



## wwPDB EM Validation Summary Report ⓘ

Nov 13, 2022 – 11:34 AM EST

PDB ID : 6WOU  
EMDB ID : EMD-21861  
Title : Cryo-EM structure of recombinant mouse Ryanodine Receptor type 2 mutant R176Q in complex with FKBP12.6 in nanodisc  
Authors : Iyer, K.A.; Hu, Y.; Kurebayashi, N.; Murayama, T.; Samso, M.  
Deposited on : 2020-04-25  
Resolution : 3.27 Å (reported)  
Based on initial model : 5L1D

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

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

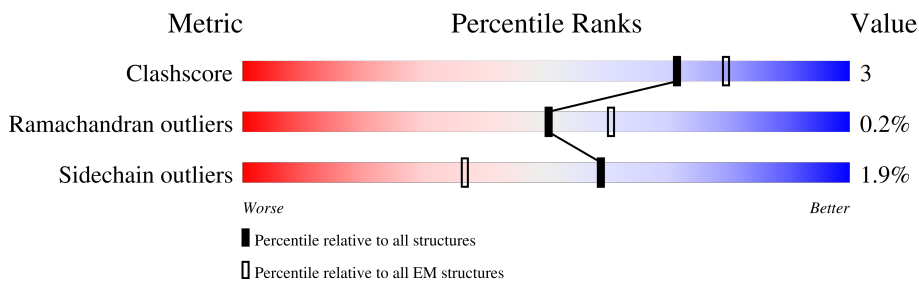
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.27 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  $\geq 3$ , 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  $\leq 5\%$ . 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	4966	
1	B	4966	
1	C	4966	
1	D	4966	
2	E	107	
2	F	107	
2	G	107	
2	H	107	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 245683 atoms, of which 120439 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	H	N	O	S		
1	A	3921	59779	19348	29287	5250	5702	192	0	0
1	B	3921	59778	19348	29286	5250	5702	192	0	0
1	C	3921	59778	19348	29286	5250	5702	192	0	0
1	D	3921	59776	19348	29284	5250	5702	192	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	GLN	ARG	engineered mutation	UNP E9Q401
B	176	GLN	ARG	engineered mutation	UNP E9Q401
C	176	GLN	ARG	engineered mutation	UNP E9Q401
D	176	GLN	ARG	engineered mutation	UNP E9Q401

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	E	107	1642	516	824	144	154	4	0	0
2	F	107	1642	516	824	144	154	4	0	0
2	G	107	1642	516	824	144	154	4	0	0
2	H	107	1642	516	824	144	154	4	0	0

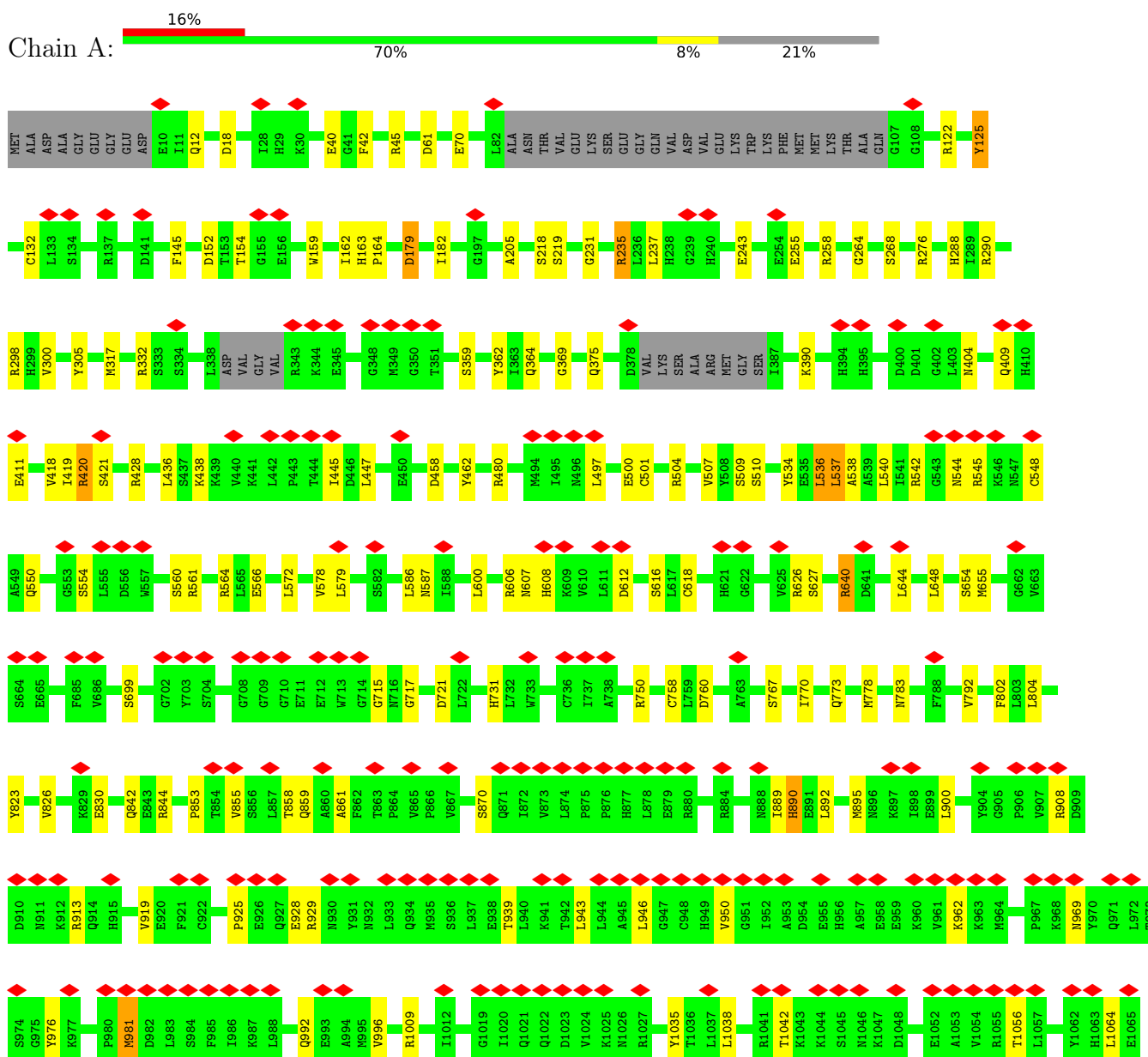
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
3	A	1	Total 1	Zn 1	0
3	B	1	Total 1	Zn 1	0
3	C	1	Total 1	Zn 1	0
3	D	1	Total 1	Zn 1	0

### 3 Residue-property plots

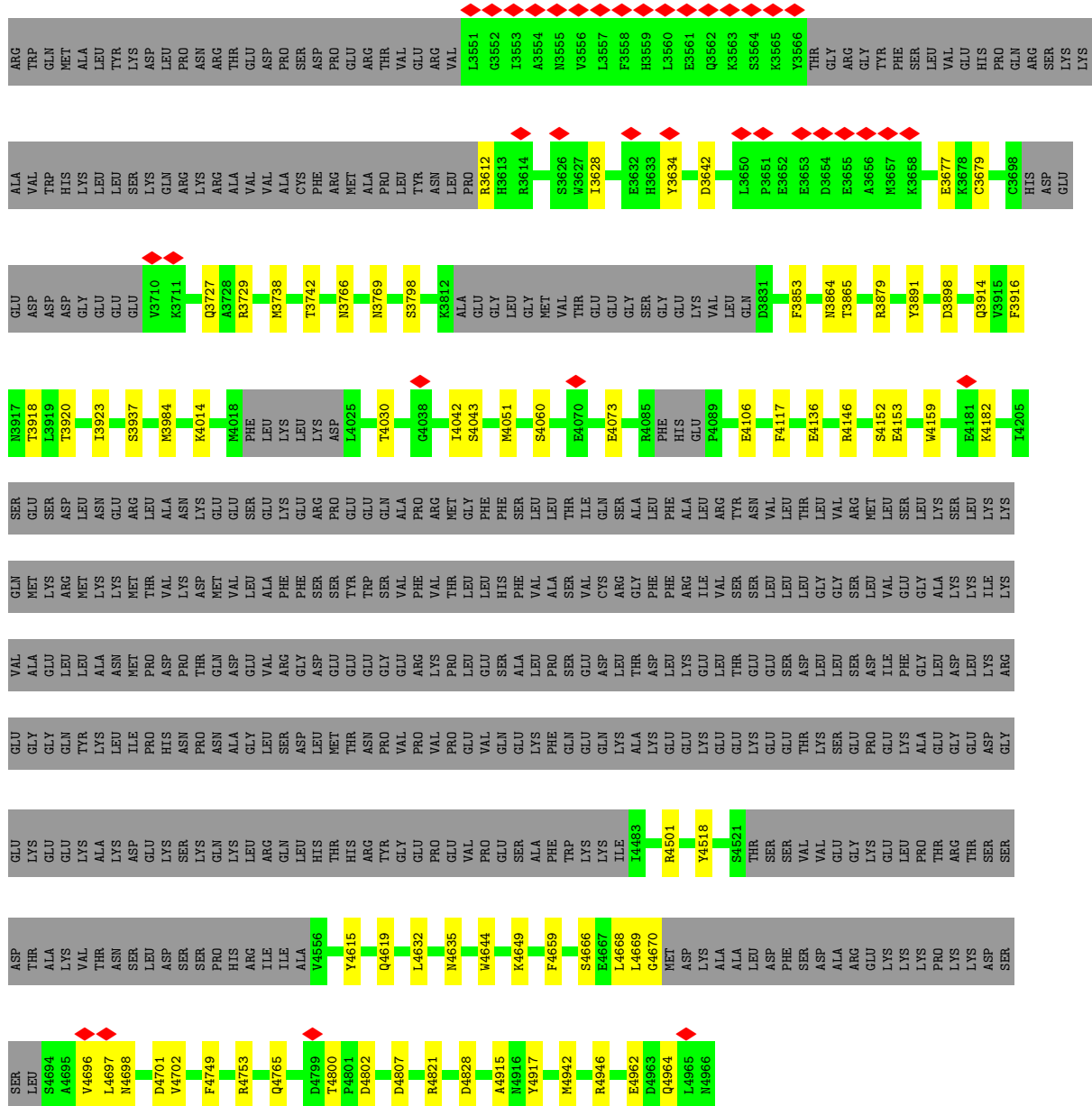
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

