



wwPDB EM Validation Summary Report i

Dec 7, 2022 – 04:08 PM JST

PDB ID : 7VMN
EMDB ID : EMD-33937
Title : Structure of recombinant RyR2 (EGTA dataset, class 2, closed state)
Authors : Kobayashi, T.; Tsutsumi, A.; Kurebayashi, N.; Kodama, M.; Kikkawa, M.; Murayama, T.; Ogawa, H.
Deposited on : 2021-10-09
Resolution : 3.50 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:

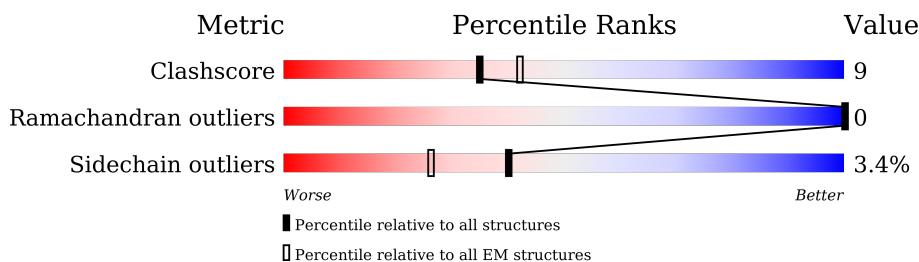
EMDB validation analysis : 0.0.1.dev43
MolProbit : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 123564 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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	4044	30071	19035	5243	5617	176	0	0
1	B	4044	30071	19035	5243	5617	176	0	0
1	C	4044	30071	19035	5243	5617	176	0	0
1	D	4044	30071	19035	5243	5617	176	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	107	819	516	144	155	4	0	0
2	H	107	819	516	144	155	4	0	0
2	I	107	819	516	144	155	4	0	0
2	J	107	819	516	144	155	4	0	0

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-67	MET	-	initiating methionine	UNP P68106
G	-66	GLY	-	expression tag	UNP P68106
G	-65	SER	-	expression tag	UNP P68106
G	-64	SER	-	expression tag	UNP P68106
G	-63	HIS	-	expression tag	UNP P68106
G	-62	HIS	-	expression tag	UNP P68106
G	-61	HIS	-	expression tag	UNP P68106
G	-60	HIS	-	expression tag	UNP P68106
G	-59	HIS	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-58	HIS	-	expression tag	UNP P68106
G	-57	SER	-	expression tag	UNP P68106
G	-56	SER	-	expression tag	UNP P68106
G	-55	GLY	-	expression tag	UNP P68106
G	-54	LEU	-	expression tag	UNP P68106
G	-53	VAL	-	expression tag	UNP P68106
G	-52	PRO	-	expression tag	UNP P68106
G	-51	ARG	-	expression tag	UNP P68106
G	-50	GLY	-	expression tag	UNP P68106
G	-49	SER	-	expression tag	UNP P68106
G	-48	HIS	-	expression tag	UNP P68106
G	-47	MET	-	expression tag	UNP P68106
G	-46	ALA	-	expression tag	UNP P68106
G	-45	SER	-	expression tag	UNP P68106
G	-44	MET	-	expression tag	UNP P68106
G	-43	ASP	-	expression tag	UNP P68106
G	-42	GLU	-	expression tag	UNP P68106
G	-41	LYS	-	expression tag	UNP P68106
G	-40	THR	-	expression tag	UNP P68106
G	-39	THR	-	expression tag	UNP P68106
G	-38	GLY	-	expression tag	UNP P68106
G	-37	TRP	-	expression tag	UNP P68106
G	-36	ARG	-	expression tag	UNP P68106
G	-35	GLY	-	expression tag	UNP P68106
G	-34	GLY	-	expression tag	UNP P68106
G	-33	HIS	-	expression tag	UNP P68106
G	-32	VAL	-	expression tag	UNP P68106
G	-31	VAL	-	expression tag	UNP P68106
G	-30	GLU	-	expression tag	UNP P68106
G	-29	GLY	-	expression tag	UNP P68106
G	-28	LEU	-	expression tag	UNP P68106
G	-27	ALA	-	expression tag	UNP P68106
G	-26	GLY	-	expression tag	UNP P68106
G	-25	GLU	-	expression tag	UNP P68106
G	-24	LEU	-	expression tag	UNP P68106
G	-23	GLU	-	expression tag	UNP P68106
G	-22	GLN	-	expression tag	UNP P68106
G	-21	LEU	-	expression tag	UNP P68106
G	-20	ARG	-	expression tag	UNP P68106
G	-19	ALA	-	expression tag	UNP P68106
G	-18	ARG	-	expression tag	UNP P68106
G	-17	LEU	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-16	GLU	-	expression tag	UNP P68106
G	-15	HIS	-	expression tag	UNP P68106
G	-14	HIS	-	expression tag	UNP P68106
G	-13	PRO	-	expression tag	UNP P68106
G	-12	GLN	-	expression tag	UNP P68106
G	-11	GLY	-	expression tag	UNP P68106
G	-10	GLN	-	expression tag	UNP P68106
G	-9	ARG	-	expression tag	UNP P68106
G	-8	GLU	-	expression tag	UNP P68106
G	-7	PRO	-	expression tag	UNP P68106
G	-6	GLY	-	expression tag	UNP P68106
G	-5	SER	-	expression tag	UNP P68106
G	-4	GLY	-	expression tag	UNP P68106
G	-3	GLY	-	expression tag	UNP P68106
G	-2	SER	-	expression tag	UNP P68106
G	-1	GLY	-	expression tag	UNP P68106
G	0	GLY	-	expression tag	UNP P68106
G	1	THR	-	expression tag	UNP P68106
H	-67	MET	-	initiating methionine	UNP P68106
H	-66	GLY	-	expression tag	UNP P68106
H	-65	SER	-	expression tag	UNP P68106
H	-64	SER	-	expression tag	UNP P68106
H	-63	HIS	-	expression tag	UNP P68106
H	-62	HIS	-	expression tag	UNP P68106
H	-61	HIS	-	expression tag	UNP P68106
H	-60	HIS	-	expression tag	UNP P68106
H	-59	HIS	-	expression tag	UNP P68106
H	-58	HIS	-	expression tag	UNP P68106
H	-57	SER	-	expression tag	UNP P68106
H	-56	SER	-	expression tag	UNP P68106
H	-55	GLY	-	expression tag	UNP P68106
H	-54	LEU	-	expression tag	UNP P68106
H	-53	VAL	-	expression tag	UNP P68106
H	-52	PRO	-	expression tag	UNP P68106
H	-51	ARG	-	expression tag	UNP P68106
H	-50	GLY	-	expression tag	UNP P68106
H	-49	SER	-	expression tag	UNP P68106
H	-48	HIS	-	expression tag	UNP P68106
H	-47	MET	-	expression tag	UNP P68106
H	-46	ALA	-	expression tag	UNP P68106
H	-45	SER	-	expression tag	UNP P68106
H	-44	MET	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-43	ASP	-	expression tag	UNP P68106
H	-42	GLU	-	expression tag	UNP P68106
H	-41	LYS	-	expression tag	UNP P68106
H	-40	THR	-	expression tag	UNP P68106
H	-39	THR	-	expression tag	UNP P68106
H	-38	GLY	-	expression tag	UNP P68106
H	-37	TRP	-	expression tag	UNP P68106
H	-36	ARG	-	expression tag	UNP P68106
H	-35	GLY	-	expression tag	UNP P68106
H	-34	GLY	-	expression tag	UNP P68106
H	-33	HIS	-	expression tag	UNP P68106
H	-32	VAL	-	expression tag	UNP P68106
H	-31	VAL	-	expression tag	UNP P68106
H	-30	GLU	-	expression tag	UNP P68106
H	-29	GLY	-	expression tag	UNP P68106
H	-28	LEU	-	expression tag	UNP P68106
H	-27	ALA	-	expression tag	UNP P68106
H	-26	GLY	-	expression tag	UNP P68106
H	-25	GLU	-	expression tag	UNP P68106
H	-24	LEU	-	expression tag	UNP P68106
H	-23	GLU	-	expression tag	UNP P68106
H	-22	GLN	-	expression tag	UNP P68106
H	-21	LEU	-	expression tag	UNP P68106
H	-20	ARG	-	expression tag	UNP P68106
H	-19	ALA	-	expression tag	UNP P68106
H	-18	ARG	-	expression tag	UNP P68106
H	-17	LEU	-	expression tag	UNP P68106
H	-16	GLU	-	expression tag	UNP P68106
H	-15	HIS	-	expression tag	UNP P68106
H	-14	HIS	-	expression tag	UNP P68106
H	-13	PRO	-	expression tag	UNP P68106
H	-12	GLN	-	expression tag	UNP P68106
H	-11	GLY	-	expression tag	UNP P68106
H	-10	GLN	-	expression tag	UNP P68106
H	-9	ARG	-	expression tag	UNP P68106
H	-8	GLU	-	expression tag	UNP P68106
H	-7	PRO	-	expression tag	UNP P68106
H	-6	GLY	-	expression tag	UNP P68106
H	-5	SER	-	expression tag	UNP P68106
H	-4	GLY	-	expression tag	UNP P68106
H	-3	GLY	-	expression tag	UNP P68106
H	-2	SER	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	GLY	-	expression tag	UNP P68106
H	0	GLY	-	expression tag	UNP P68106
H	1	THR	-	expression tag	UNP P68106
I	-67	MET	-	initiating methionine	UNP P68106
I	-66	GLY	-	expression tag	UNP P68106
I	-65	SER	-	expression tag	UNP P68106
I	-64	SER	-	expression tag	UNP P68106
I	-63	HIS	-	expression tag	UNP P68106
I	-62	HIS	-	expression tag	UNP P68106
I	-61	HIS	-	expression tag	UNP P68106
I	-60	HIS	-	expression tag	UNP P68106
I	-59	HIS	-	expression tag	UNP P68106
I	-58	HIS	-	expression tag	UNP P68106
I	-57	SER	-	expression tag	UNP P68106
I	-56	SER	-	expression tag	UNP P68106
I	-55	GLY	-	expression tag	UNP P68106
I	-54	LEU	-	expression tag	UNP P68106
I	-53	VAL	-	expression tag	UNP P68106
I	-52	PRO	-	expression tag	UNP P68106
I	-51	ARG	-	expression tag	UNP P68106
I	-50	GLY	-	expression tag	UNP P68106
I	-49	SER	-	expression tag	UNP P68106
I	-48	HIS	-	expression tag	UNP P68106
I	-47	MET	-	expression tag	UNP P68106
I	-46	ALA	-	expression tag	UNP P68106
I	-45	SER	-	expression tag	UNP P68106
I	-44	MET	-	expression tag	UNP P68106
I	-43	ASP	-	expression tag	UNP P68106
I	-42	GLU	-	expression tag	UNP P68106
I	-41	LYS	-	expression tag	UNP P68106
I	-40	THR	-	expression tag	UNP P68106
I	-39	THR	-	expression tag	UNP P68106
I	-38	GLY	-	expression tag	UNP P68106
I	-37	TRP	-	expression tag	UNP P68106
I	-36	ARG	-	expression tag	UNP P68106
I	-35	GLY	-	expression tag	UNP P68106
I	-34	GLY	-	expression tag	UNP P68106
I	-33	HIS	-	expression tag	UNP P68106
I	-32	VAL	-	expression tag	UNP P68106
I	-31	VAL	-	expression tag	UNP P68106
I	-30	GLU	-	expression tag	UNP P68106
I	-29	GLY	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-28	LEU	-	expression tag	UNP P68106
I	-27	ALA	-	expression tag	UNP P68106
I	-26	GLY	-	expression tag	UNP P68106
I	-25	GLU	-	expression tag	UNP P68106
I	-24	LEU	-	expression tag	UNP P68106
I	-23	GLU	-	expression tag	UNP P68106
I	-22	GLN	-	expression tag	UNP P68106
I	-21	LEU	-	expression tag	UNP P68106
I	-20	ARG	-	expression tag	UNP P68106
I	-19	ALA	-	expression tag	UNP P68106
I	-18	ARG	-	expression tag	UNP P68106
I	-17	LEU	-	expression tag	UNP P68106
I	-16	GLU	-	expression tag	UNP P68106
I	-15	HIS	-	expression tag	UNP P68106
I	-14	HIS	-	expression tag	UNP P68106
I	-13	PRO	-	expression tag	UNP P68106
I	-12	GLN	-	expression tag	UNP P68106
I	-11	GLY	-	expression tag	UNP P68106
I	-10	GLN	-	expression tag	UNP P68106
I	-9	ARG	-	expression tag	UNP P68106
I	-8	GLU	-	expression tag	UNP P68106
I	-7	PRO	-	expression tag	UNP P68106
I	-6	GLY	-	expression tag	UNP P68106
I	-5	SER	-	expression tag	UNP P68106
I	-4	GLY	-	expression tag	UNP P68106
I	-3	GLY	-	expression tag	UNP P68106
I	-2	SER	-	expression tag	UNP P68106
I	-1	GLY	-	expression tag	UNP P68106
I	0	GLY	-	expression tag	UNP P68106
I	1	THR	-	expression tag	UNP P68106
J	-67	MET	-	initiating methionine	UNP P68106
J	-66	GLY	-	expression tag	UNP P68106
J	-65	SER	-	expression tag	UNP P68106
J	-64	SER	-	expression tag	UNP P68106
J	-63	HIS	-	expression tag	UNP P68106
J	-62	HIS	-	expression tag	UNP P68106
J	-61	HIS	-	expression tag	UNP P68106
J	-60	HIS	-	expression tag	UNP P68106
J	-59	HIS	-	expression tag	UNP P68106
J	-58	HIS	-	expression tag	UNP P68106
J	-57	SER	-	expression tag	UNP P68106
J	-56	SER	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-55	GLY	-	expression tag	UNP P68106
J	-54	LEU	-	expression tag	UNP P68106
J	-53	VAL	-	expression tag	UNP P68106
J	-52	PRO	-	expression tag	UNP P68106
J	-51	ARG	-	expression tag	UNP P68106
J	-50	GLY	-	expression tag	UNP P68106
J	-49	SER	-	expression tag	UNP P68106
J	-48	HIS	-	expression tag	UNP P68106
J	-47	MET	-	expression tag	UNP P68106
J	-46	ALA	-	expression tag	UNP P68106
J	-45	SER	-	expression tag	UNP P68106
J	-44	MET	-	expression tag	UNP P68106
J	-43	ASP	-	expression tag	UNP P68106
J	-42	GLU	-	expression tag	UNP P68106
J	-41	LYS	-	expression tag	UNP P68106
J	-40	THR	-	expression tag	UNP P68106
J	-39	THR	-	expression tag	UNP P68106
J	-38	GLY	-	expression tag	UNP P68106
J	-37	TRP	-	expression tag	UNP P68106
J	-36	ARG	-	expression tag	UNP P68106
J	-35	GLY	-	expression tag	UNP P68106
J	-34	GLY	-	expression tag	UNP P68106
J	-33	HIS	-	expression tag	UNP P68106
J	-32	VAL	-	expression tag	UNP P68106
J	-31	VAL	-	expression tag	UNP P68106
J	-30	GLU	-	expression tag	UNP P68106
J	-29	GLY	-	expression tag	UNP P68106
J	-28	LEU	-	expression tag	UNP P68106
J	-27	ALA	-	expression tag	UNP P68106
J	-26	GLY	-	expression tag	UNP P68106
J	-25	GLU	-	expression tag	UNP P68106
J	-24	LEU	-	expression tag	UNP P68106
J	-23	GLU	-	expression tag	UNP P68106
J	-22	GLN	-	expression tag	UNP P68106
J	-21	LEU	-	expression tag	UNP P68106
J	-20	ARG	-	expression tag	UNP P68106
J	-19	ALA	-	expression tag	UNP P68106
J	-18	ARG	-	expression tag	UNP P68106
J	-17	LEU	-	expression tag	UNP P68106
J	-16	GLU	-	expression tag	UNP P68106
J	-15	HIS	-	expression tag	UNP P68106
J	-14	HIS	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-13	PRO	-	expression tag	UNP P68106
J	-12	GLN	-	expression tag	UNP P68106
J	-11	GLY	-	expression tag	UNP P68106
J	-10	GLN	-	expression tag	UNP P68106
J	-9	ARG	-	expression tag	UNP P68106
J	-8	GLU	-	expression tag	UNP P68106
J	-7	PRO	-	expression tag	UNP P68106
J	-6	GLY	-	expression tag	UNP P68106
J	-5	SER	-	expression tag	UNP P68106
J	-4	GLY	-	expression tag	UNP P68106
J	-3	GLY	-	expression tag	UNP P68106
J	-2	SER	-	expression tag	UNP P68106
J	-1	GLY	-	expression tag	UNP P68106
J	0	GLY	-	expression tag	UNP P68106
J	1	THR	-	expression tag	UNP P68106

