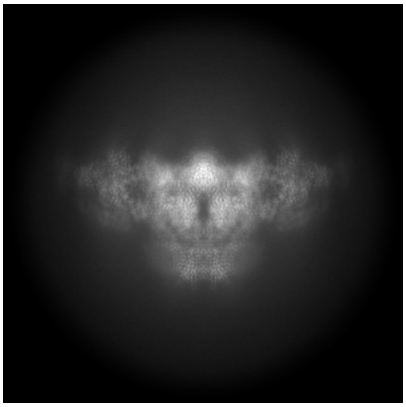
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19466. These allow visual inspection of the internal detail of the map and identification of artifacts.

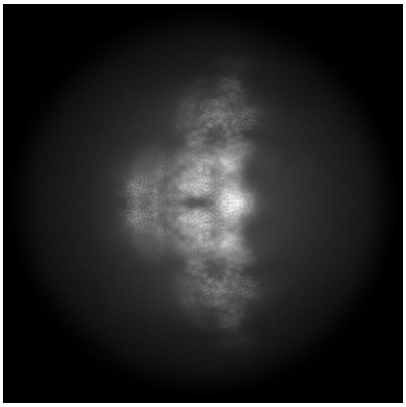
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

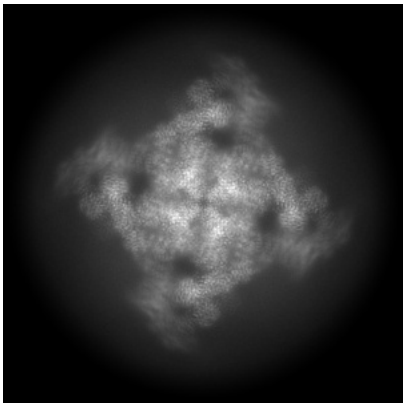
6.1.1 Primary map



X



Y

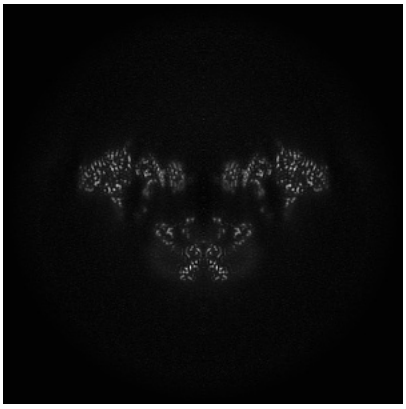


Z

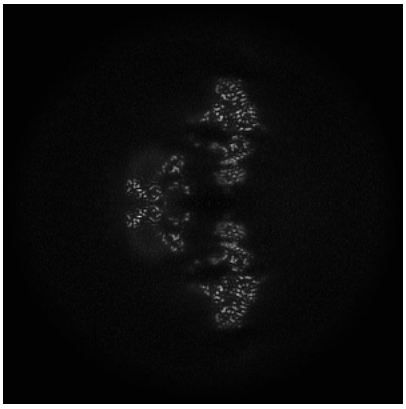
The images above show the map projected in three orthogonal directions.