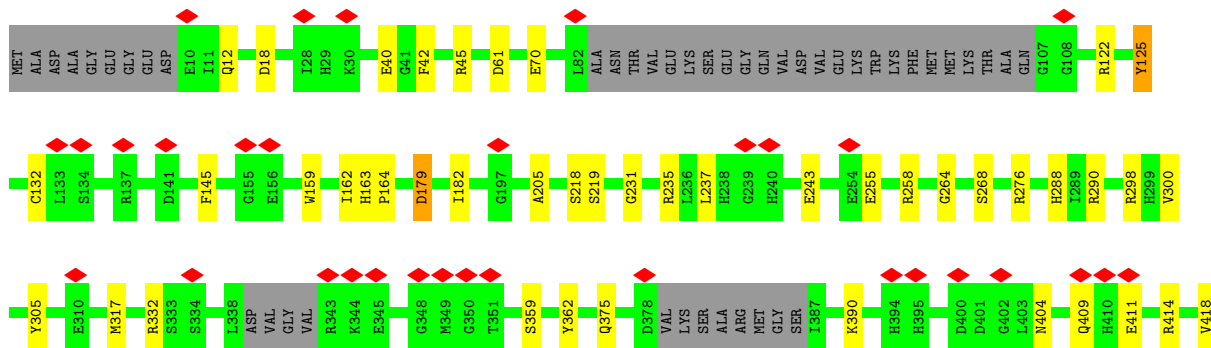




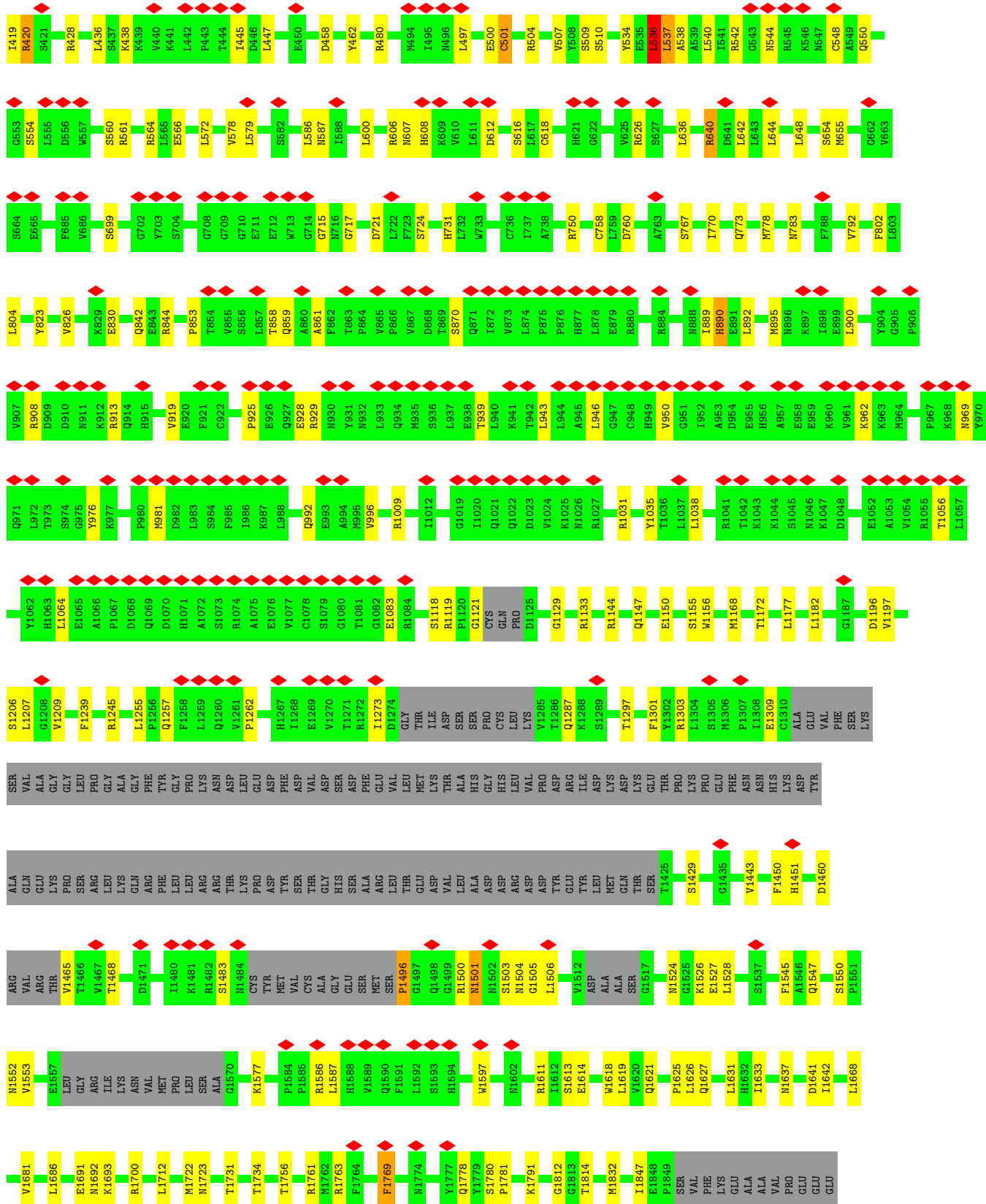
L3464	L3465	Y3404	A3343	D3202	A3058	PRO	ASP	M2846	W2786	H2726	W2626
L3466	L3467	W3405	R3344	V3203	D3061	LEU	LEU	Y2847	R2787	S2727	E2636
Y3406	A3467	G3345	G3345	C3204	A3064	ILE	ASP	H2848	I2788	H2728	I2647
S3408	S3408	D3346	D3346	F3205	A3064	GLN	ASP	N2849	D2789	D2729	L2651
H3409	H3409	M3347	M3347	N3206	E3065	THR	THR	I2850	K2790	K2730	K2654
N3410	N3410	I3282	I3282	I3207	E3068	PHE	ILE	W2851	T2791	W2731	K2655
F3411	F3411	I3283	I3283	S3208	H3069	LYS	ILE	A2852	R2792	S2732	W2654
K3412	K3412	I3284	I3284	P3209	T3070	ASN	GLU	K2853	E2793	M2733	Y2656
L3413	L3413	Y3285	Y3285	L3210	M3071	HIS	LYS	K2854	D2794	D2734	E2657
E3414	E3414	N3286	N3286	T2145	E3072	ARG	ARG	D2855	D2795	K2735	E2658
Q3415	Q3415	L3287	L3287	Q3076	Q3076	TYR	PHE	K2856	S2796	L2736	L2660
R3416	R3416	G3288	G3288	G3077	Q3077	SER	TYR	L2857	A2737	A2737	L2661
S3417	S3417	I3289	I3289	Q3078	Q3078	THR	THR	L2858	N2797	N2738	P2666
T3418	T3418	D3290	D3290	F3079	F3079	PHE	SER	E2859	L2798	G2739	P2677
Y3419	Y3419	E3291	E3291	T3080	T3080	LEU	GLN	E2860	L2799	G2739	D2678
C3420	C3420	G3292	G3292	H3081	H3081	GLN	GLN	E2861	Y2800	W2740	Y2679
Q3421	Q3421	A3292	A3292	T3082	T3082	GLN	GLN	S2861	N2801	I2741	M2687
N3422	N3422	T3228	T3228	Q3085	Q3085	LEU	ARG	K2862	ARG	I2742	P2677
E3423	E3423	Q3229	Q3229	P3086	P3086	ILE	ARG	G2863	THR	G2743	D2678
S3424	S3424	M3230	M3230	A3099	A3099	TYR	TYR	H2867	ARG	E2744	Y2679
K3425	K3425	F3231	F3231	V3098	V3098	ASP	ASP	P2868	ARG	I2745	M2687
N3426	N3426	R3232	R3232	L3100	L3100	GLU	VAL	L2869	ILE	Y2746	Y2679
D3427	D3427	M3233	M3233	P3102	P3102	ALA	ALA	L2870	THR	S2747	M2687
E3428	E3428	A3234	A3234	M3103	M3103	HIS	HIS	L2871	THR	D2748	Q2691
L3429	L3429	P3235	P3235	A3099	A3099	GLY	GLY	L2872	THR	S2749	S2692
S3430	S3430	V3236	V3236	L3100	L3100	LEU	LEU	P2872	GLN	S2750	S2693
K3431	K3431	F3237	F3237	P3102	P3102	LEU	LEU	Y2873	VAL	K2751	S2694
N3432	N3432	M3240	M3240	M3103	M3103	GLU	PHE	D2874	ASP	I2752	ASP
D3433	D3433	A3241	A3241	LEU	LEU	ILE	ASP	L2875	ASP	Q2753	GLU
E3434	E3434	P3242	P3242	LEU	LEU	PHE	GLY	T2876	A2816	P2754	GLY
L3435	L3435	C3243	C3243	LEU	LEU	GLY	GLY	T2877	A2817	P2754	ASN
S3436	S3436	N3244	N3244	LEU	LEU	ASP	ASP	A2878	H2818	L2755	ASN
K3437	K3437	H3245	H3245	LEU	LEU	THR	THR	K2879	G2819	M2756	PHE
N3438	N3438	T3246	T3246	GLU	GLU	ALA	ALA	Y2820	ASN	K2757	ASN
D3439	D3439	M3246	M3246	HIS	HIS	LYS	LYS	E2880	LYS	P2758	PRO
E3440	E3440	R3247	R3247	ILE	ILE	GLY	GLY	K2881	GLY	Y2759	PRO
A3441	A3441	W3248	W3248	ILE	ILE	ILE	ILE	A2882	P2822	Y2759	PRO
S3442	S3442	N3249	N3249	VAL	VAL	VAL	VAL	A2883	R2823	K2760	V2705
K3382	K3382	E3250	E3250	GLN	GLN	ASN	HIS	K2883	A2824	L2761	D2706
W3383	W3383	H3251	H3251	HIS	HIS	CYS	PHE	D2884	L2825	L2762	T2707
L3384	L3384	G3252	G3252	GLN	GLN	LEU	THR	K2885	D2826	S2763	S2708
K3385	K3385	P3253	P3253	PHE	PHE	ILE	GLY	E2886	M2827	E2764	H2709
E3386	E3386	G3254	G3254	GLU	GLU	ILE	GLU	K2887	S2828	K2765	I2710
P3387	P3387	E3254	E3254	ASP	ASP	ILE	ILE	L2876	S2828	E2766	I2711
N3388	N3388	N3255	N3255	LEU	LEU	ASP	ASP	T2877	N2829	E2766	T2712
K3389	K3389	H3256	H3256	LEU	LEU	PHE	PHE	Q2889	M2830	K2767	I2712
GLU	GLU	P3257	P3257	ASP	ASP	ALA	ALA	D2890	V2830	E2768	P2713
ALA	ALA	E3258	E3258	VAL	VAL	LYS	LYS	T2891	L2832	I2769	E2714
GLU	GLU	A3260	A3260	VAL	VAL	VAL	VAL	F2892	L2833	Y2770	K2715
GLU	GLU	E3261	E3261	VAL	VAL	VAL	VAL	K2893	R2834	R2771	L2716
GLU	GLU	C3264	C3264	VAL	VAL	VAL	VAL	F2894	D2835	E2771	L2716
ALA	ALA	E3270	E3270	VAL	VAL	VAL	VAL	K2895	L2836	E2772	E2717
GLU	GLU	H3271	H3271	VAL	VAL	VAL	VAL	F2896	L2837	W2773	E2718
LEU	LEU	M3272	M3272	CYS	CYS	TYR	TYR	Q2897	H2837	I2774	F2719
PHE	PHE	N3273	N3273	TYR	TYR	ARG	ARG	L2897	M2838	K2775	I2720
ILE	ILE	L3274	L3274	ARG	ARG	ARG	ARG	S2898	M2839	S2776	N2721
								G2899	A2840	E2777	K2722
								Y2900	E2841	S2777	Y2723
								V2901	M2842	L2778	A2724
								S2903	M2843	K2779	E2725
								ARG	E2845	T2780	
								GLY		M2781	
								PHE		L2782	
								LYS		A2783	
										W2784	
										W2785	