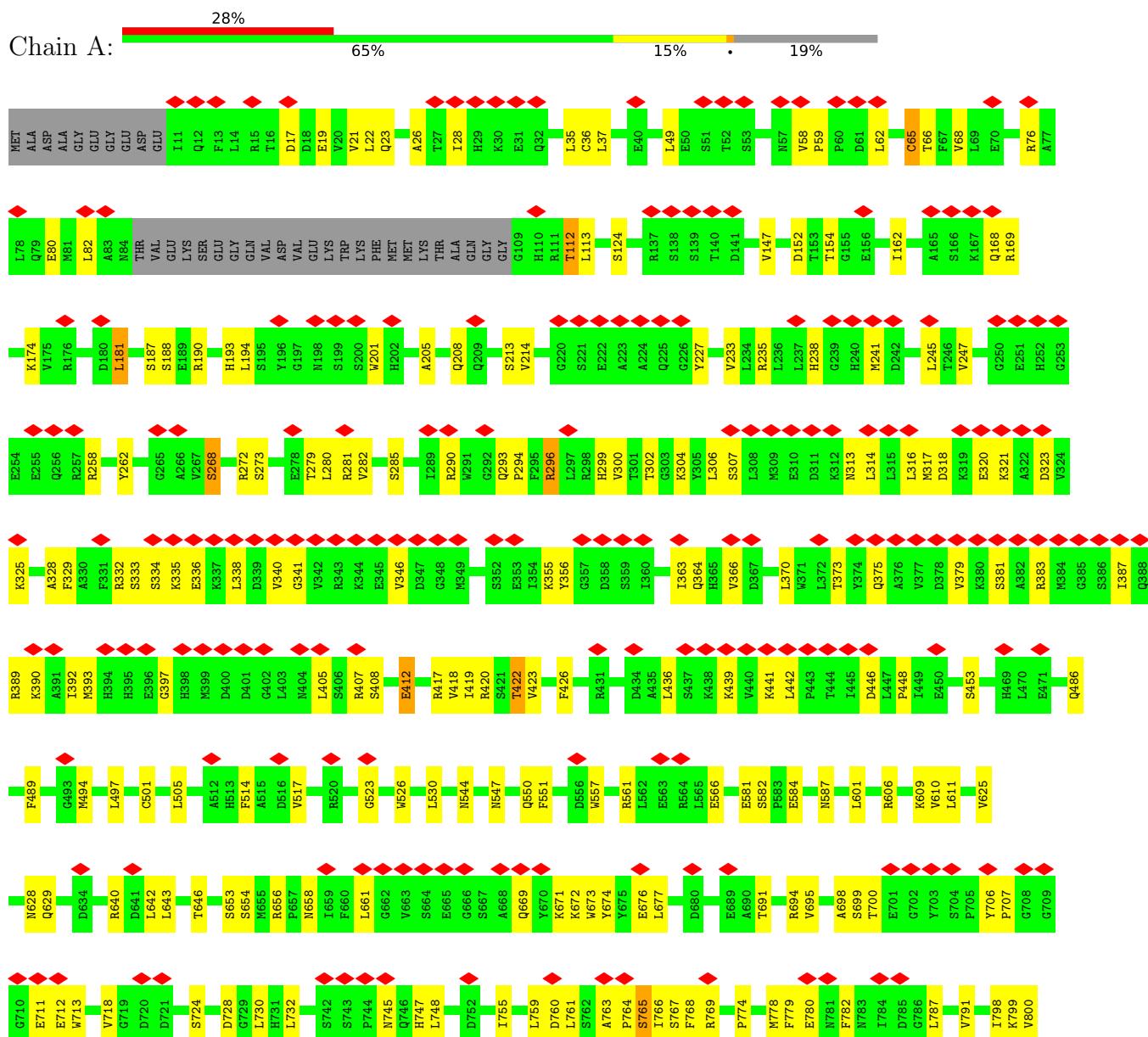
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

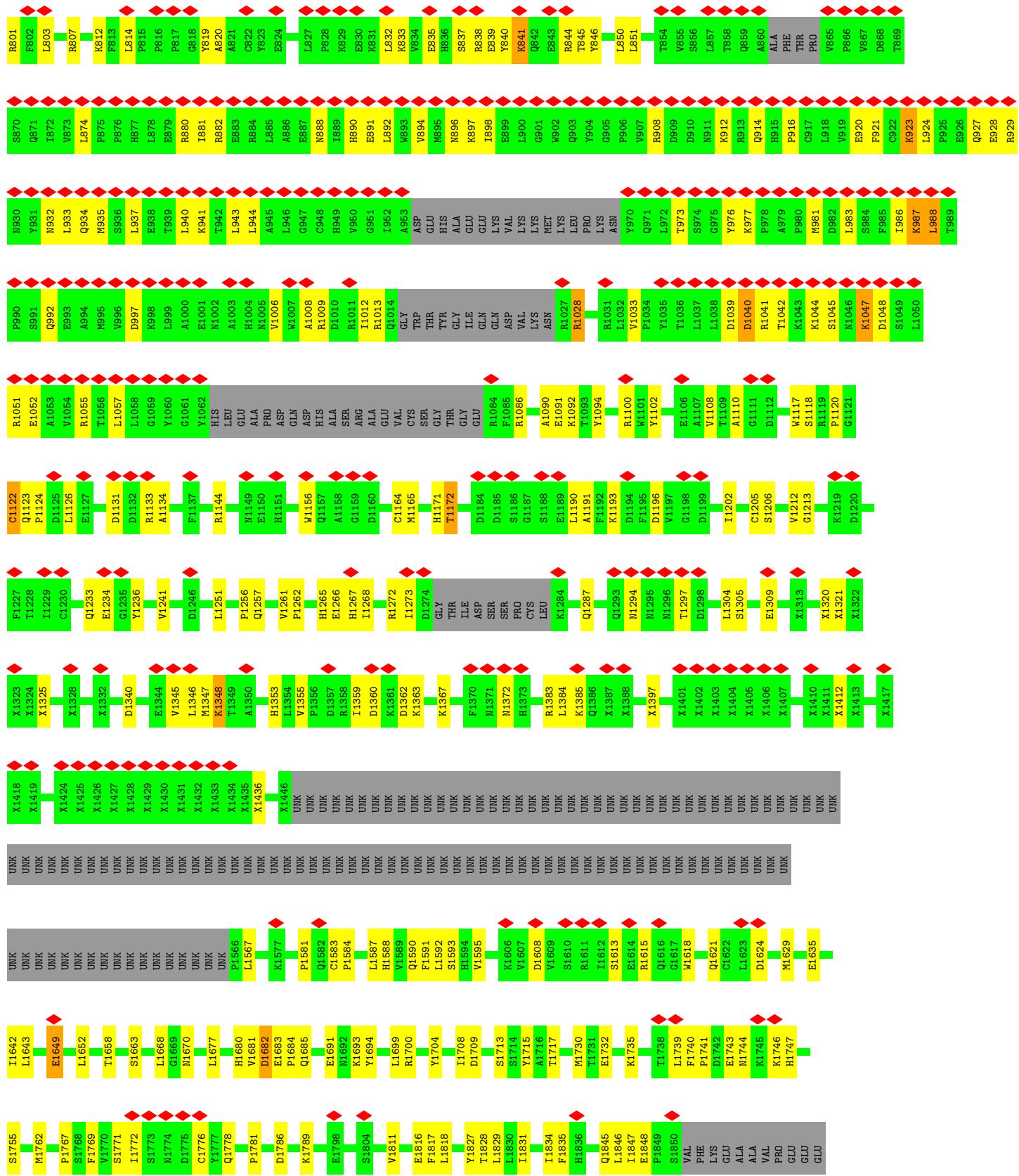
Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Zn 1 1	0
3	B	1	Total Zn 1 1	0
3	C	1	Total Zn 1 1	0
3	D	1	Total Zn 1 1	0

3 Residue-property plots

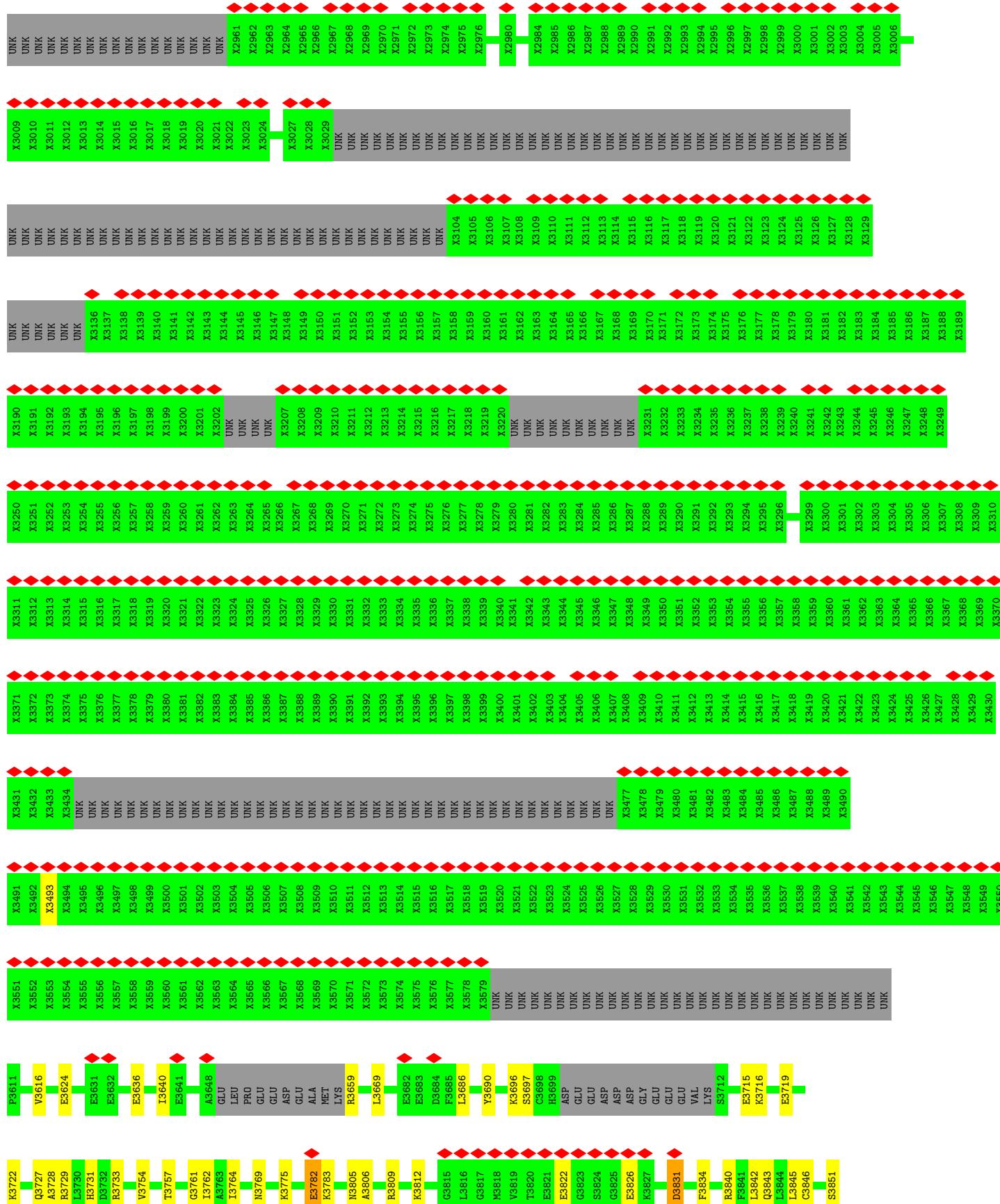
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