6.2 Central slices

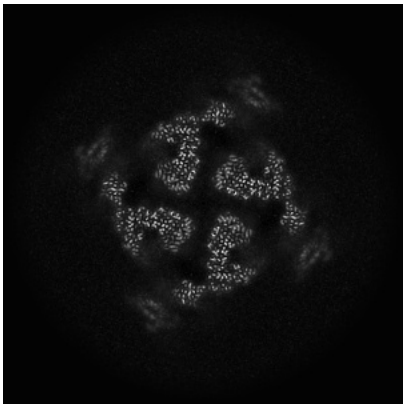
6.2.1 Primary map



X Index: 168



Y Index: 168



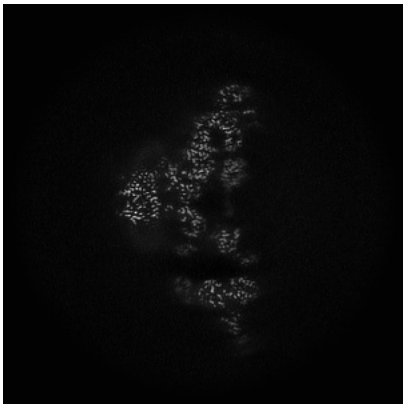
Z Index: 168

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

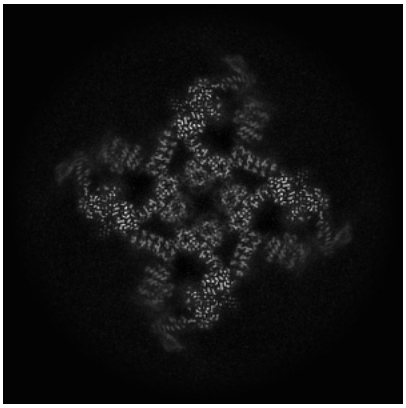
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 178



Y Index: 178

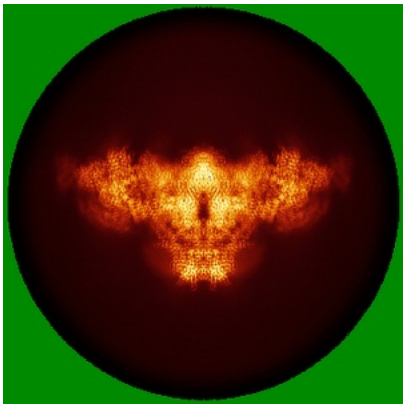


Z Index: 187

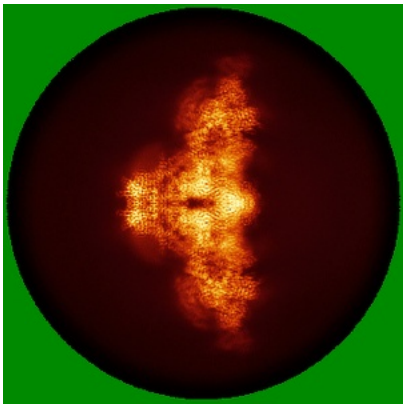
The images above show the largest variance slices of the map in three orthogonal directions.

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

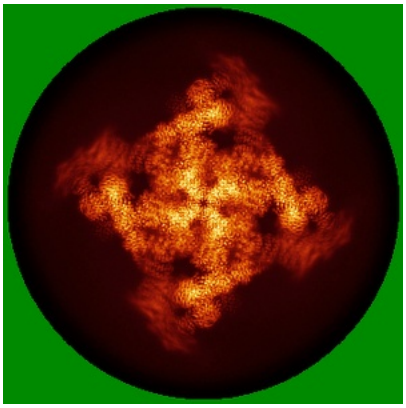
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