• Molecule 1: Ryanodine receptor 2



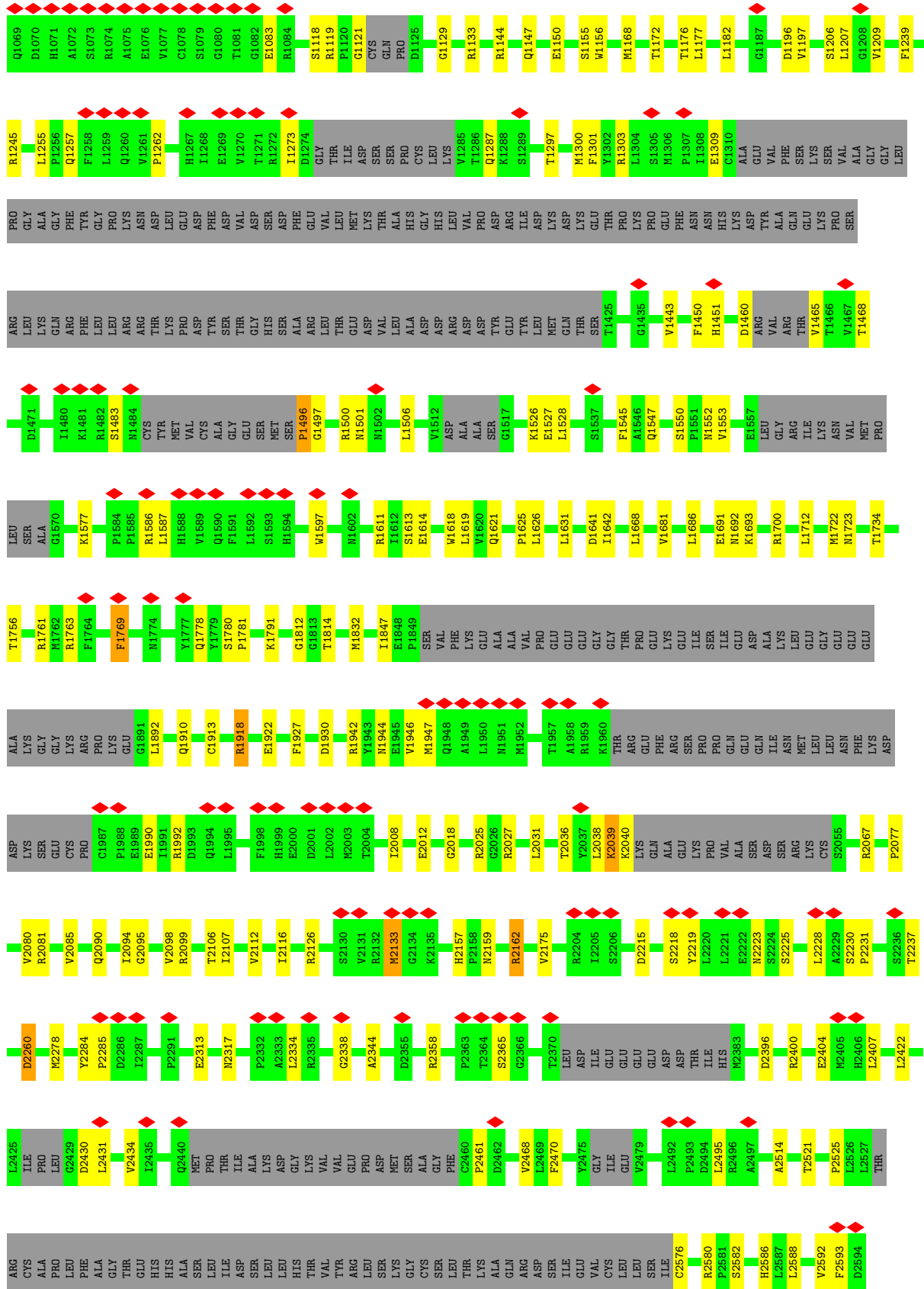






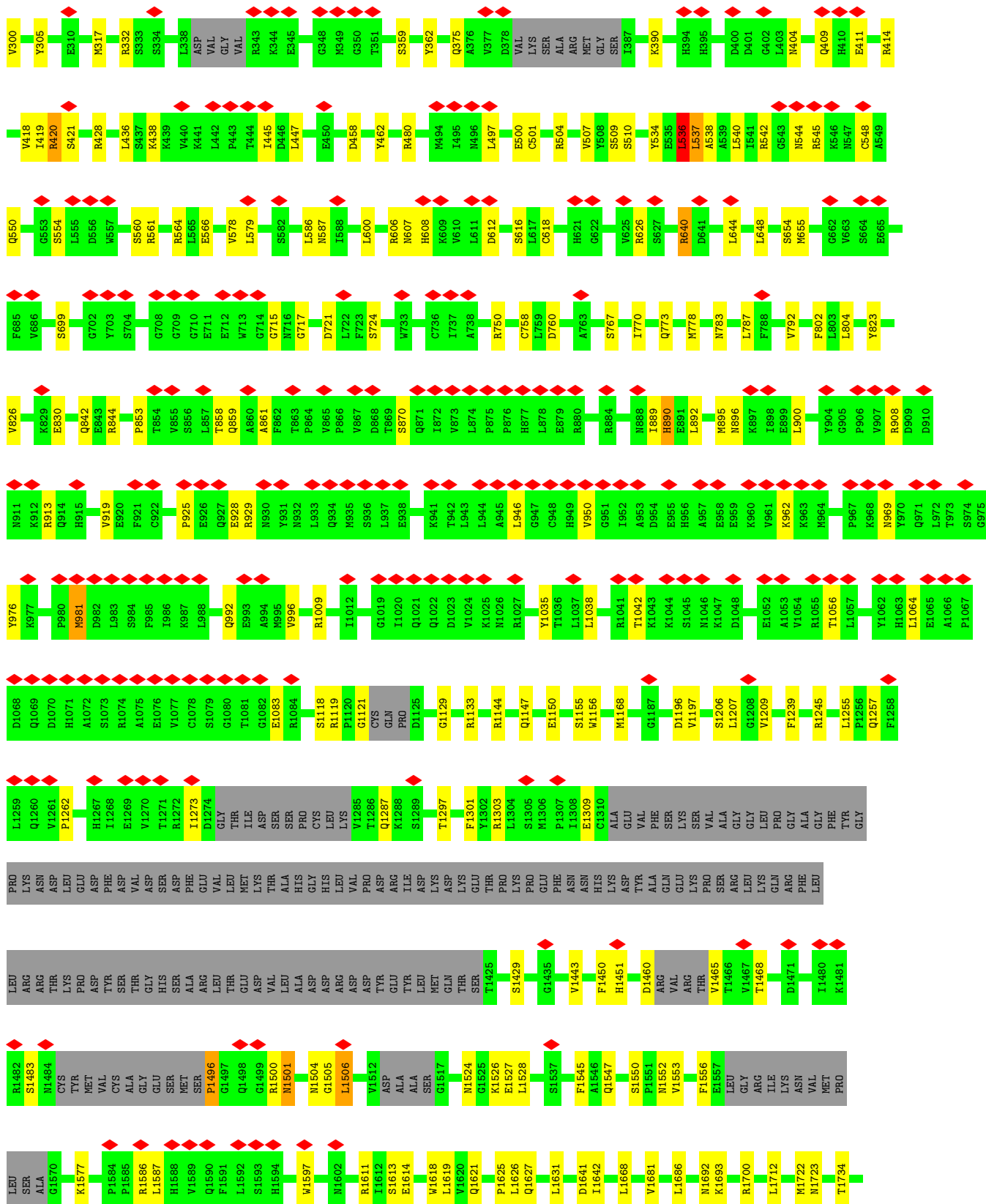






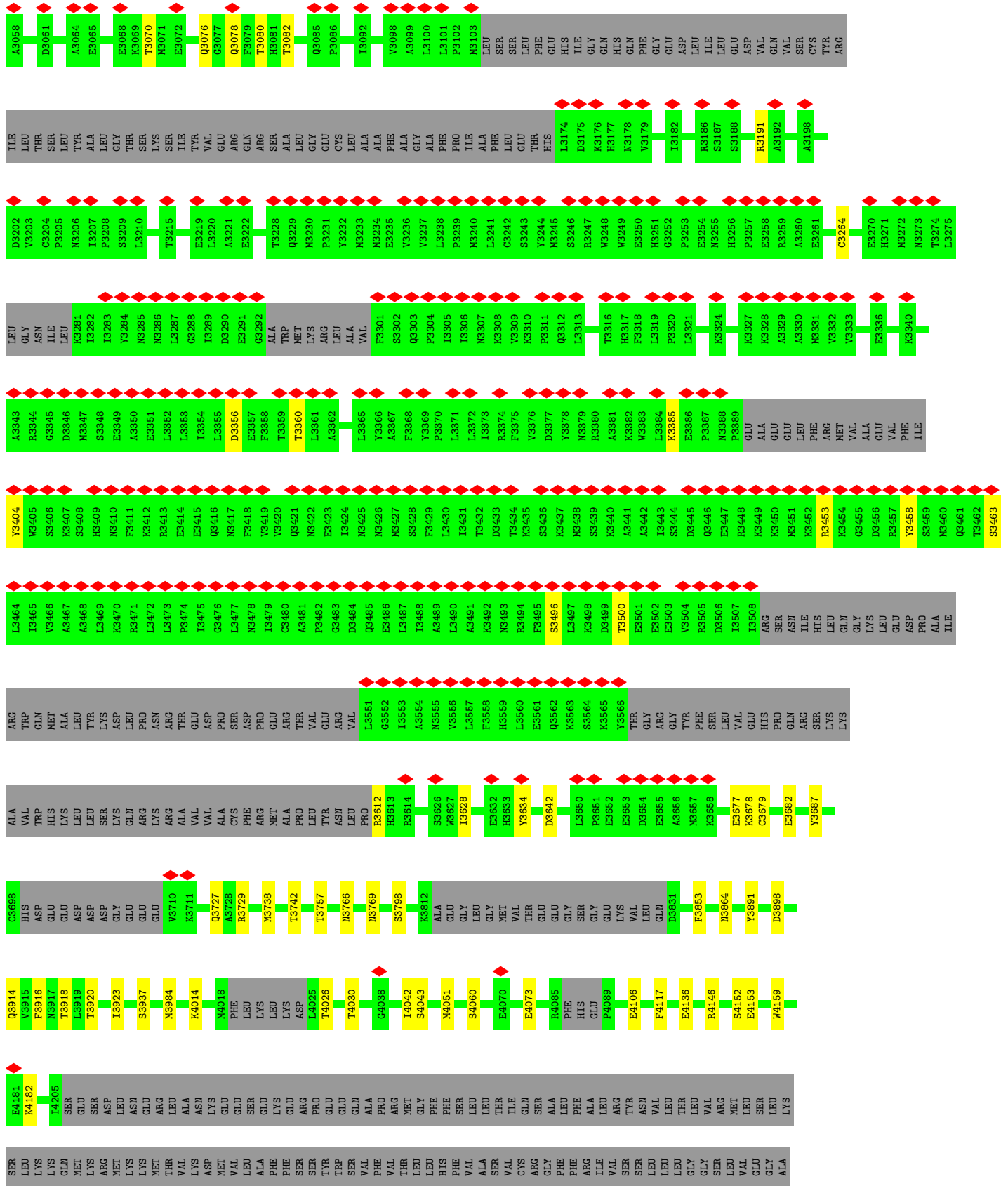
L2609	L2720	T2780	A2840	V2902	PHE	S3054	SER	A3192	M3272	E3336	GLU	M3460
E2614	N2721	M2781	E2841	S2903	ALA	A3065	CYS	A3196	N3273	R3340	VAL	Q3461
K2618	K2722	L2782	M2842	ARG	LYS	L3056	TYR		T3274		PHE	T3462
V2619	Y2723	A2783	M2843	GLY	VAL	R3057	ARG		L3275		ILE	S3463
Y2620	A2724	K2784	A2844	PHE	LEU	A3058	LEU	D3202	LEU	A3343	Y3404	W3405
W2626	E2725	W2785	E2845	ASP	PRO	D3061	THR	V3203	GLY	R3344	W3406	S3407
E2636	H2726	W2786	Y2846	ASP	LEU	A3064	SER	C3204	ASN	G3345	S3408	V3466
	S2727	R2787	Y2847	ASP	LEU	E3065	LEU	C3205	ASN	D3346	S3409	A3467
	H2728	R2788	H2848	LEU	LEU	E3068	TYR	N3206	K3281	M3347	H3409	S3468
	D2729	E2789	M2849	LEU	ASP	K3069	ALA	P3208	I3282	I3283	N3410	A3469
	K2730	R2790	L2850	THR	THR	M3071	GLY	S3209	Y3284	A3350	F3411	R3470
	W2731	T2791	W2851	PRO	LYS	E3072	THR	L3210	M3285	E3351	K3412	R3471
	S2732	R2792	A2852	ILE	HIS	T3070	LYS	T3215	N3286	L3352	R3413	L3472
	M2733	E2793	K2853	GLU	ARG	M3078	SER	E3219	M3287	L3353	E3414	L3473
	D2734	G2794	K2854	LYS	LEU	F3079	ILE	L3220	L3288	L3354	E3415	F3474
	K2735	G2795	K2855	PHE	TYR	T3080	VAL	E3219	I3289	L3355	Q3416	I3475
	L2736	L2796	K2856	ALA	PHE	Q3076	GLU	E3219	I3289	D3356	M3417	G3476
	A2737	M2797	L2857	SER	PHE	G3077	ARG	E3222	D3290	E3357	F3418	L3477
	N2738	R2798	E2858	PHE	PHE	F3078	GLN	T3228	ALA	F3357	V3419	M3478
	G2739	L2799	L2859	LEU	LEU	T3081	THR	M3229	TRP	T3358	V3420	I3479
	W2740	Y2800	E2860	GLN	LEU	H3082	VAL	Q3230	MET	T3360	Q3421	C3480
	I2741	L2801	S2861	ILE	ILE	T3082	ALA	F3231	LYS	L3361	N3422	C3481
	S2661	M2801	K2862	ARG	ARG	Q3085	ALA	Y3232	ARG	A3362	E3423	F3482
	F2666	ARG	G2863	TYR	TYR	P3086	ALA	M3233	LEU		L3424	C3483
	Y2666	THR		VAL		I3092	ALA	M3234	ALA		N3425	C3484
	Y2679	ARG	H2867	VAL	ASP		PHE	E3235	F3301	Y3366	N3426	Q3485