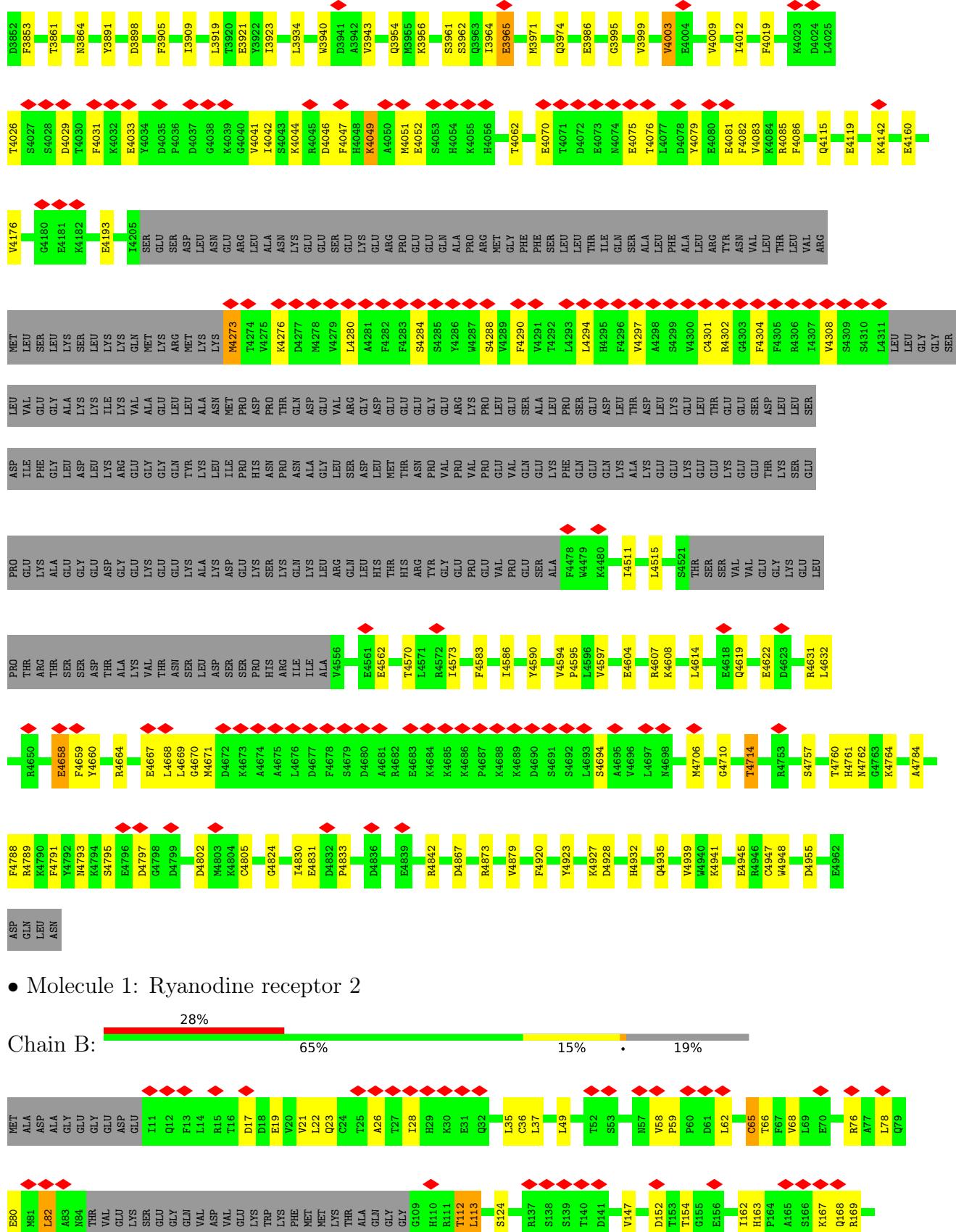
- Molecule 1: Ryanodine receptor 2

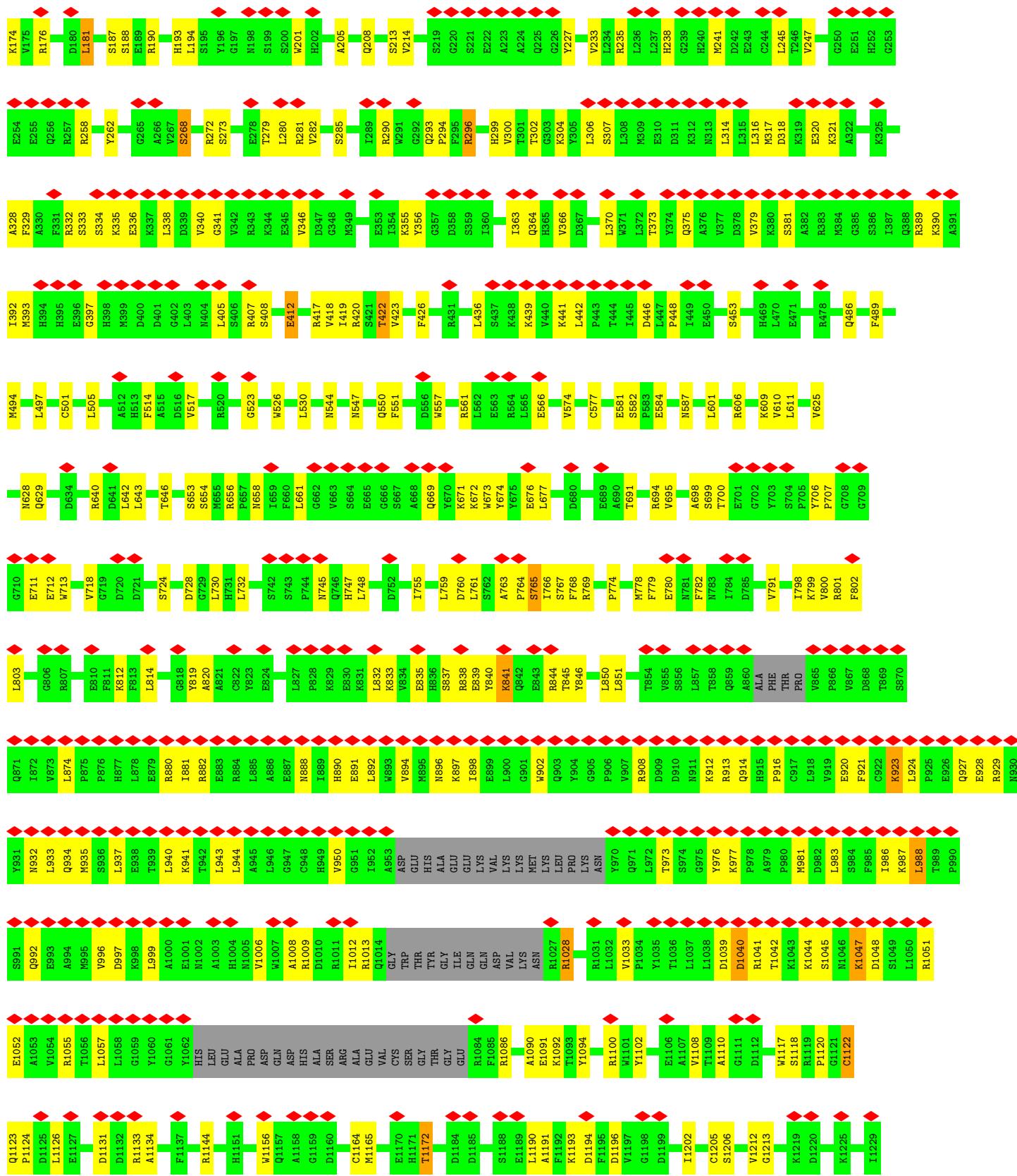


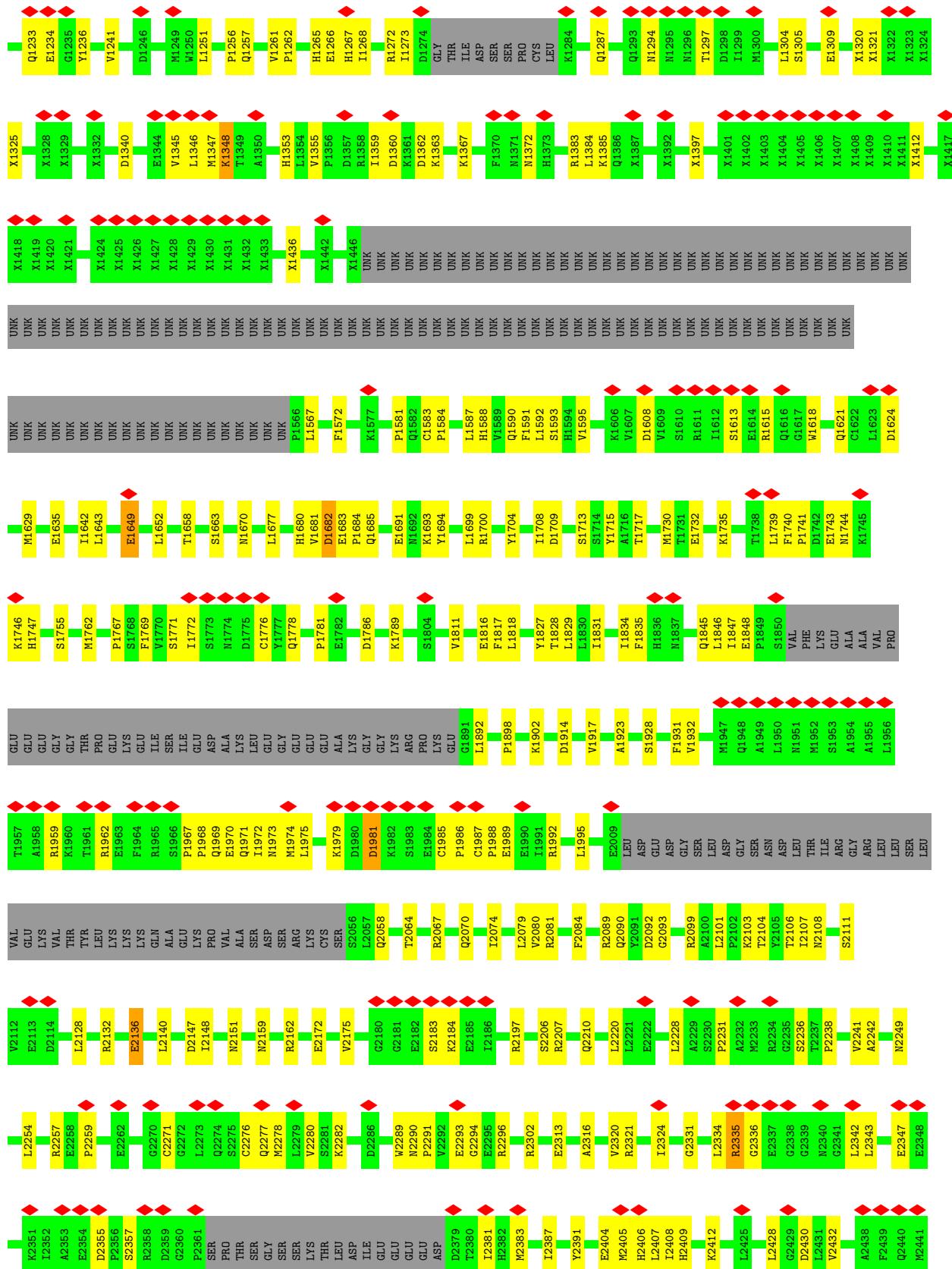


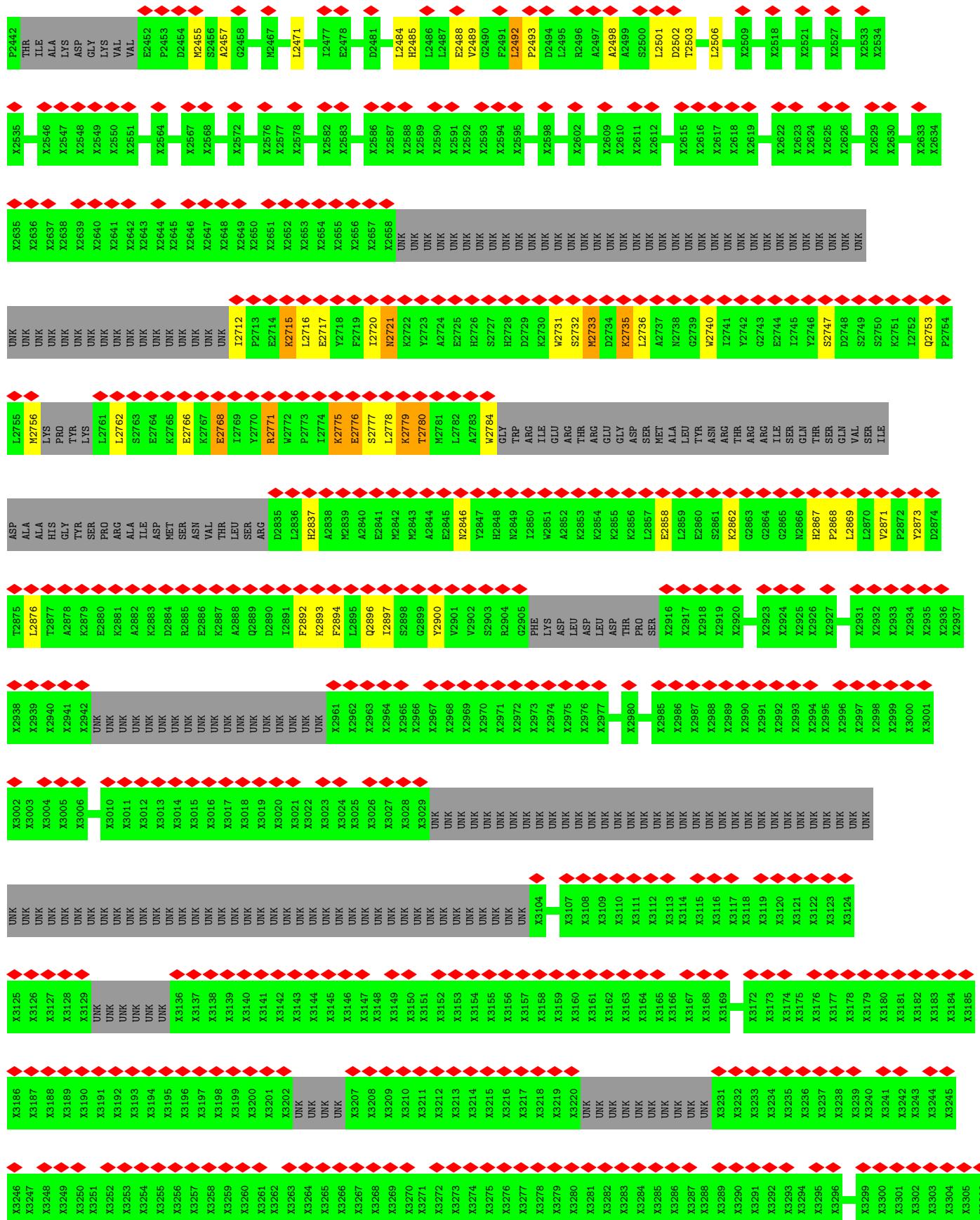


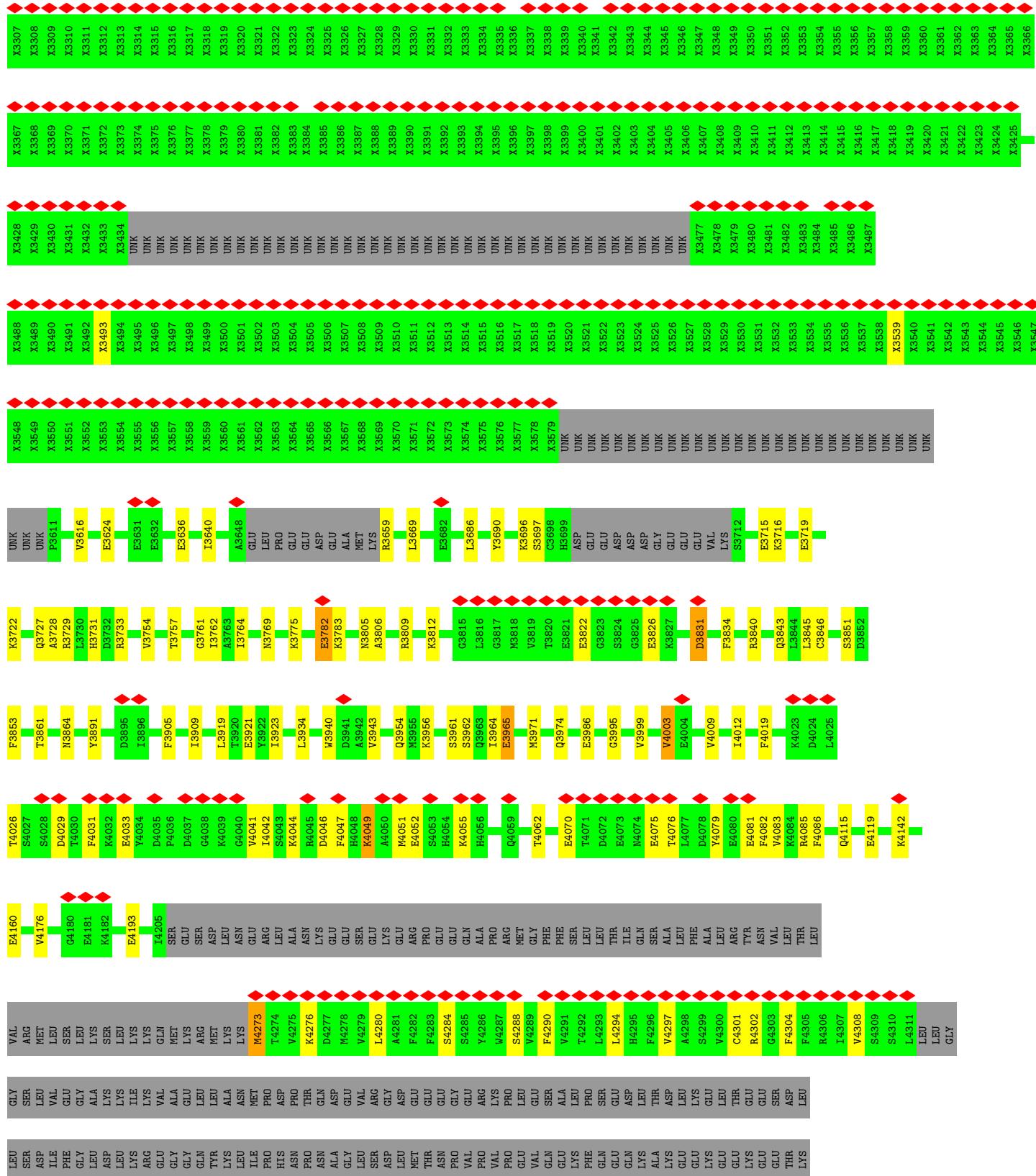


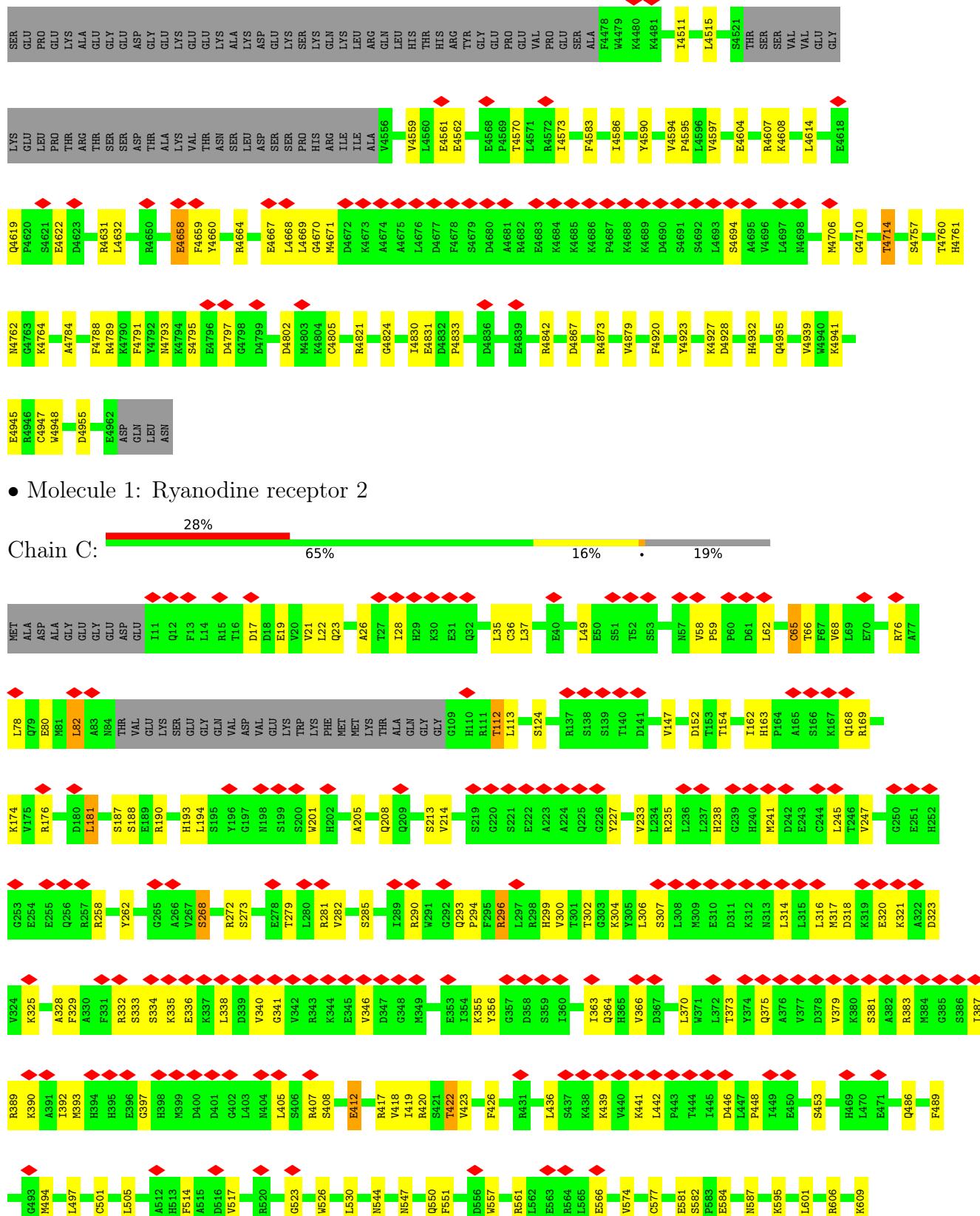


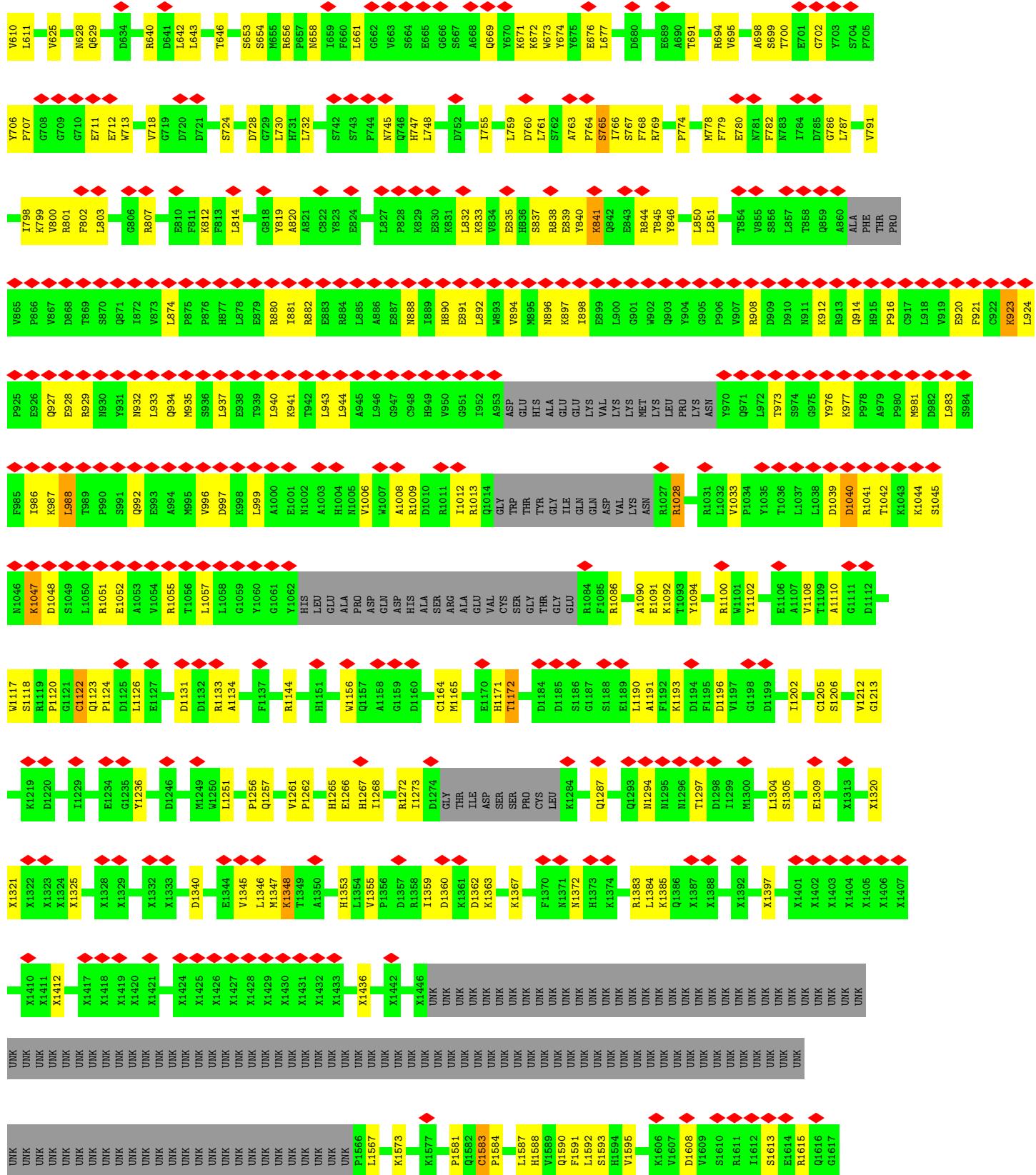


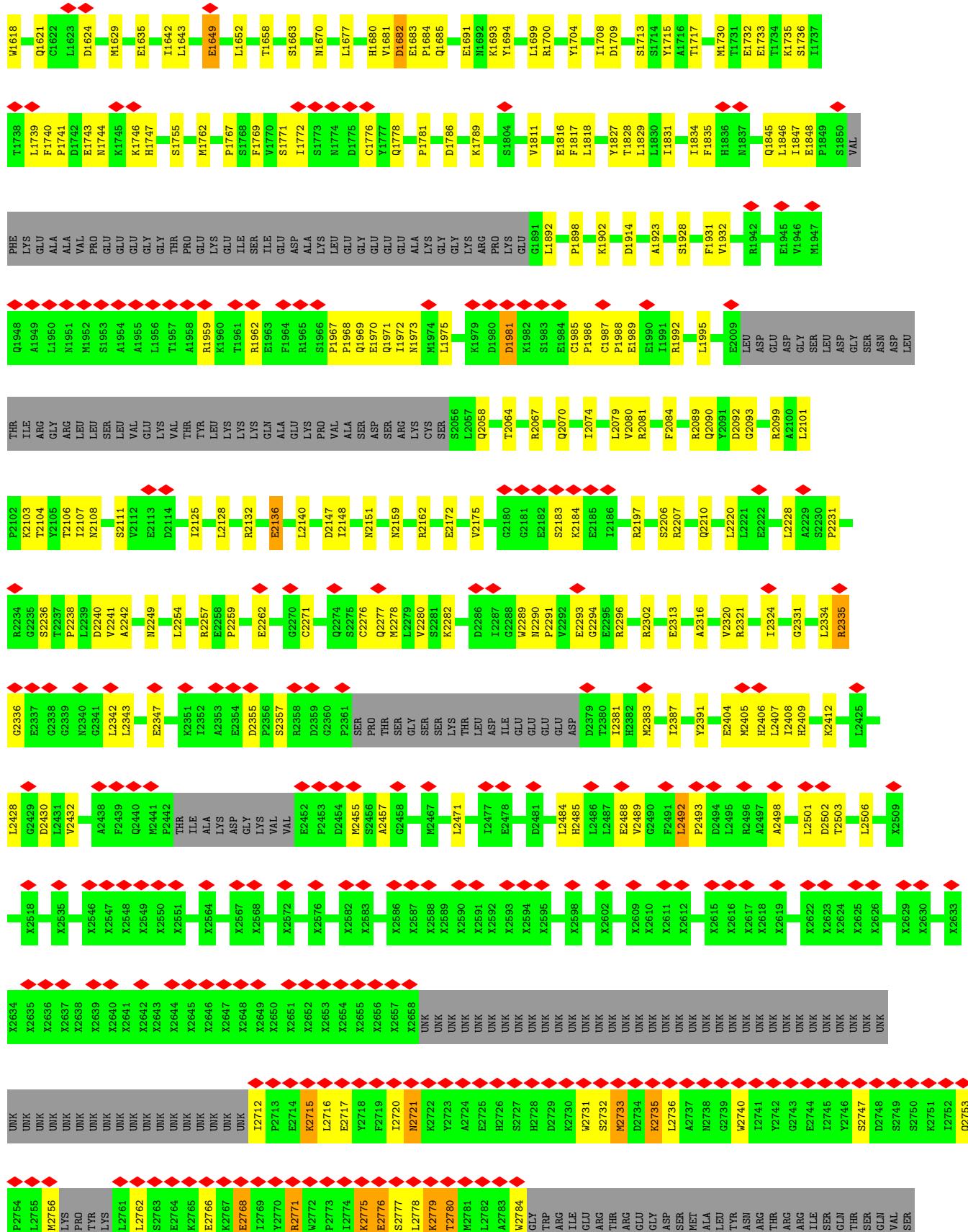




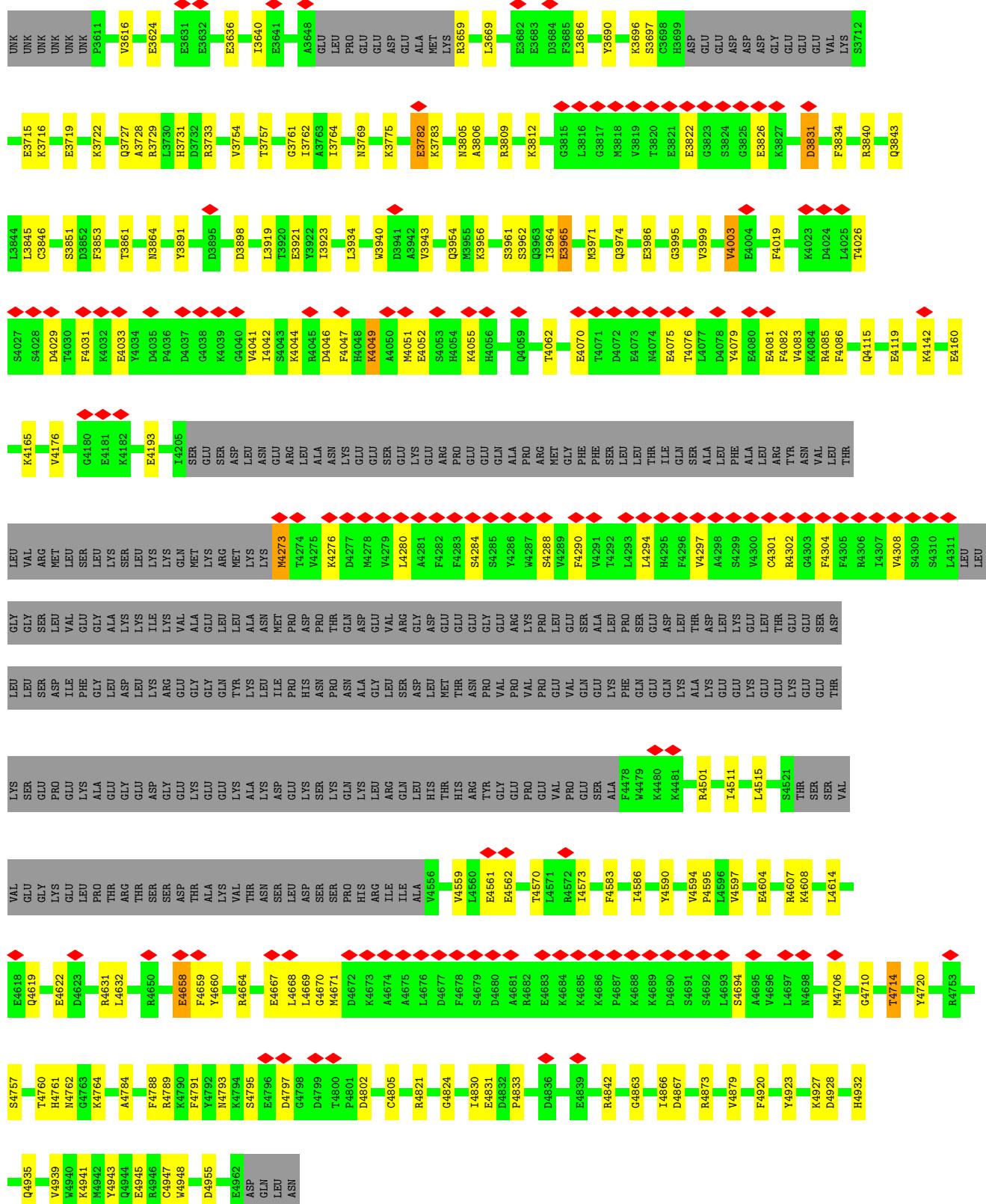








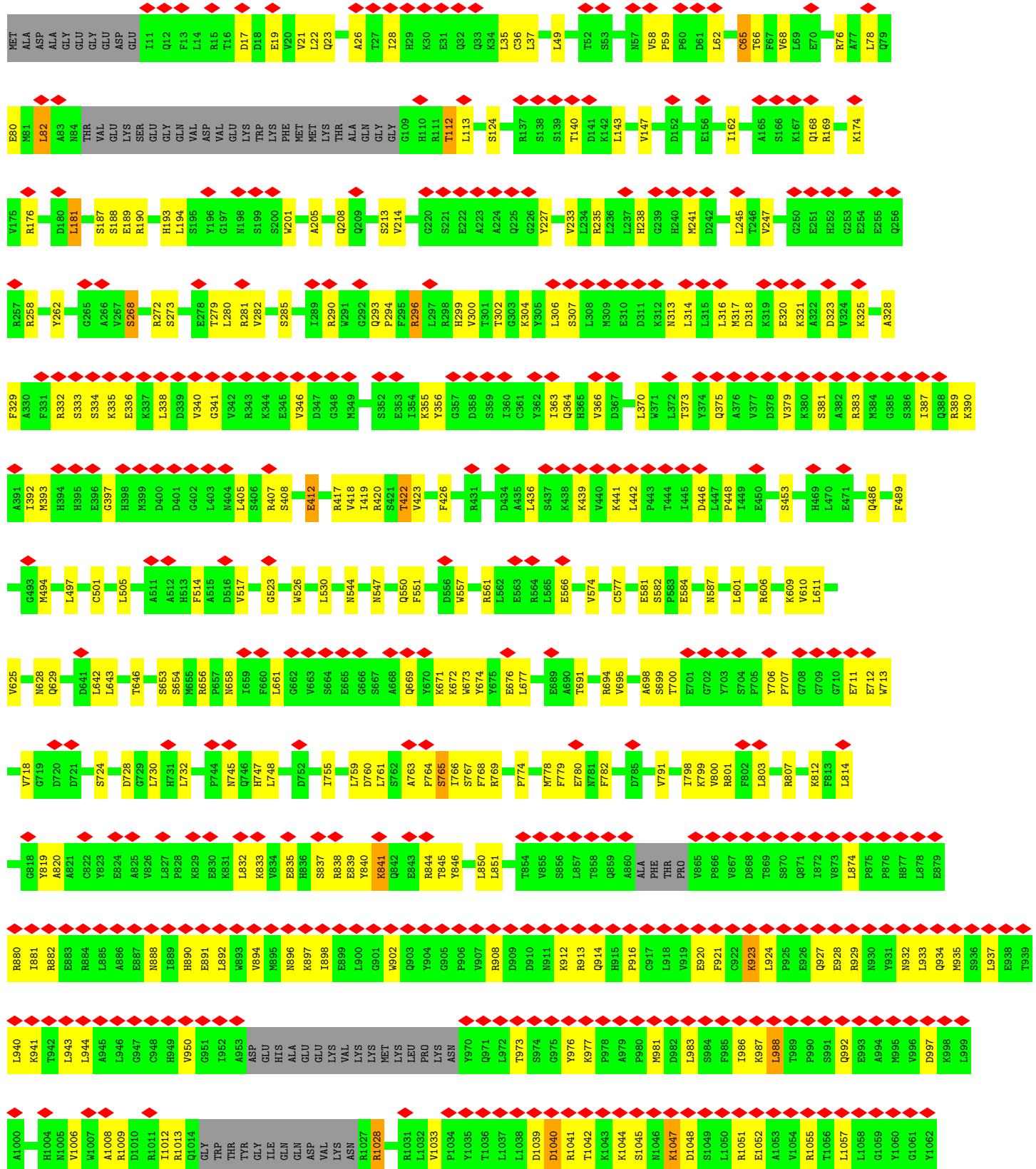
X3545	X3304	X3183	X3122	D2874
X3546	X3305	X3184	X3123	T2875
X3547	X3306	X3185	X3124	L2876
X3548	X3307	X3186	X3125	T2877
X3549	X3308	X3187	X3126	GLY
X3490	X3309	X3188	X3127	TYR
X3491	X3310	X3189	X3128	SER
X3551	X3311	X3190	X3129	PRO
X3552	X3312	X3191	X3130	ARG
X3553	X3313	X3192	X3011	ALA
X3554	X3314	X3193	X3012	ALA
X3555	X3315	X3194	X3013	ALA
X3556	X3316	X3195	X3014	ALA
X3557	X3317	X3196	X3015	ALA