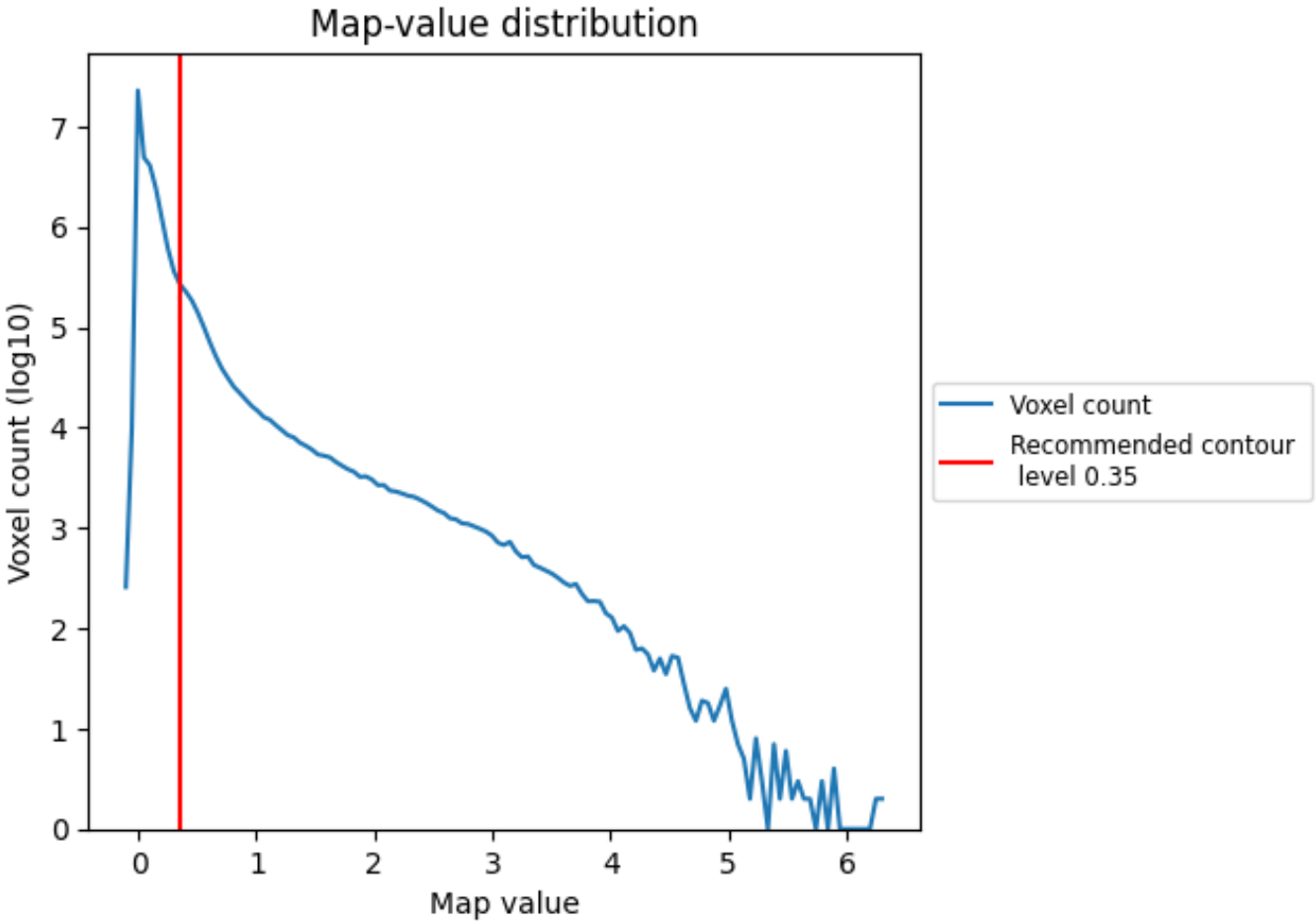
6.6 Mask visualisation (i)