	M2687	ILE	P2868	LEU	GLU		ALA	E3236	S3302	A3367	M3427	E3486
	S2693	GLN	L2870	ALA	ALA		ALA	V3236	Q3302	F3368	S3428	L3487
	R2694	THR	V2871	HIS	THR		ALA	V3237	Q3303	F3369	F3429	L3488
ASP	VAL	THR	P2872	GLN	PHE		PRO	L3238	P3304	P3370	L3430	A3489
ASP	GLY	SER	P2873	LEU	ILE		ILE	P3239	I3305	L3371	I3431	L3490
GLY	ILE	ASP	D2874	GLY	LEU		ALA	M3240	M3307	L3372	T3432	A3491
ASN	ASP	ASP	T2875	PHE	LEU		LEU	L3241	K3308	L3373	K3433	R3492
ASN	GLY	GLY	L2876	GLY	LEU		THR	S3243	V3309	R3374	T3434	K3493
PRO	ASN	ASN	A2878	ASN	ASN		GLU	C3242	K3310	F3375	K3435	R3494
GLN	ASN	ASN	K2879	PRO	PHE		LEU	M3245	K3311	V3376	S3436	F3495
PRO	GLN	GLY	E2880	THR	THR		PHE	S3246	P3312	D3377	K3437	S3496
PRO	PRO	ASP	K2881	ILE	ILE		ALA	R3248	Q3312	Y3378	M3438	K3497
PRO	PRO	ASP	L2882	VAL	VAL		LEU	M3248	L3313	M3379	R3439	R3498
PRO	PRO	ASP	P2882	GLY	GLY		GLY	Y3244	T3316	R3380	K3440	D3499
PRO	PRO	ASP	K2883	CYS	CYS		THR	M3249	H3317	A3381	A3441	T3500
PRO	PRO	ASP	D2884	LEU	LEU		THR	E3250	F3318	K3382	A3442	E3501
PRO	PRO	ASP	R2885	HIS	HIS		THR	H3251	L3319	W3383	I3443	E3502
PRO	PRO	ASP	E2886	LEU	ILE		THR	G3252	P3320	L3384	I3444	E3503
PRO	PRO	ASP	K2887	ASP	ASP		THR	F3253	L3321	E3385	D3445	V3504
PRO	PRO	ASP	Q2888	LEU	LEU		THR	E3254	K3324	F3387	Q3446	R3506
PRO	PRO	ASP	A2888	ILE	ILE		THR	N3255	K3324	M3388	E3447	D3506
PRO	PRO	ASP	D2889	LEU	LEU		THR	H3256		P3389	R3448	I3507
PRO	PRO	ASP	T2890	GLU	GLU		THR	P3257	K3327	GLU	K3449	I3508
PRO	PRO	ASP	T2891	LYS	LYS		THR	E3258	K3328	ALA	M3450	ARG
PRO	PRO	ASP	F2892	LEU	LEU		THR	A3260	A3329	GLU	K3451	SER
PRO	PRO	ASP	K2893	GLY	GLY		THR	A3260	A3330	LEU	K3452	ASN
PRO	PRO	ASP	F2894	ILE	ILE		THR	E3261	K3331	PHE	R3453	ILE
PRO	PRO	ASP	L2895	ASP	ASP		THR	C3264	M3331	ARG	K3454	ILE
PRO	PRO	ASP	Q2896	GLU	GLU		THR	E3270	V3332	MET	G3455	LEU
PRO	PRO	ASP	S2898	LEU	LEU		THR	H3271	V3333	VAL	R3456	GLN
PRO	PRO	ASP	Q2899	PHE	PHE		THR			ALA	R3457	LYS
PRO	PRO	ASP	Y2900				THR				Y3458	LEU
PRO	PRO	ASP	S2901				THR				S3459	GLU