X3558	X3318	X3197	X3016	ALA
X3559	X3319	X3198	X3017	ALA
X3560	X3320	X3199	X3018	ALA
X3561	X3321	X3200	X3019	ALA
X3562	X3322	X3201	X3020	ALA
X3563	X3323	X3202	X3021	ALA
X3564	X3324	X3203	X3022	ALA
X3565	X3325	X3204	X3023	ALA
X3566	X3326	X3205	X3024	ALA
X3567	X3327	X3206	X3025	ALA
X3568	X3328	X3207	X2901	ALA
X3569	X3329	X3208	X2902	ALA
X3570	X3330	X3209	X2903	ALA
X3571	X3331	X3210	X2904	ALA
X3572	X3332	X3211	X2905	ALA
X3573	X3333	X3212	X2906	ALA
X3574	X3334	X3213	X2907	ALA
X3575	X3335	X3214	X2908	ALA
X3576	X3336	X3215	X2909	ALA
X3577	X3337	X3216	X2910	ALA
X3578	X3338	X3217	X2911	ALA
X3579	X3339	X3218	X2912	ALA
UNK	X3580	X3219	X2913	ALA
X3581	X3340	X3220	X2914	ALA
X3582	X3341	X3221	X2915	ALA
X3583	X3342	X3222	X2916	ALA
X3584	X3343	X3223	X2917	ALA
X3585	X3344	X3224	X2918	ALA
X3586	X3345	X3225	X2919	ALA
X3587	X3346	X3226	X2920	ALA
X3588	X3347	X3227	X2921	ALA
X3589	X3348	X3228	X2922	ALA