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

7 Map analysis

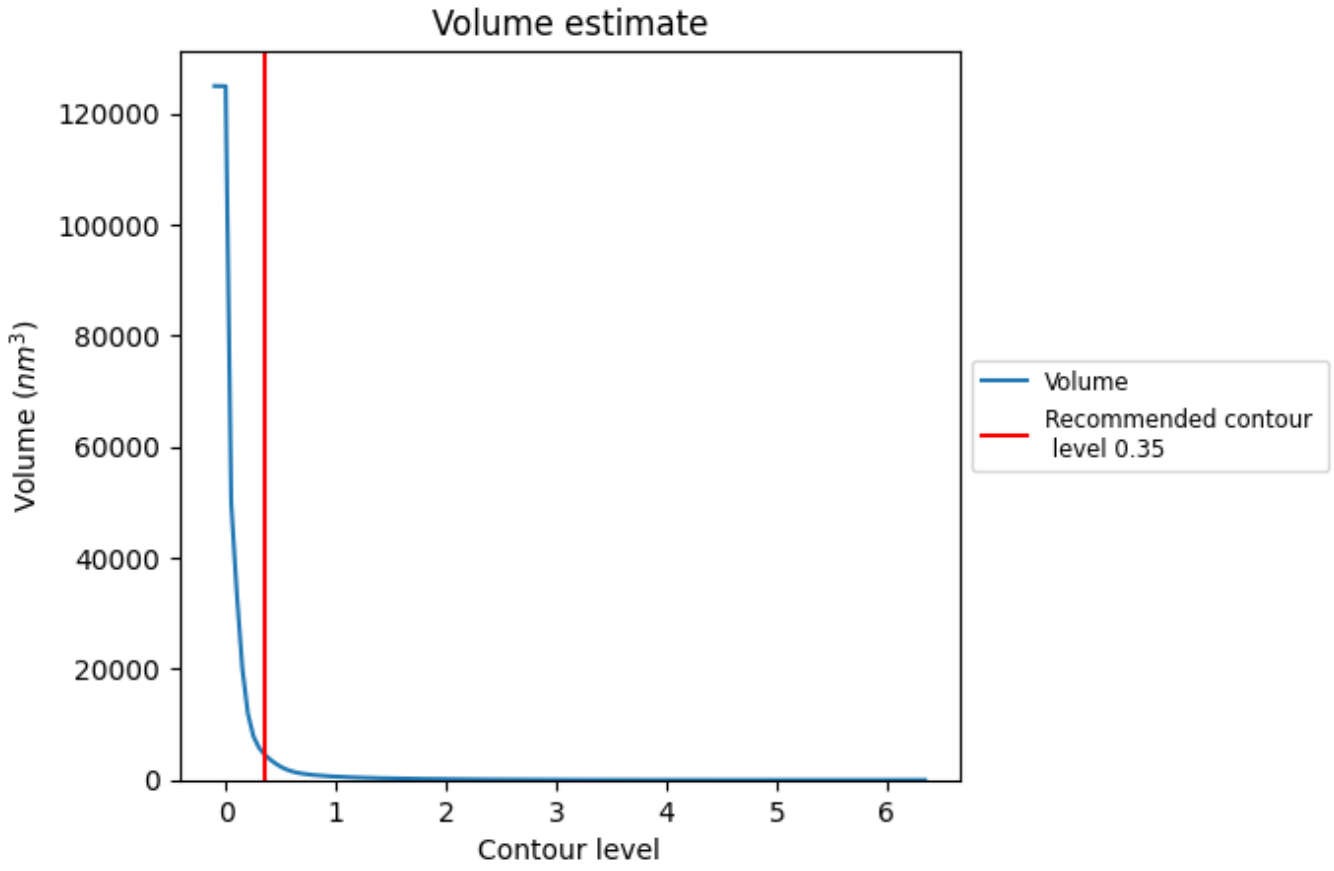
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