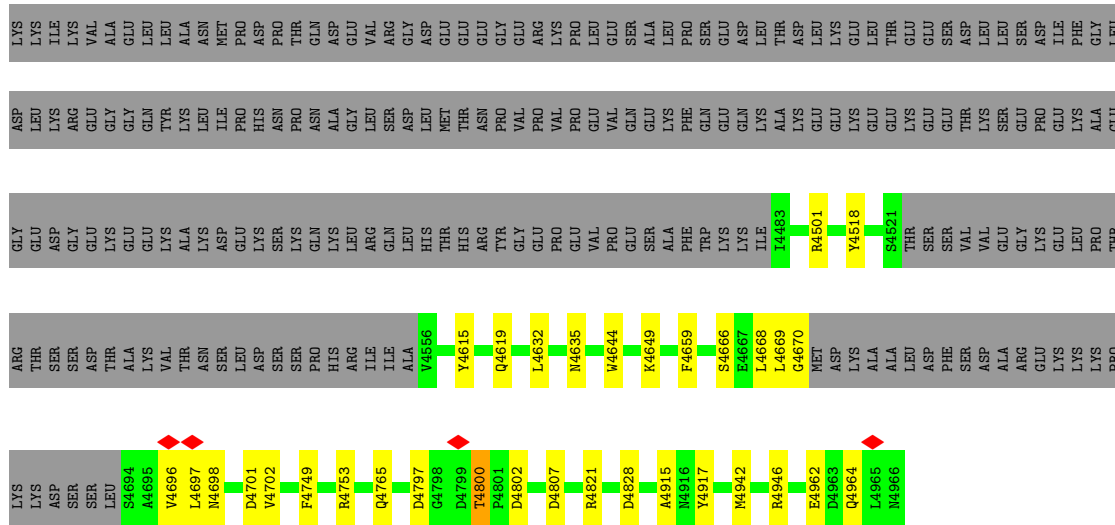




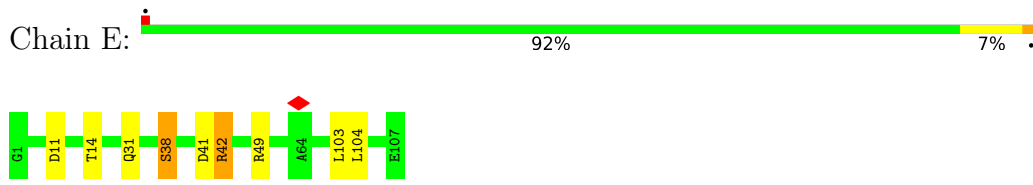




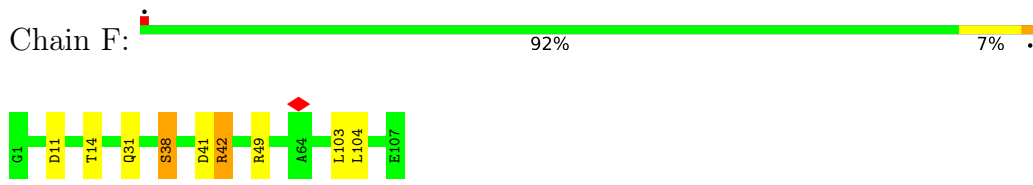




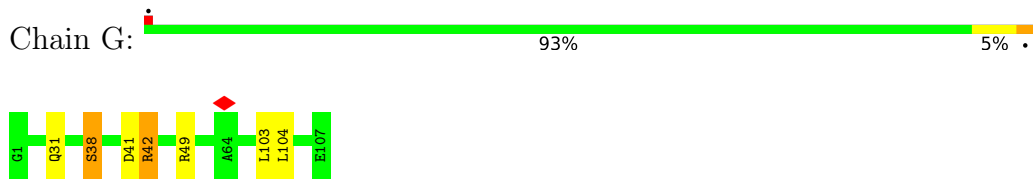
● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



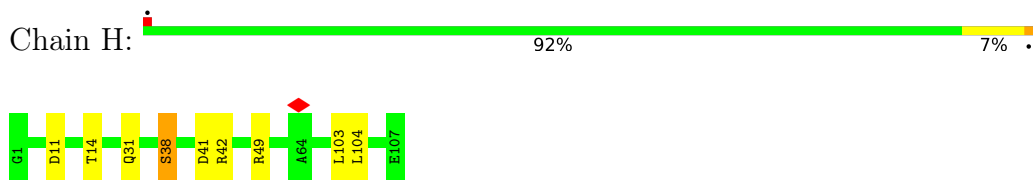
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	282778	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50, 50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.715	Depositor
Minimum map value	-0.955	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.132	Depositor
Map size ( $\text{\AA}$ )	501.12003, 501.12003, 501.12003	wwPDB
Map dimensions	464, 464, 464	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.08, 1.08, 1.08	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	0.38	0/31107	0.67	22/42056 (0.1%)
1	B	0.38	0/31107	0.67	16/42056 (0.0%)
1	C	0.38	0/31107	0.67	17/42056 (0.0%)
1	D	0.38	0/31107	0.67	19/42056 (0.0%)
2	E	0.31	0/834	0.65	1/1123 (0.1%)
2	F	0.31	0/834	0.65	1/1123 (0.1%)
2	G	0.31	0/834	0.64	1/1123 (0.1%)
2	H	0.31	0/834	0.64	0/1123
All	All	0.38	0/127764	0.67	77/172716 (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	9
1	B	0	9
1	C	0	9
1	D	0	7
All	All	0	34

There are no bond length outliers.