X3590	X3349	X3229	X2923	ALA
X3591	X3350	X3230	X2924	ALA
X3592	X3351	X3231	X2925	ALA
X3593	X3352	X3232	X2926	ALA
X3594	X3353	X3233	X2927	ALA
X3595	X3354	X3234	X2928	ALA
X3596	X3355	X3235	X2929	ALA
X3597	X3356	X3236	X2930	ALA
X3598	X3357	X3237	X2931	ALA
X3599	X3358	X3238	X2932	ALA
X3600	X3359	X3239	X2933	ALA
X3601	X3360	X3240	X2934	ALA
X3602	X3361	X3241	X2935	ALA
X3603	X3362	X3242	X2936	ALA
X3604	X3363	X3243	X2937	ALA

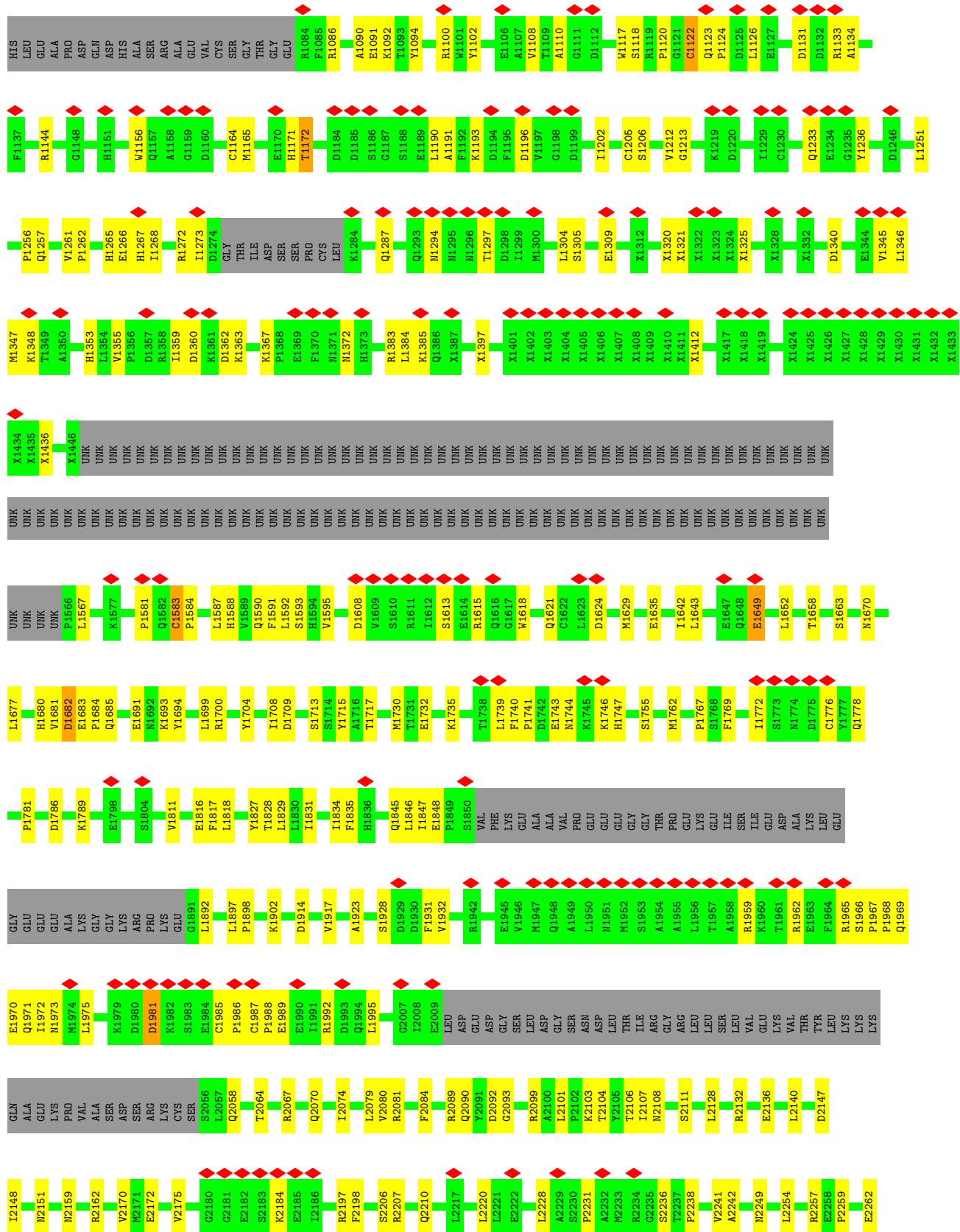


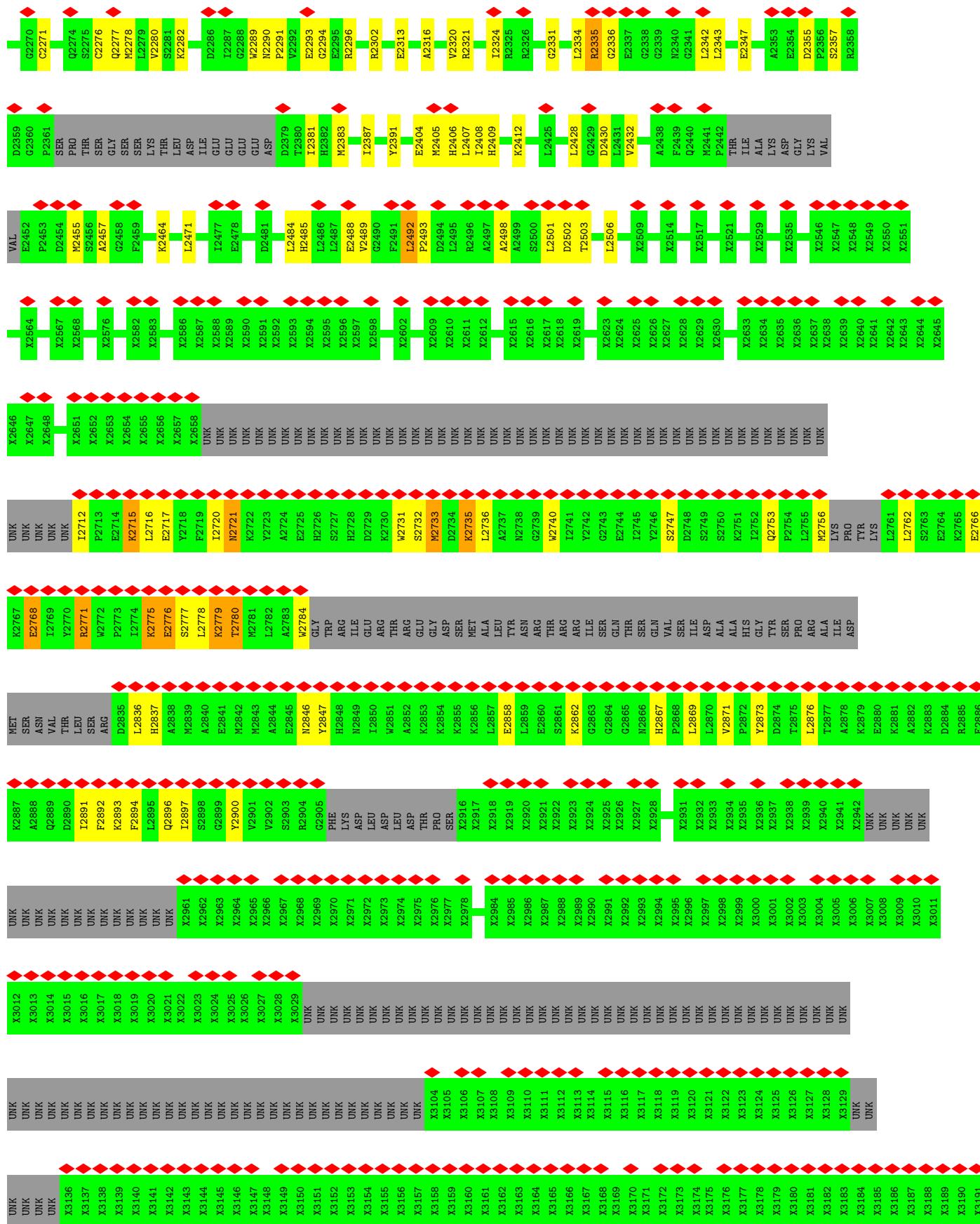
- Molecule 1: Ryanodine receptor 2

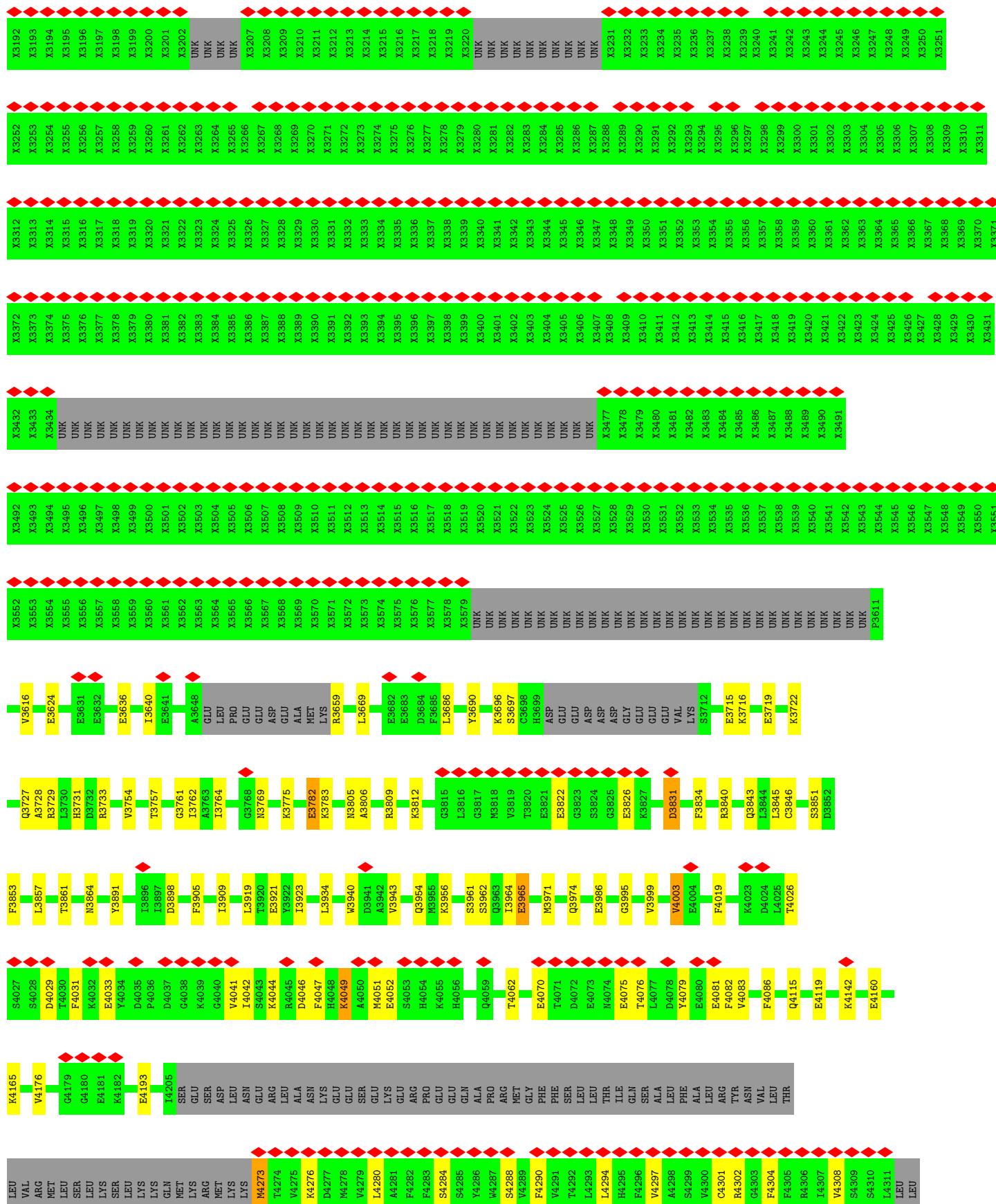
A horizontal bar chart titled "Chain D:" at the top left. The x-axis represents the percentage of each chain type, ranging from 0% to 100%. There are four bars: a red bar at 29%, a green bar at 65%, a yellow bar at 15%, and a grey bar at 19%. The bars are separated by small gaps.