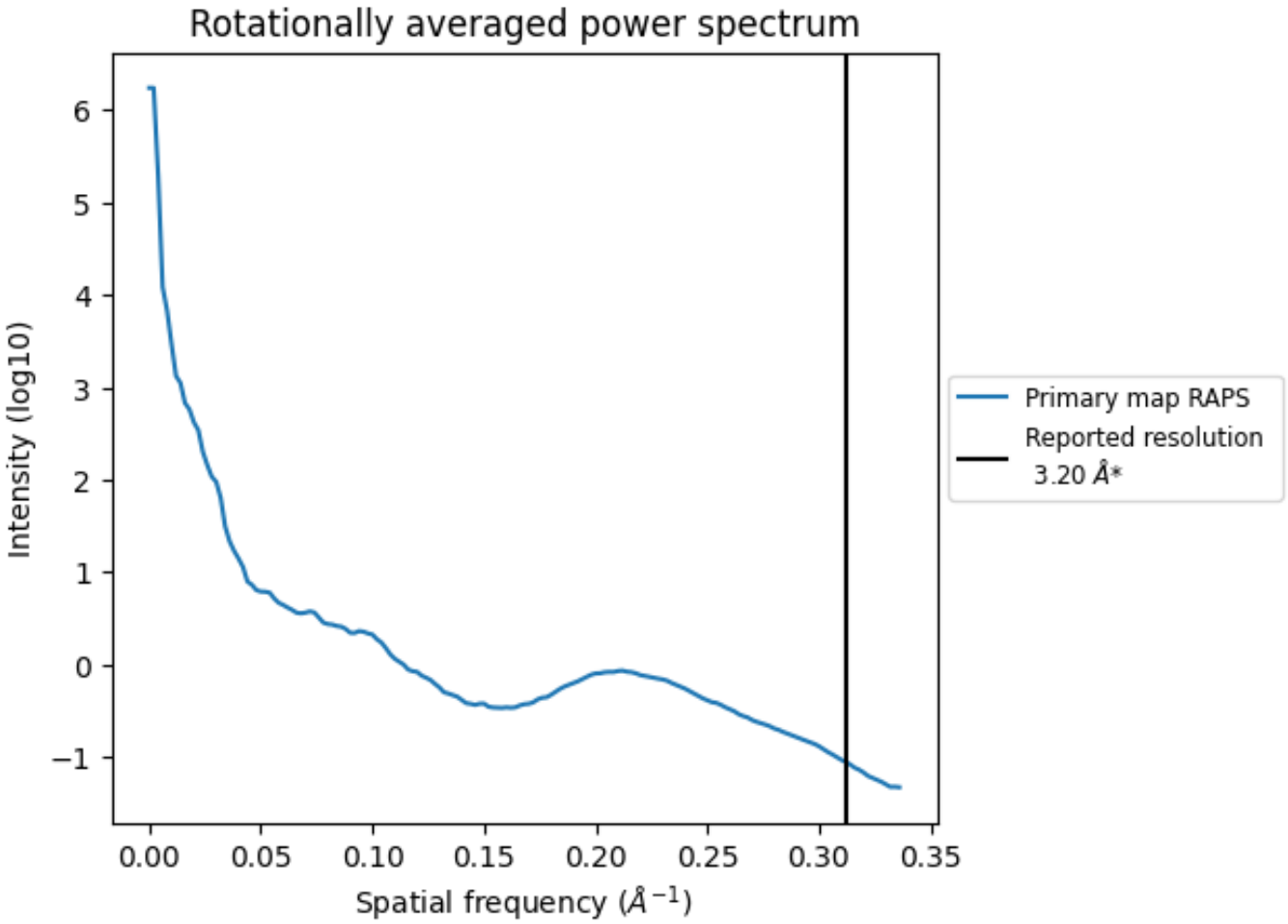
7.2 Volume estimate (i)



The volume at the recommended contour level is 4570 nm^3; this corresponds to an approximate mass of 4129 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)