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	536	LEU	CA-CB-CG	8.00	133.70	115.30
1	A	536	LEU	CA-CB-CG	7.99	133.68	115.30
1	C	536	LEU	CA-CB-CG	7.97	133.64	115.30
1	D	536	LEU	CA-CB-CG	7.96	133.62	115.30

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1303	ARG	NE-CZ-NH1	6.34	123.47	120.30

There are no chirality outliers.

5 of 34 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1552	ASN	Peptide
1	A	159	TRP	Peptide
1	A	1769	PHE	Peptide
1	A	1780	SER	Peptide
1	A	618	CYS	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	30492	29287	29275	204	0
1	B	30492	29286	29275	212	0
1	C	30492	29286	29275	206	0
1	D	30492	29284	29275	215	0
2	E	818	824	824	4	0
2	F	818	824	824	4	0
2	G	818	824	824	3	0
2	H	818	824	824	4	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	125244	120439	120396	848	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 3.

The worst 5 of 848 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:612:ASP:O	1:D:616:SER:OG	2.07	0.72
1:C:612:ASP:O	1:C:616:SER:OG	2.07	0.70
1:B:612:ASP:O	1:B:616:SER:OG	2.07	0.70
1:A:612:ASP:O	1:A:616:SER:OG	2.07	0.69
1:C:2278:MET:SD	1:C:2284:TYR:OH	2.51	0.69

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	3849/4966 (78%)	3318 (86%)	523 (14%)	8 (0%)	47	77
1	B	3849/4966 (78%)	3325 (86%)	517 (13%)	7 (0%)	47	77
1	C	3849/4966 (78%)	3323 (86%)	516 (13%)	10 (0%)	41	72
1	D	3849/4966 (78%)	3329 (86%)	512 (13%)	8 (0%)	47	77
2	E	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
2	F	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
2	G	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
2	H	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
All	All	15816/20292 (78%)	13687 (86%)	2096 (13%)	33 (0%)	50	77

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	607	ASN
1	B	607	ASN
1	B	1501	ASN
1	C	607	ASN
1	C	1497	GLY

### 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	3181/4355 (73%)	3121 (98%)	60 (2%)	57	77
1	B	3181/4355 (73%)	3120 (98%)	61 (2%)	57	77
1	C	3181/4355 (73%)	3124 (98%)	57 (2%)	59	78
1	D	3181/4355 (73%)	3117 (98%)	64 (2%)	55	76
2	E	88/88 (100%)	85 (97%)	3 (3%)	37	65
2	F	88/88 (100%)	85 (97%)	3 (3%)	37	65
2	G	88/88 (100%)	85 (97%)	3 (3%)	37	65
2	H	88/88 (100%)	85 (97%)	3 (3%)	37	65
All	All	13076/17772 (74%)	12822 (98%)	254 (2%)	59	77

5 of 254 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4518	TYR
1	D	2654	LYS
1	C	976	TYR
1	D	2651	LEU
1	D	4518	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	658	ASN
1	D	2090	GLN
1	C	1440	ASN
1	D	781	ASN
1	C	930	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

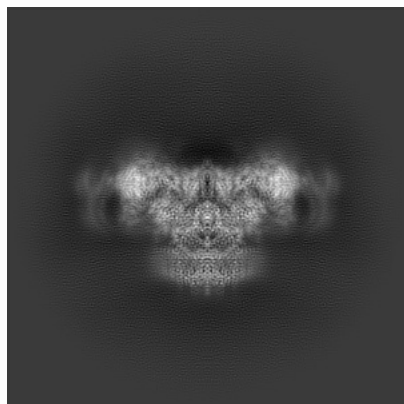
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21861. These allow visual inspection of the internal detail of the map and identification of artifacts.

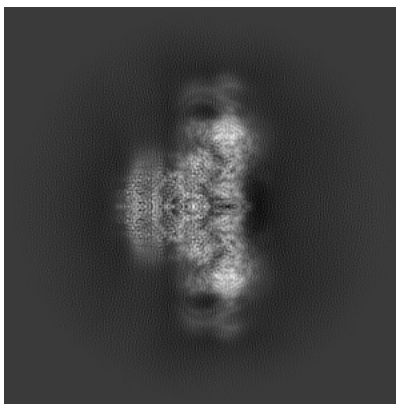
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

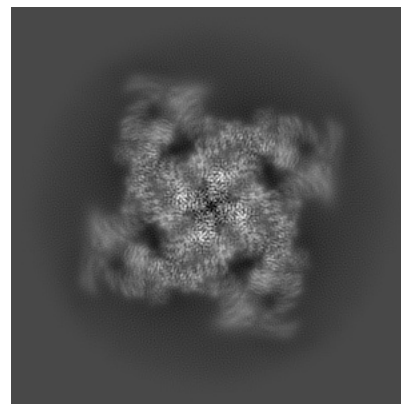
#### 6.1.1 Primary map



X

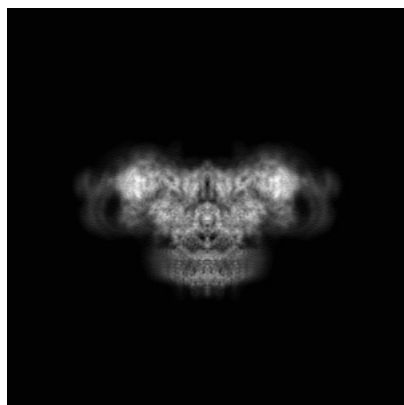


Y

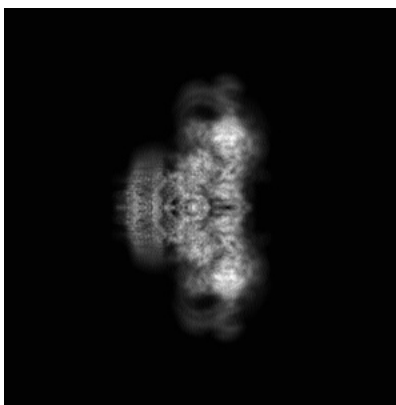


Z

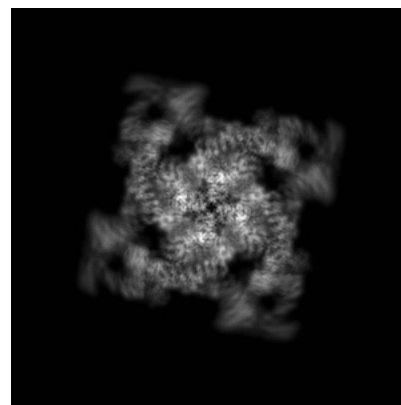
#### 6.1.2 Raw map



X



Y

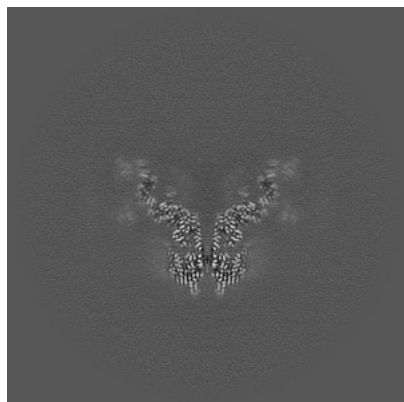


Z

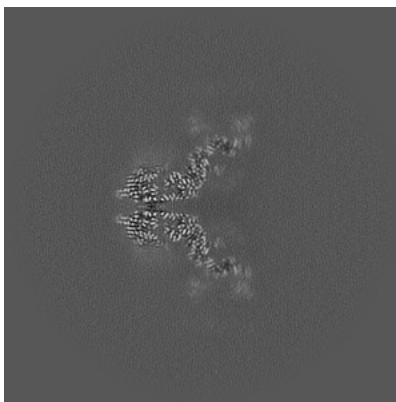
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