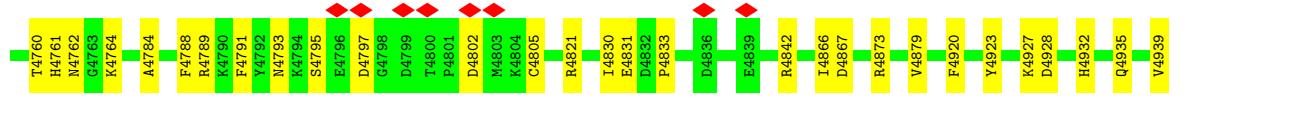
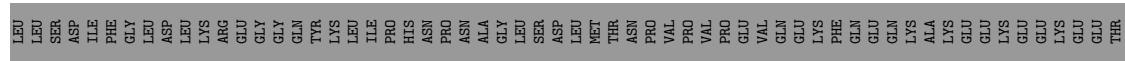
Chain Type	Percentage
Red	29%
Green	65%
Yellow	15%
Grey	19%



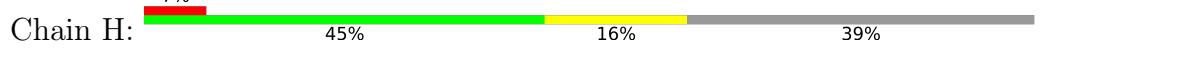




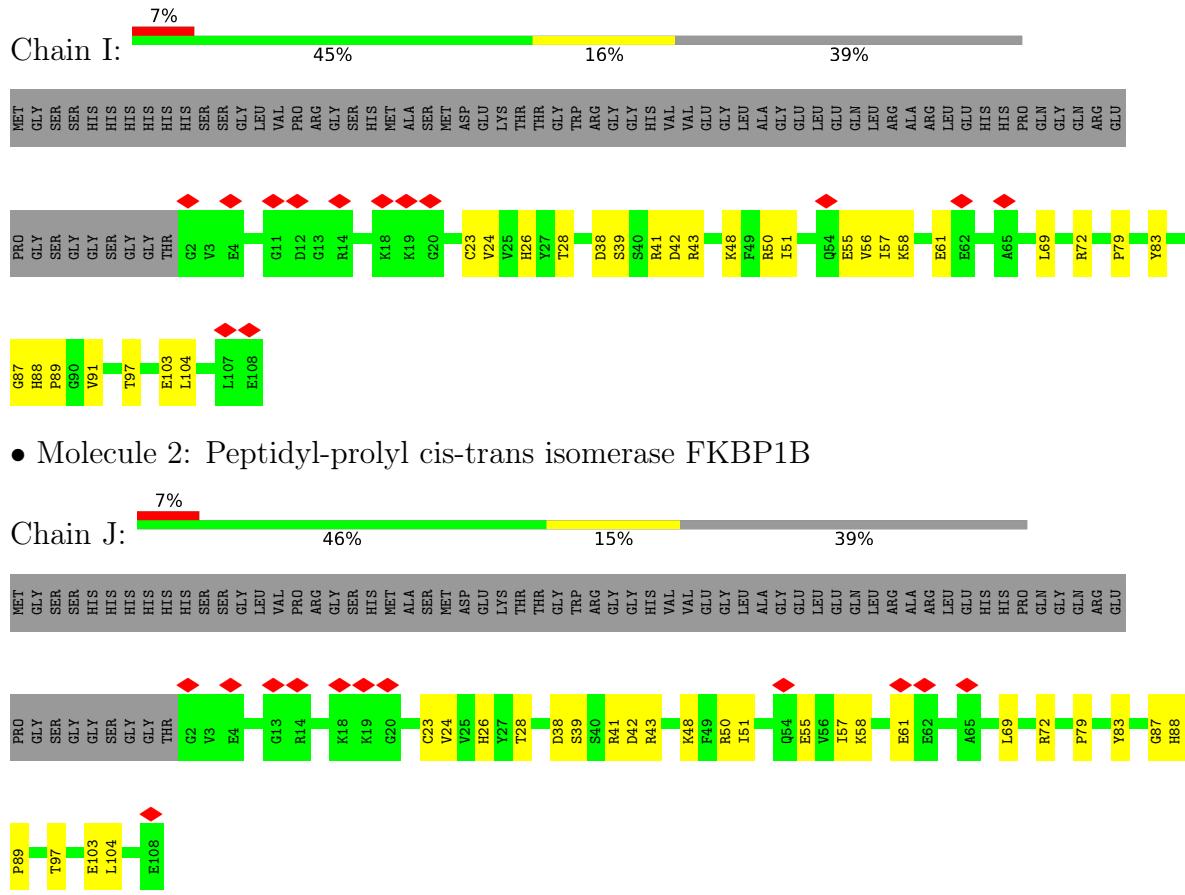




- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



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



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41197	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.120	Depositor
Minimum map value	-0.076	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	513.60004, 513.60004, 513.60004	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.284, 1.284, 1.284	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: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/26895	0.44	1/36316 (0.0%)
1	B	0.26	0/26895	0.44	1/36316 (0.0%)
1	C	0.26	0/26895	0.44	1/36316 (0.0%)
1	D	0.26	0/26895	0.44	1/36316 (0.0%)
2	G	0.27	0/835	0.47	0/1123
2	H	0.26	0/835	0.47	0/1123
2	I	0.26	0/835	0.47	0/1123
2	J	0.26	0/835	0.47	0/1123
All	All	0.26	0/110920	0.44	4/149756 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1624	ASP	CB-CG-OD1	5.96	123.67	118.30
1	B	1624	ASP	CB-CG-OD1	5.92	123.62	118.30
1	D	1624	ASP	CB-CG-OD1	5.92	123.62	118.30
1	C	1624	ASP	CB-CG-OD1	5.91	123.62	118.30

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	A	30071	0	26711	498	0
1	B	30071	0	26711	500	0
1	C	30071	0	26711	507	0
1	D	30071	0	26711	506	0
2	G	819	0	821	19	0
2	H	819	0	821	19	0
2	I	819	0	821	19	0
2	J	819	0	821	17	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	123564	0	110128	2042	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 9.

The worst 5 of 2042 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:D:1772:ILE:HD11	2:J:57:ILE:HA	1.57	0.86
1:A:1233:GLN:HG3	1:B:3493:UNK:HA	1.56	0.86
1:A:4833:PRO:HB3	1:A:4842:ARG:HD3	1.61	0.82
1:C:4833:PRO:HB3	1:C:4842:ARG:HD3	1.61	0.81
1:D:76:ARG:O	1:D:80:GLU:HB2	1.81	0.81

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	3255/4966 (66%)	3047 (94%)	208 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	3255/4966 (66%)	3047 (94%)	208 (6%)	0	100 100
1	C	3255/4966 (66%)	3046 (94%)	209 (6%)	0	100 100
1	D	3255/4966 (66%)	3047 (94%)	208 (6%)	0	100 100
2	G	105/176 (60%)	102 (97%)	3 (3%)	0	100 100
2	H	105/176 (60%)	102 (97%)	3 (3%)	0	100 100
2	I	105/176 (60%)	102 (97%)	3 (3%)	0	100 100
2	J	105/176 (60%)	102 (97%)	3 (3%)	0	100 100
All	All	13440/20568 (65%)	12595 (94%)	845 (6%)	0	100 100

There are no Ramachandran outliers to report.

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	2862/3387 (84%)	2762 (96%)	100 (4%)	36 67
1	B	2862/3387 (84%)	2762 (96%)	100 (4%)	36 67
1	C	2862/3387 (84%)	2762 (96%)	100 (4%)	36 67
1	D	2862/3387 (84%)	2762 (96%)	100 (4%)	36 67
2	G	88/140 (63%)	88 (100%)	0	100 100
2	H	88/140 (63%)	88 (100%)	0	100 100
2	I	88/140 (63%)	88 (100%)	0	100 100
2	J	88/140 (63%)	88 (100%)	0	100 100
All	All	11800/14108 (84%)	11400 (97%)	400 (3%)	40 68

5 of 400 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	988	LEU
1	C	4076	THR

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Mol	Chain	Res	Type
1	D	4802	ASP
1	C	1047	LYS
1	C	2471	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 176 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2317	ASN
1	D	888	ASN
1	C	2846	ASN
1	C	4960	GLN
1	D	1627	GLN

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

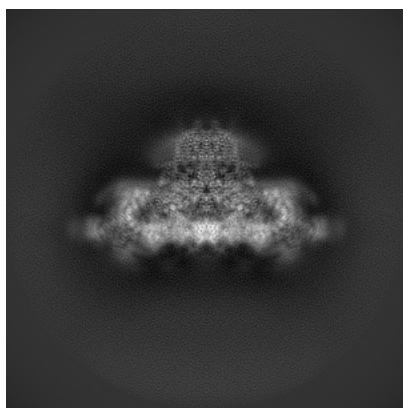
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-33937. These allow visual inspection of the internal detail of the map and identification of artifacts.

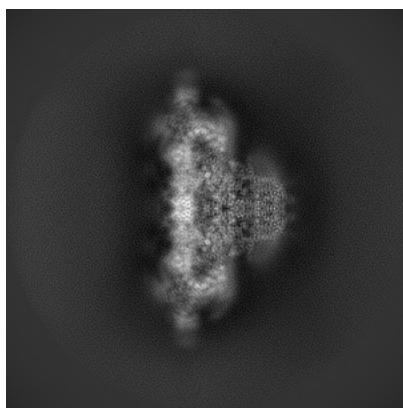
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

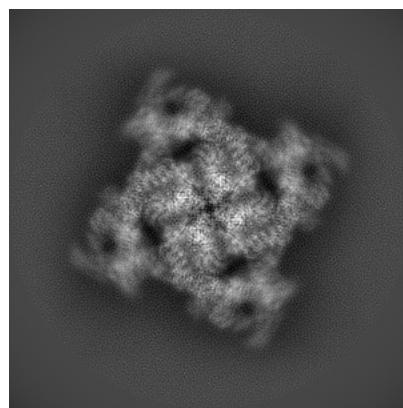
6.1.1 Primary map



X

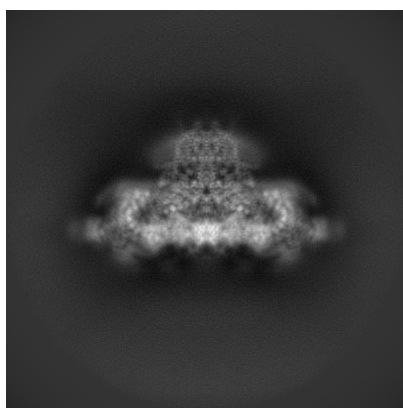


Y

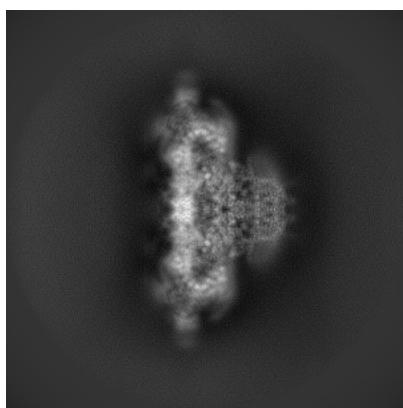


Z

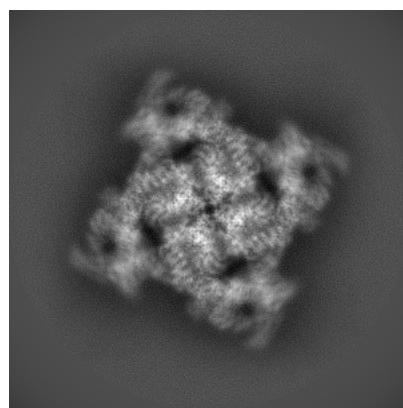
6.1.2 Raw map



X



Y

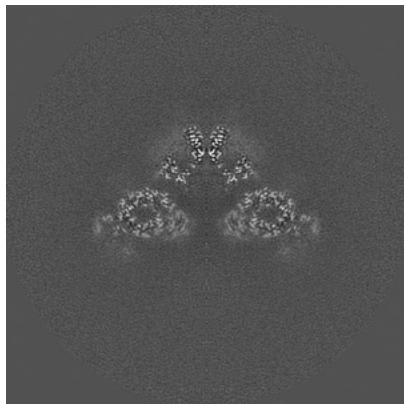


Z

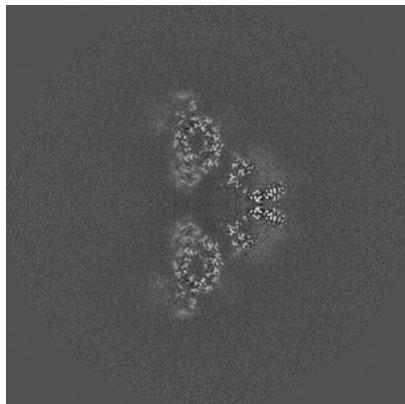
The images above show the map projected in three orthogonal directions.