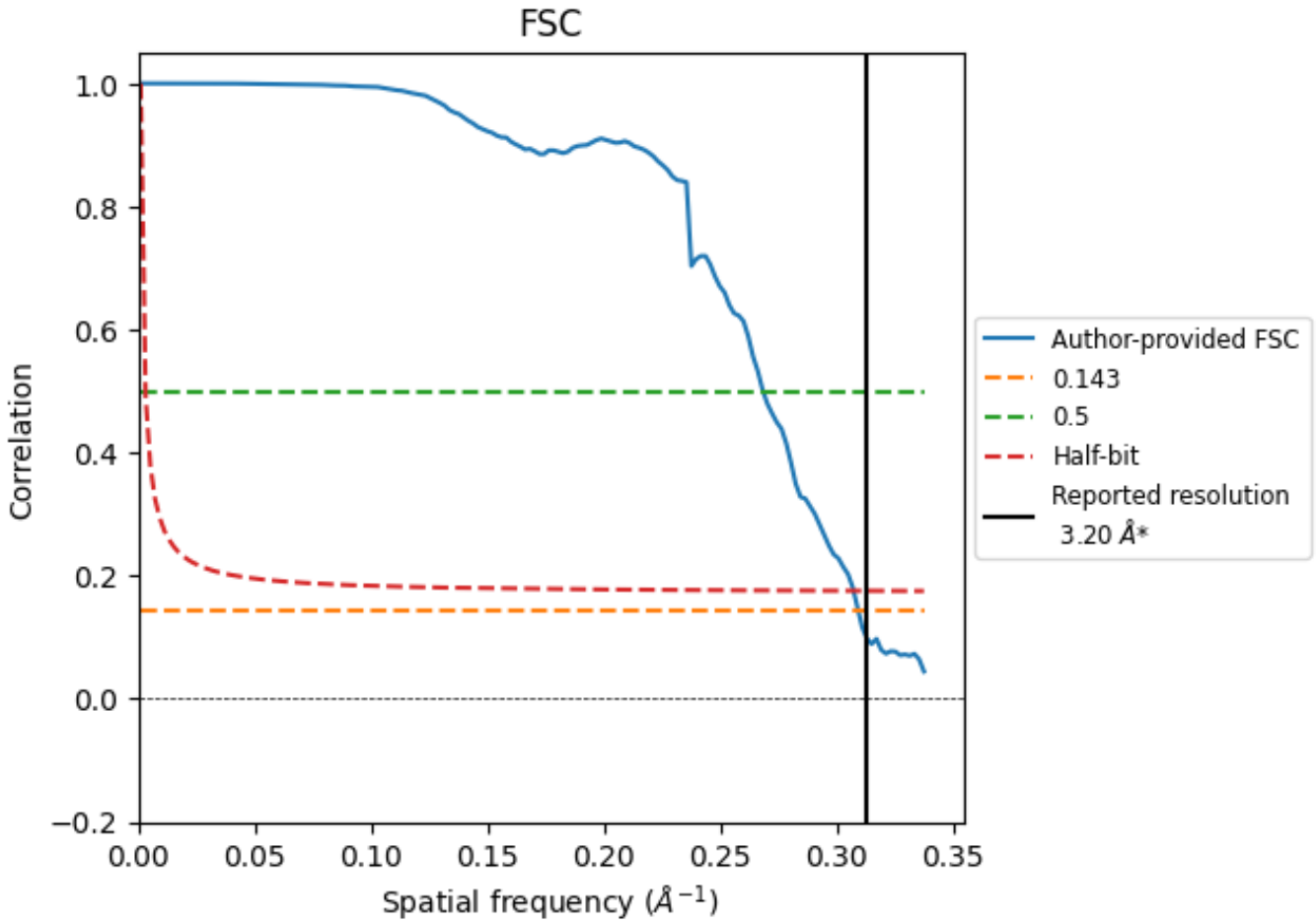


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

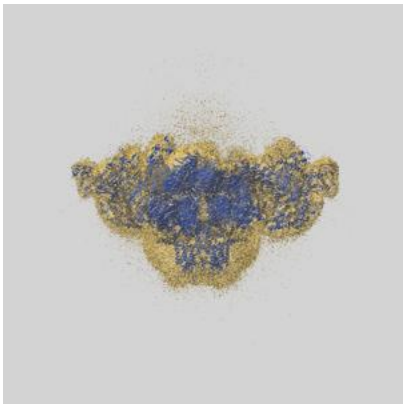
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.23	3.73	3.26
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

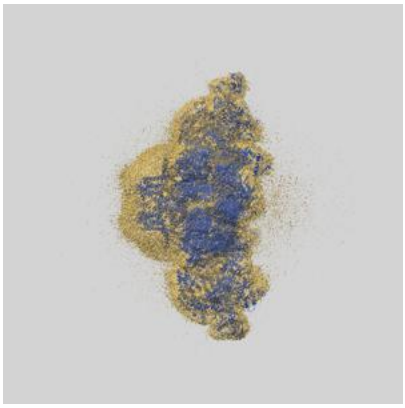
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19466 and PDB model 8RRV. Per-residue inclusion information can be found in section 3 on page 6.