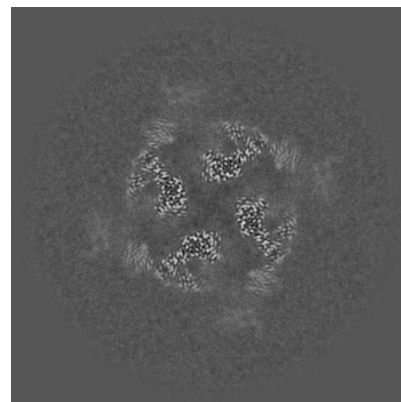
### 6.2.1 Primary map



X Index: 232

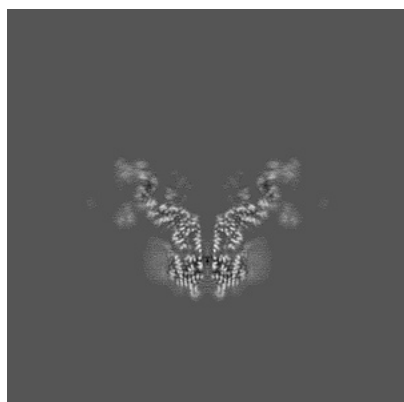


Y Index: 232

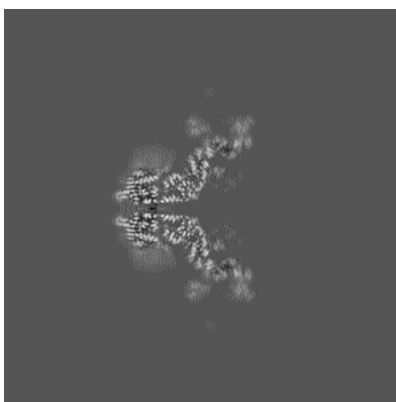


Z Index: 232

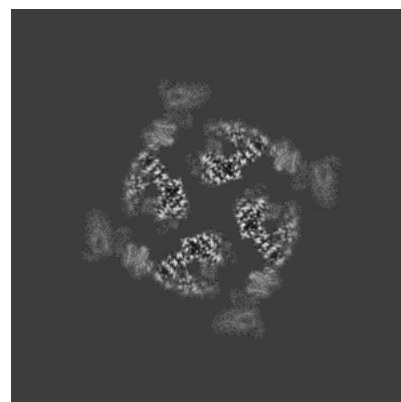
### 6.2.2 Raw map



X Index: 232



Y Index: 232



Z Index: 232

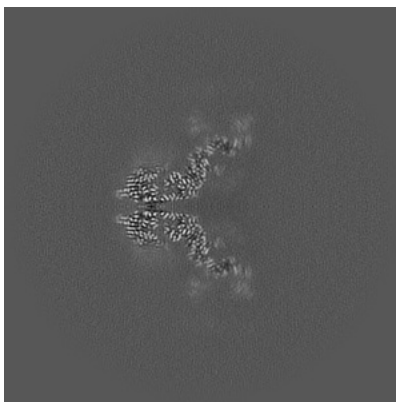
The images above show central slices of the map in three orthogonal directions.

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

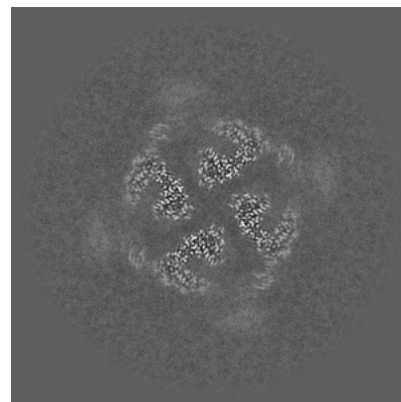
### 6.3.1 Primary map



X Index: 232

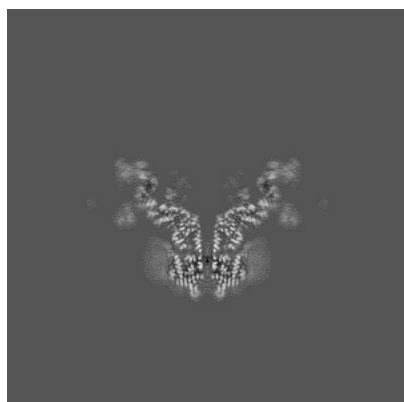


Y Index: 232

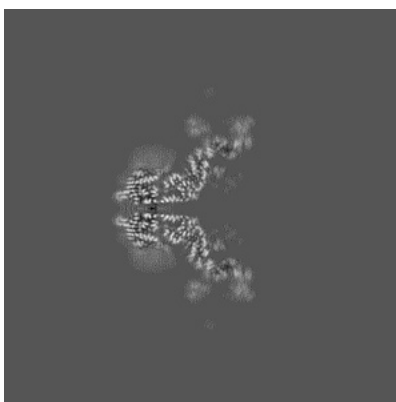


Z Index: 227

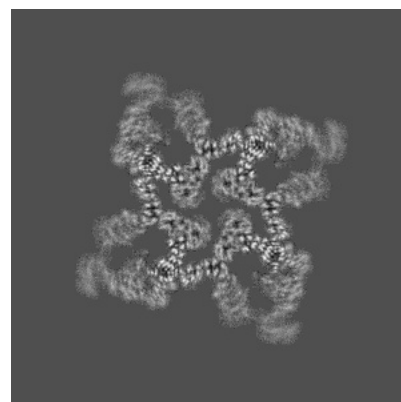
### 6.3.2 Raw map



X Index: 232



Y Index: 232



Z Index: 259

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

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

### 6.4.1 Primary map



X



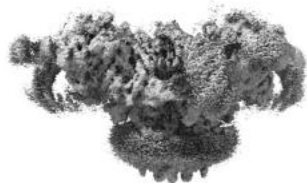
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.132. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

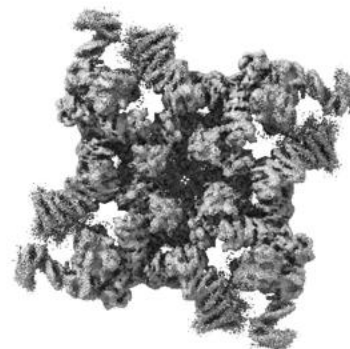
### 6.4.2 Raw map



X



Y



Z

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

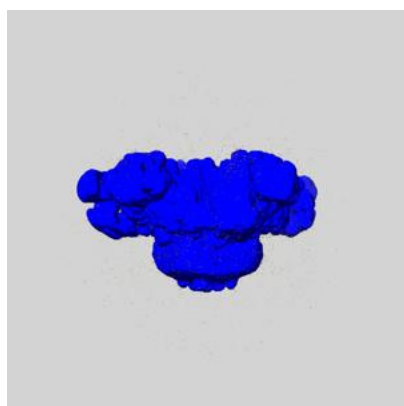
## 6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

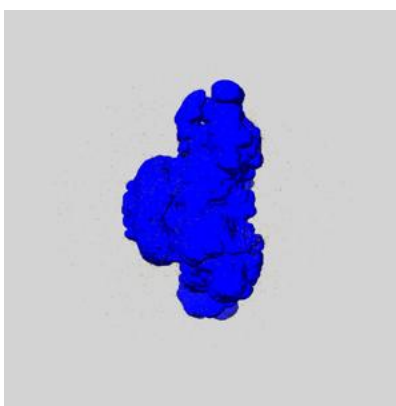
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

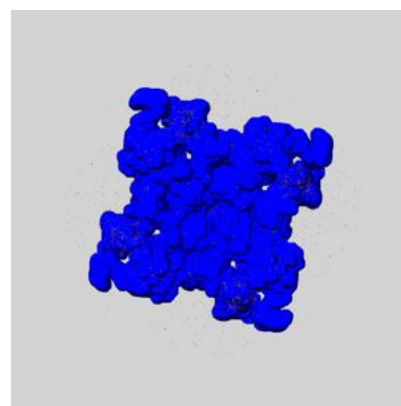
### 6.5.1 emd\_21861\_msk\_1.map [i](#)