6.2 Central slices [\(i\)](#)

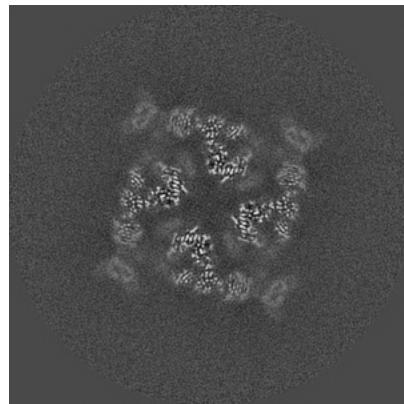
6.2.1 Primary map



X Index: 200

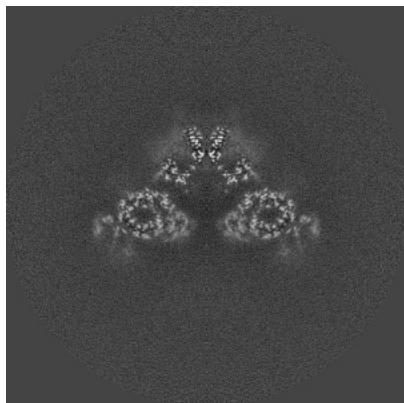


Y Index: 200

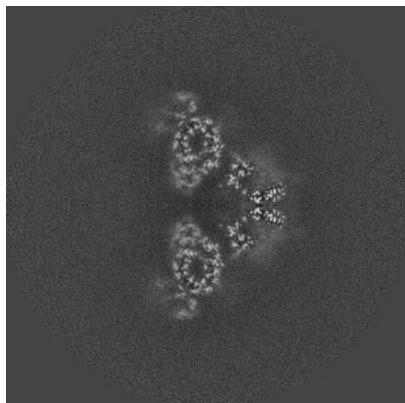


Z Index: 200

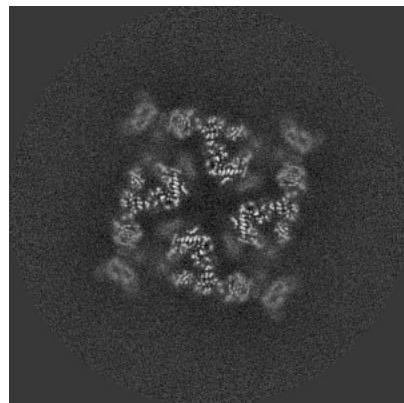
6.2.2 Raw map



X Index: 200



Y Index: 200

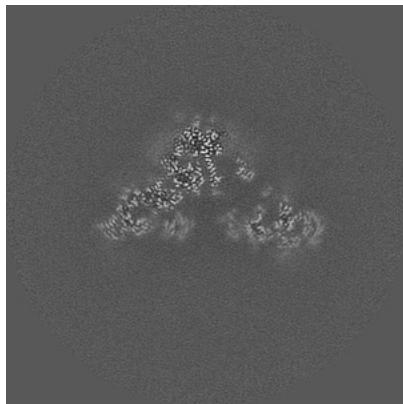


Z Index: 200

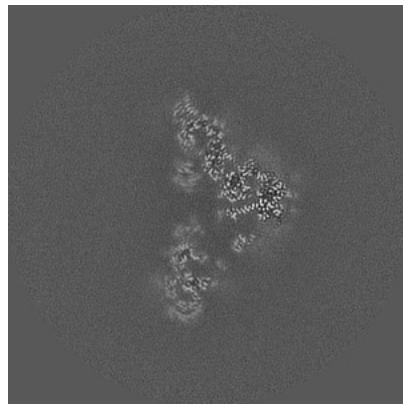
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

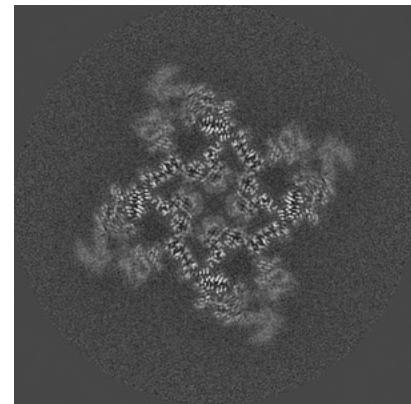
6.3.1 Primary map



X Index: 193

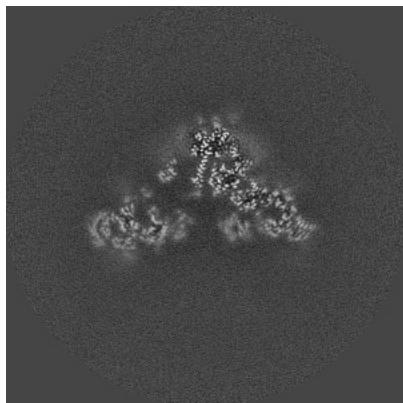


Y Index: 193

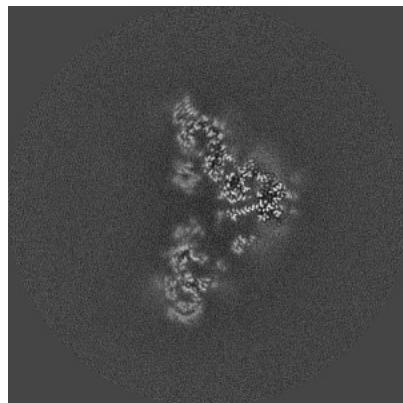


Z Index: 183

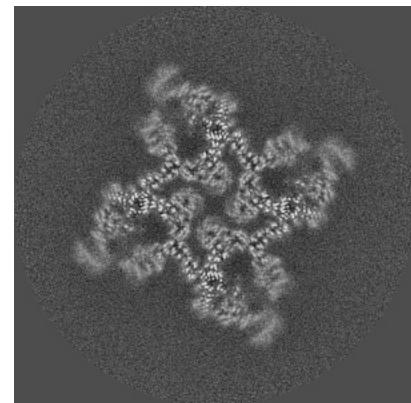
6.3.2 Raw map



X Index: 207



Y Index: 193

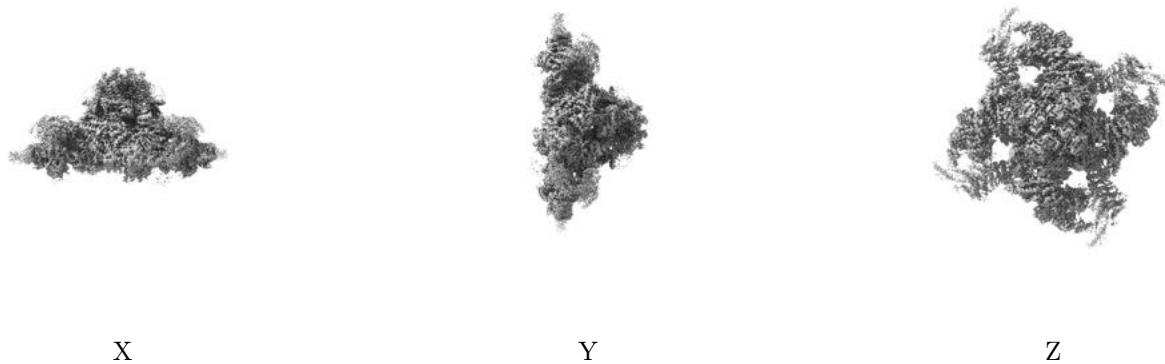


Z Index: 180

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

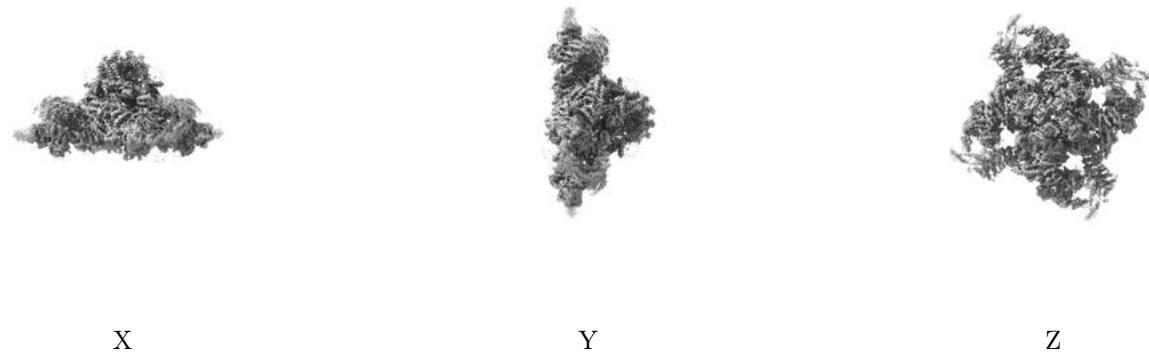
6.4 Orthogonal surface views [\(i\)](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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



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.

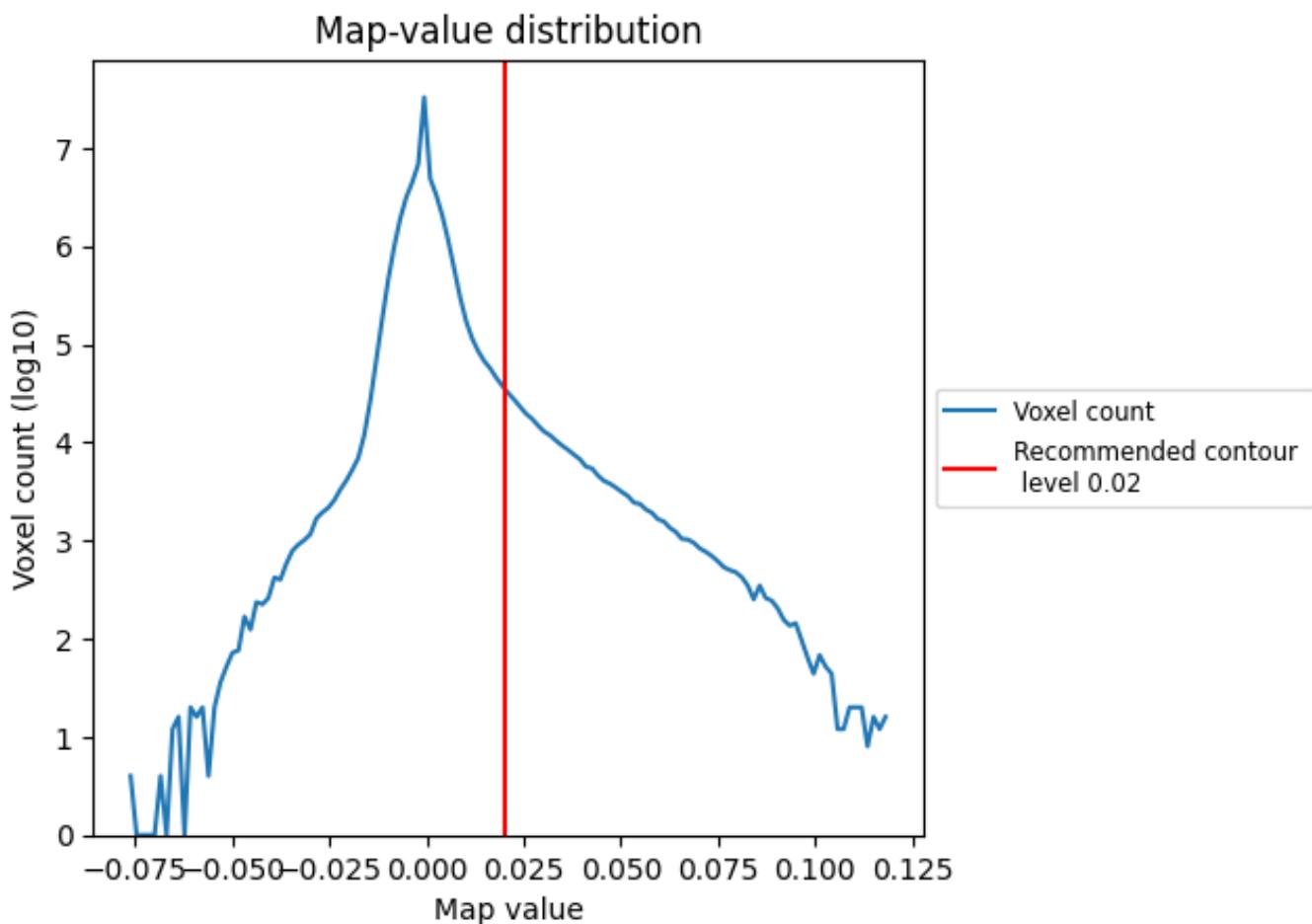
6.5 Mask visualisation [\(i\)](#)

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

7 Map analysis (i)

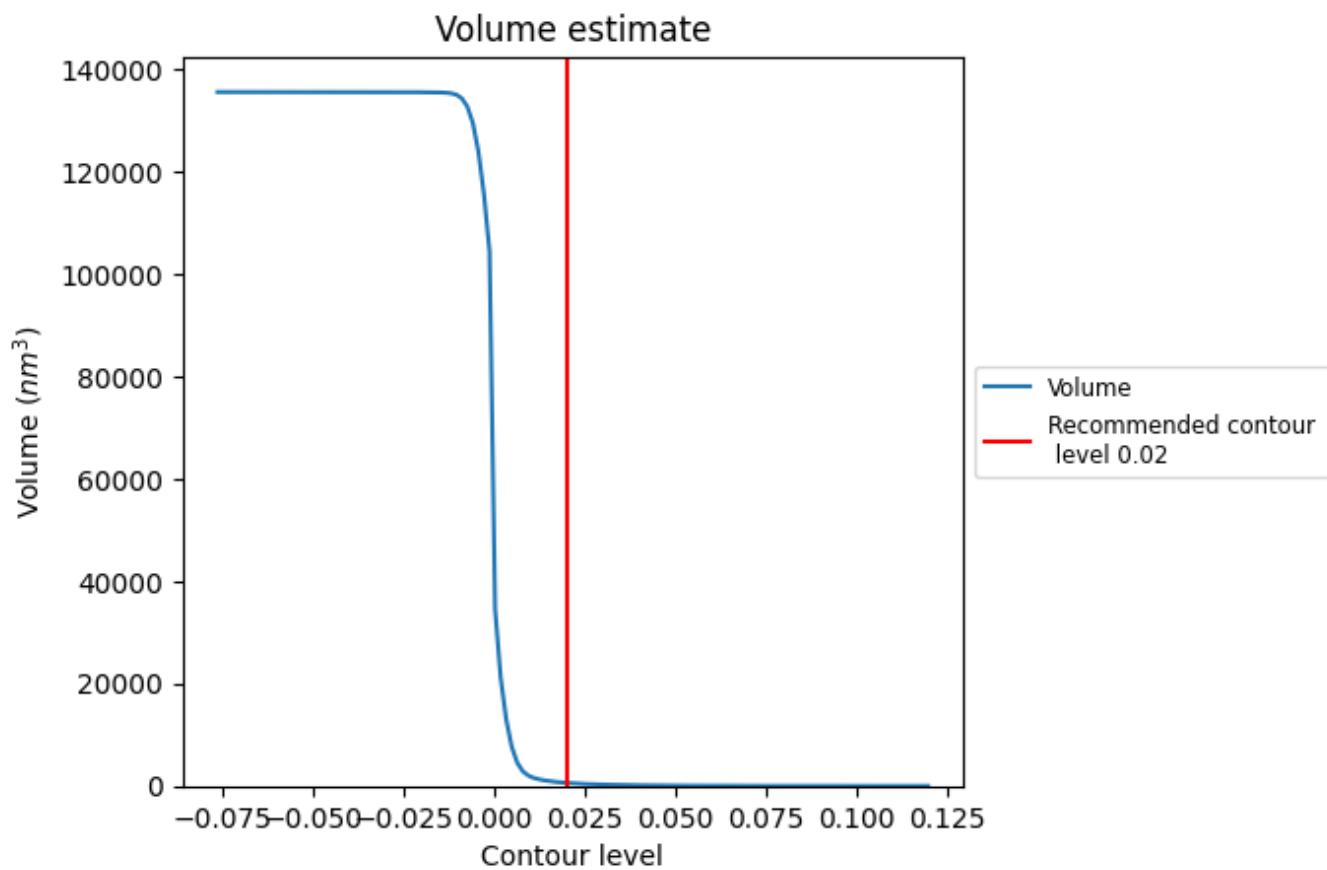
This section contains the results of statistical analysis of the map.

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.