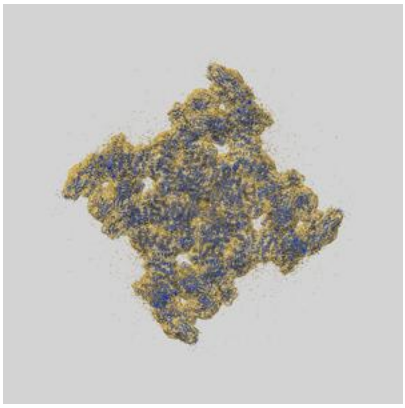
9.1 Map-model overlay



X



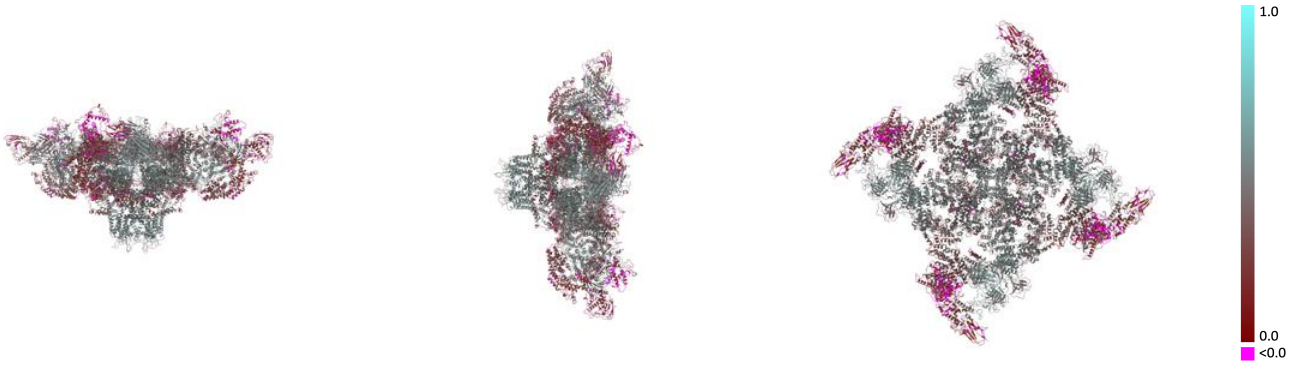
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

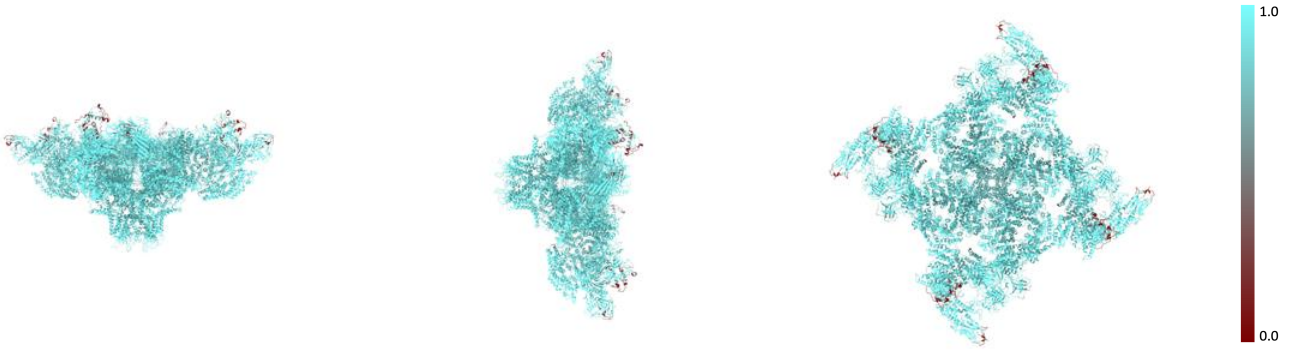
9.2 Q-score mapped to coordinate model (i)



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.

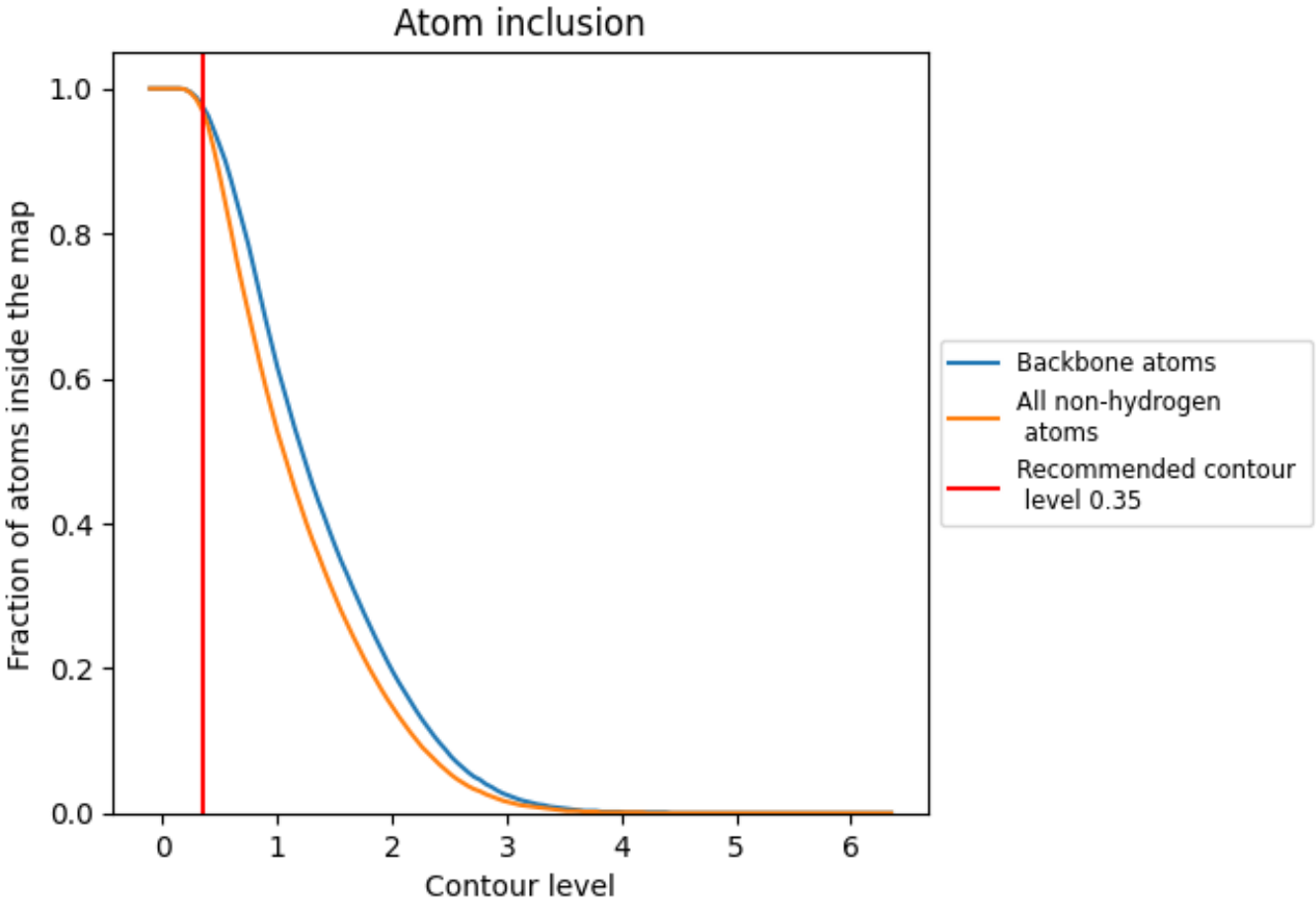
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9700	0.3800
A	0.8810	0.4120
B	0.9770	0.3850
C	0.7720	0.1480
D	0.8780	0.4170
E	0.9780	0.3850
F	0.7760	0.1480
G	0.9770	0.3850
H	0.8860	0.4150
I	0.8810	0.4170
J	0.9770	0.3860
K	0.7770	0.1480
M	0.7720	0.1500