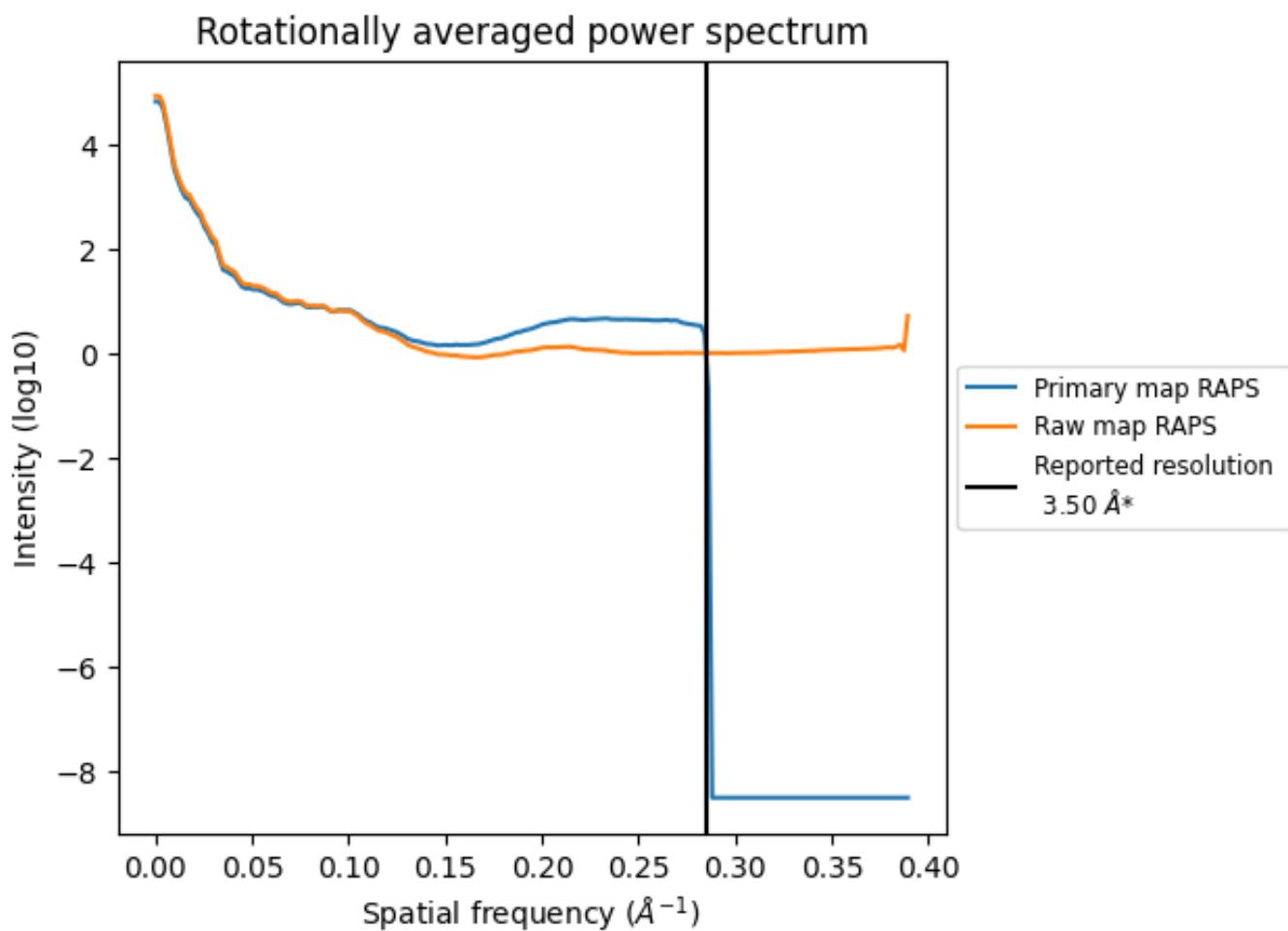
7.2 Volume estimate (i)



The volume at the recommended contour level is 601 nm³; this corresponds to an approximate mass of 542 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 [\(i\)](#)

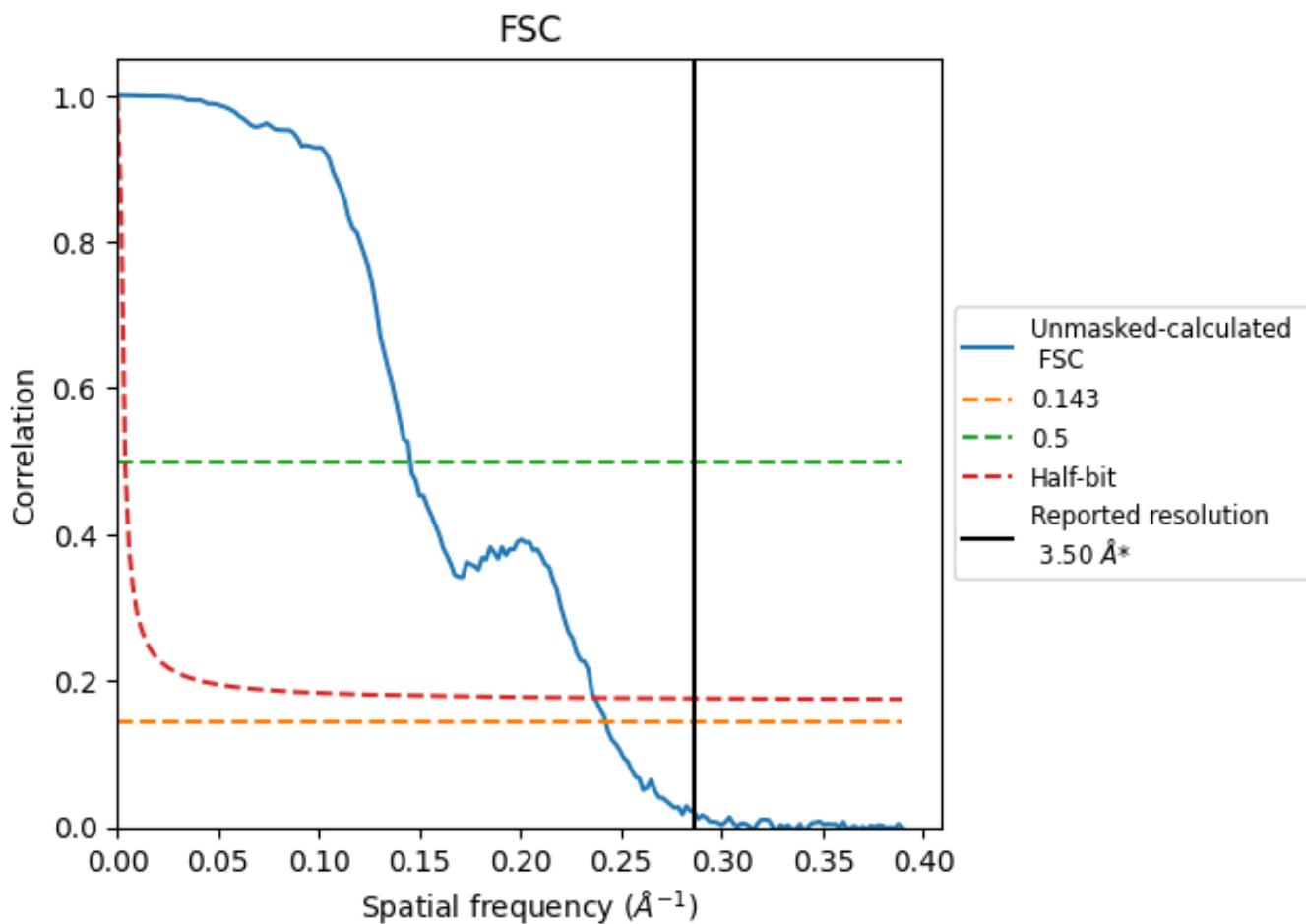


*Reported resolution corresponds to spatial frequency of 0.286 \AA^{-1}

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 0.286 \AA^{-1}

8.2 Resolution estimates [\(i\)](#)

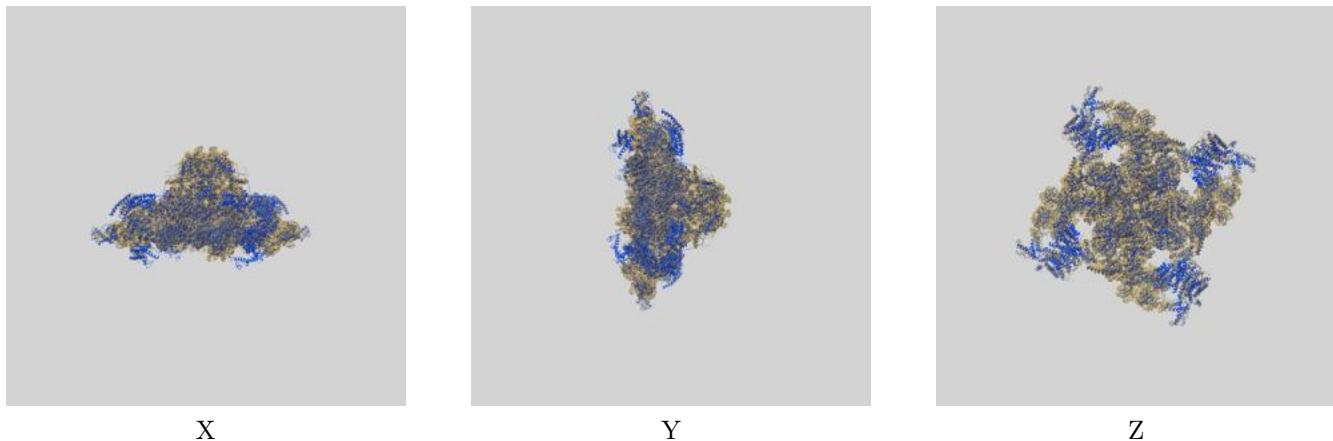
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.13	6.88	4.22

*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 4.13 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [\(i\)](#)

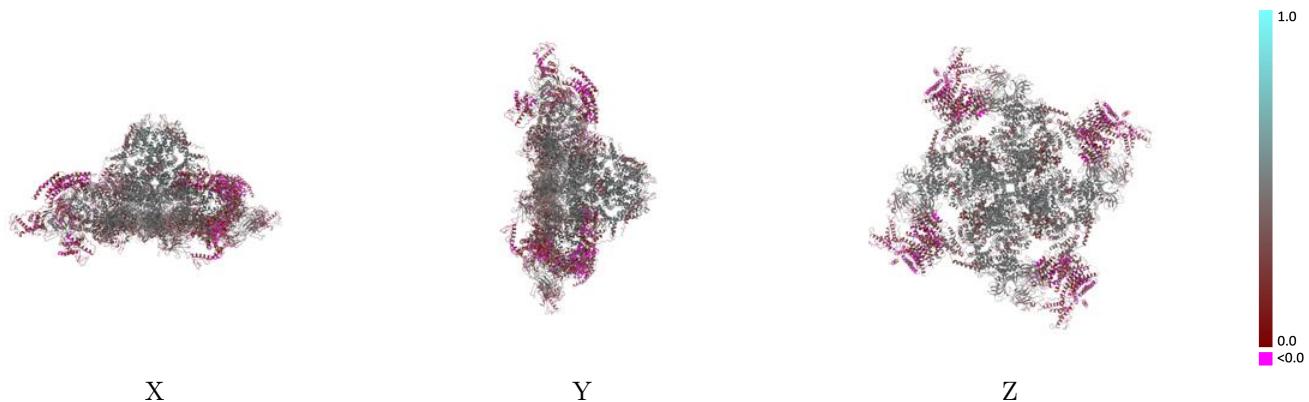
This section contains information regarding the fit between EMDB map EMD-33937 and PDB model 7VMN. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [\(i\)](#)



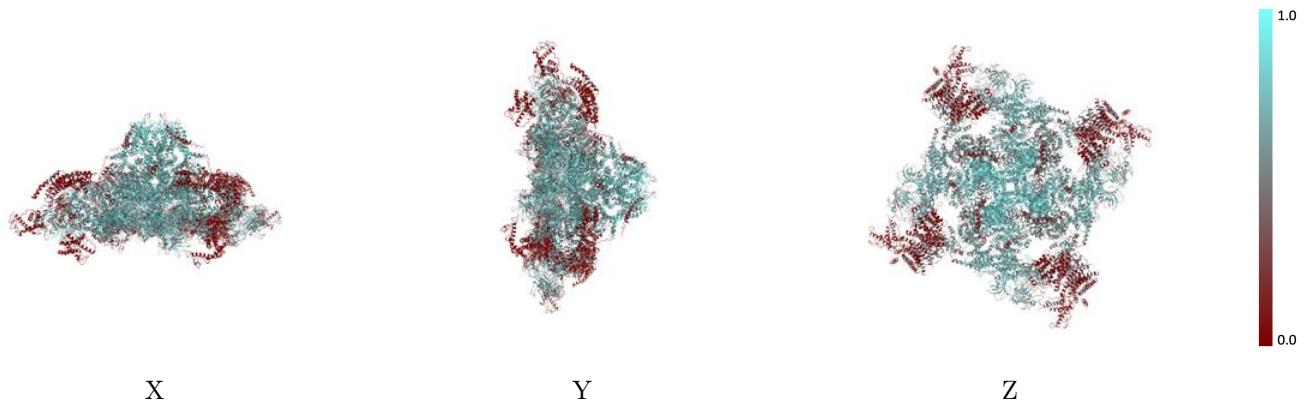
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [\(i\)](#)



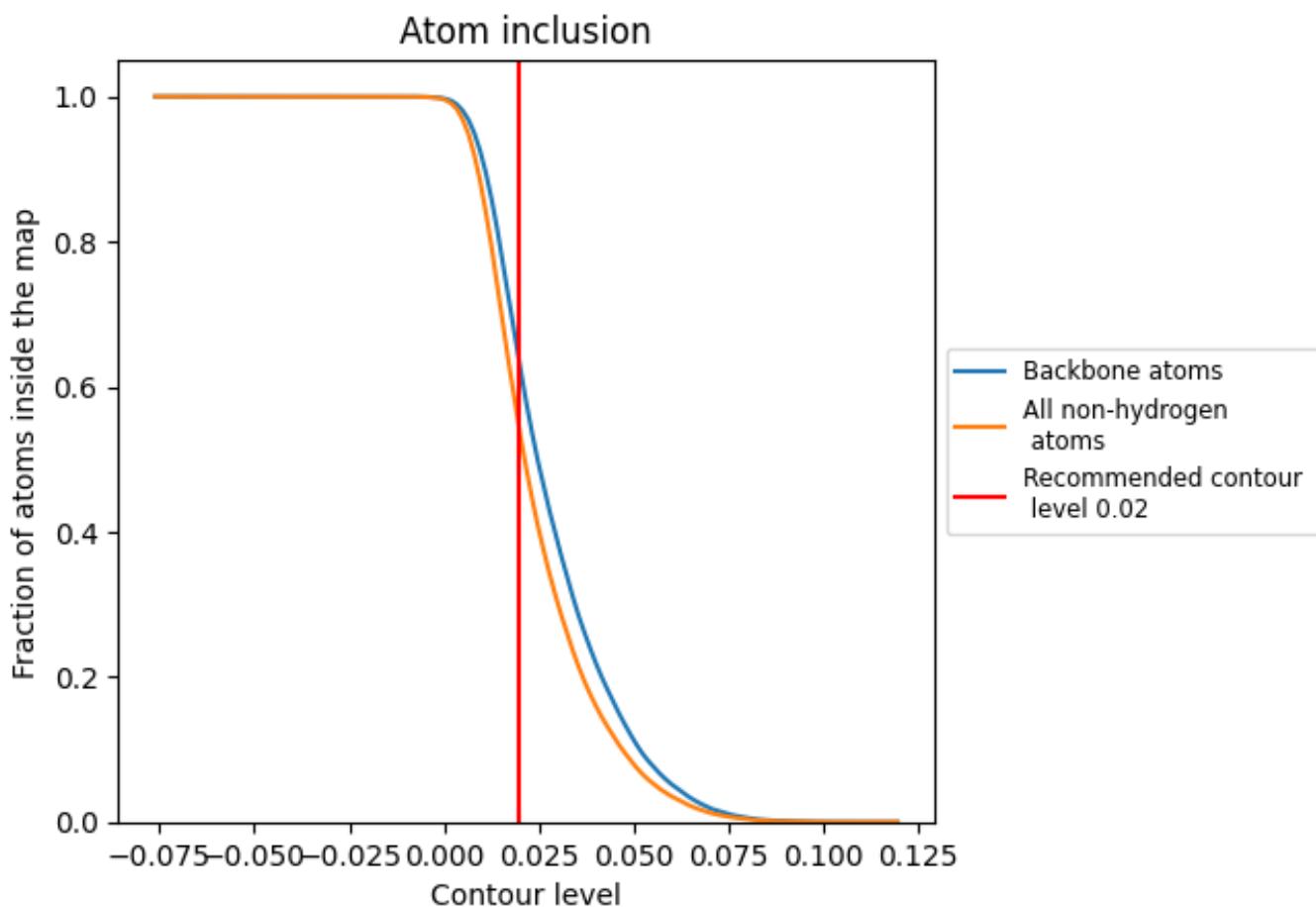
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [\(i\)](#)



At the recommended contour level, 63% of all backbone atoms, 54% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5384	0.3770
A	0.5349	0.3750
B	0.5370	0.3760
C	0.5358	0.3760
D	0.5360	0.3740
G	0.6295	0.4370
H	0.6307	0.4350
I	0.6320	0.4300
J	0.6295	0.4350