X



Y

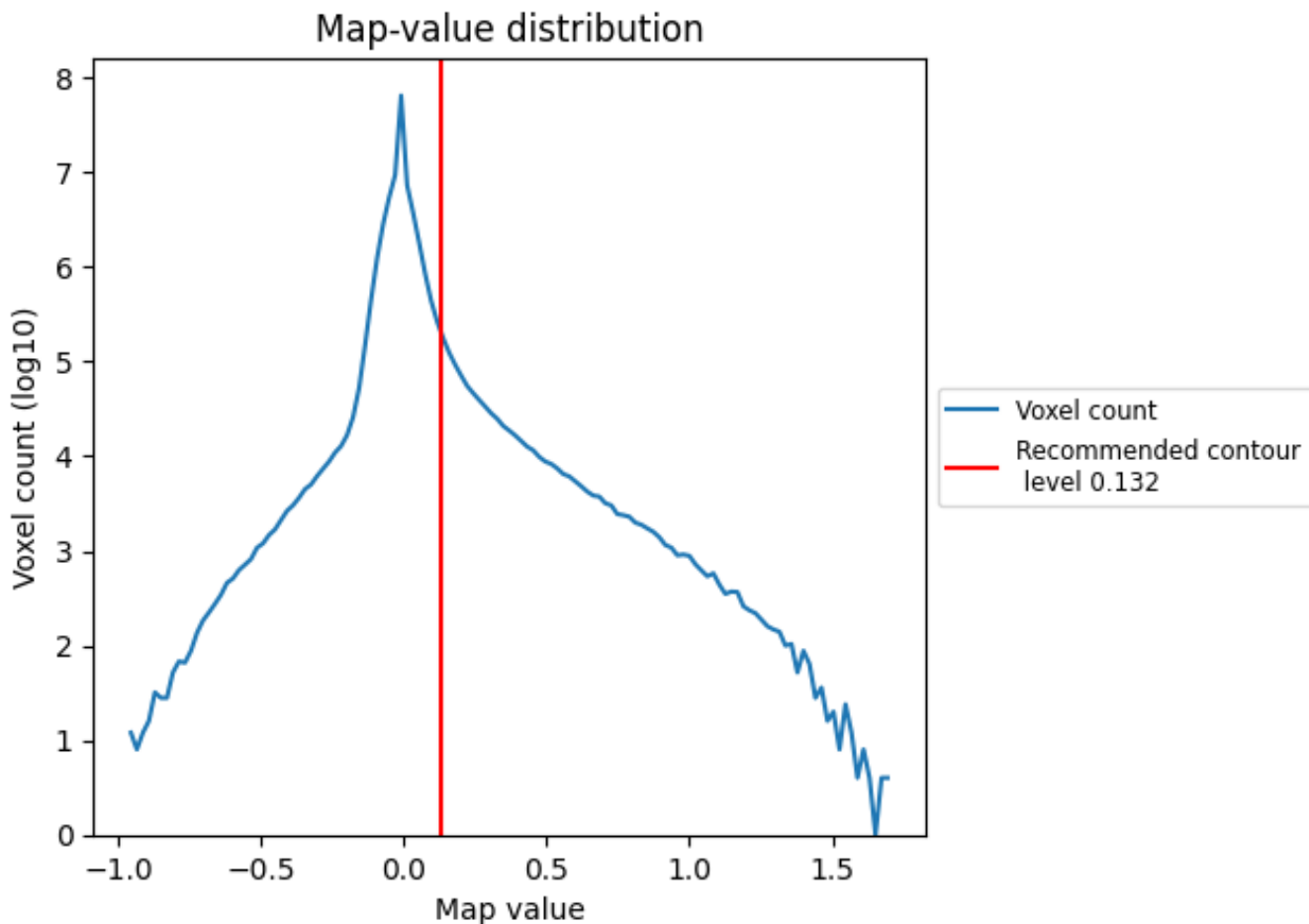


Z

## 7 Map analysis [i](#)

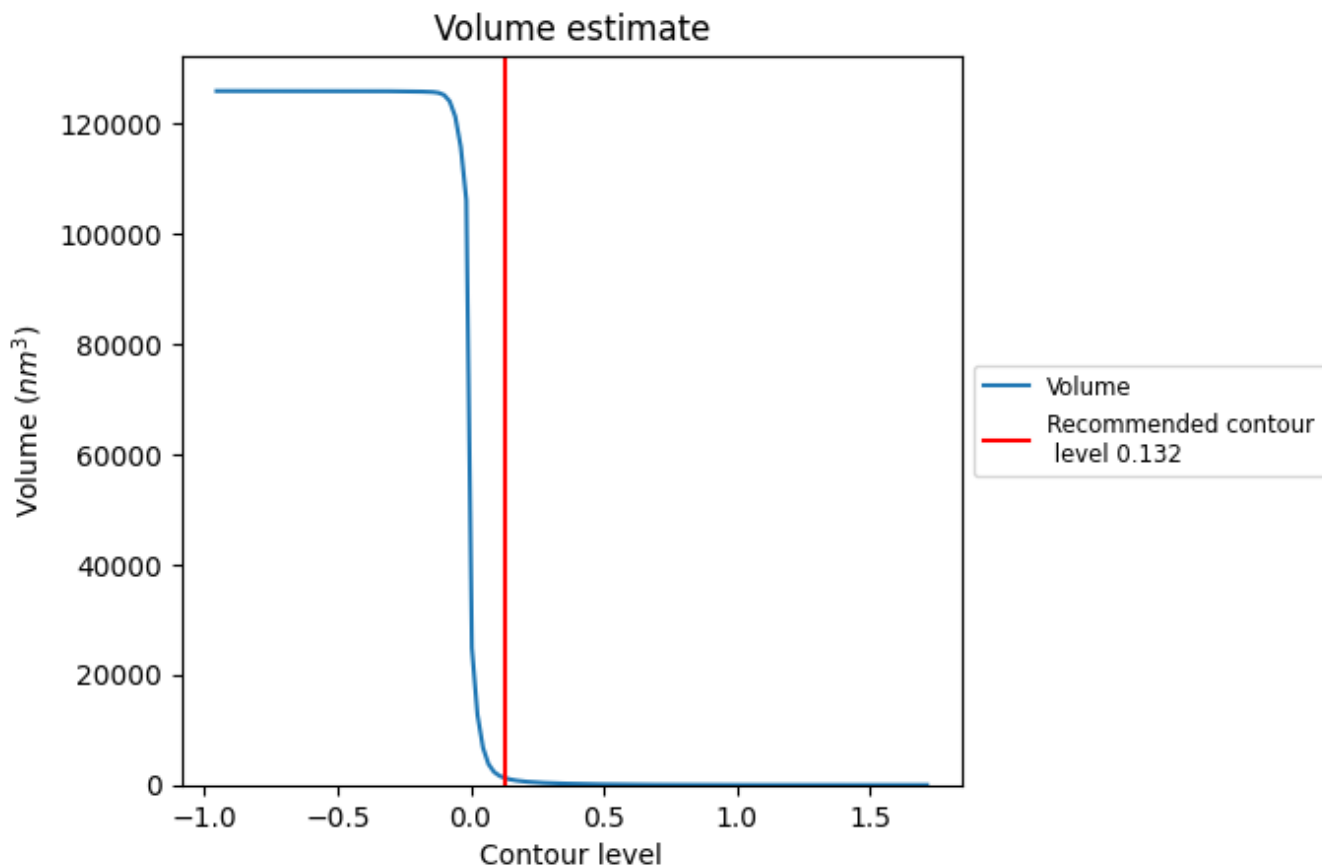
This section contains the results of statistical analysis of the map.

### 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](#)

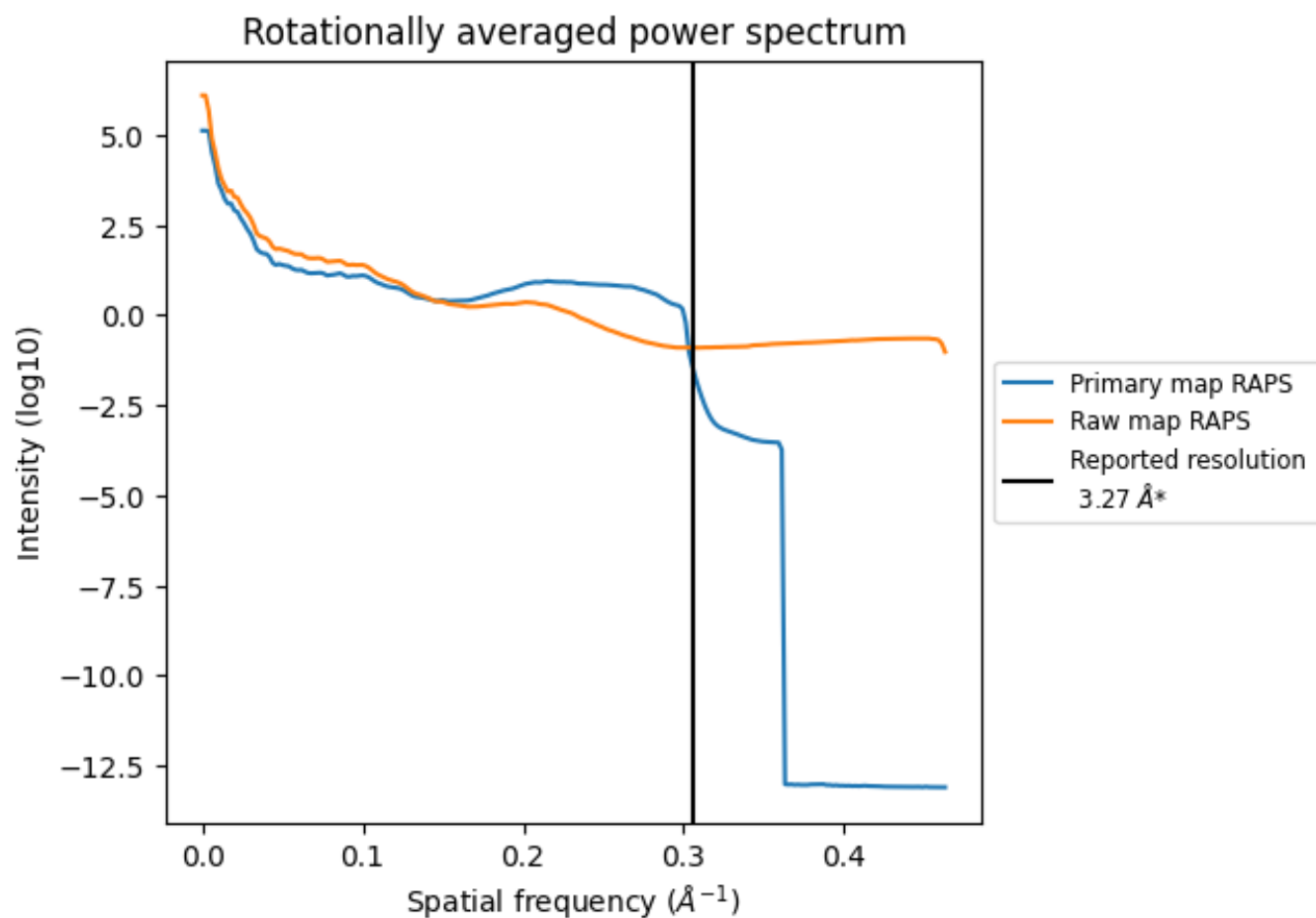


The volume at the recommended contour level is 1213  $\text{nm}^3$ ; this corresponds to an approximate mass of 1096 kDa.

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

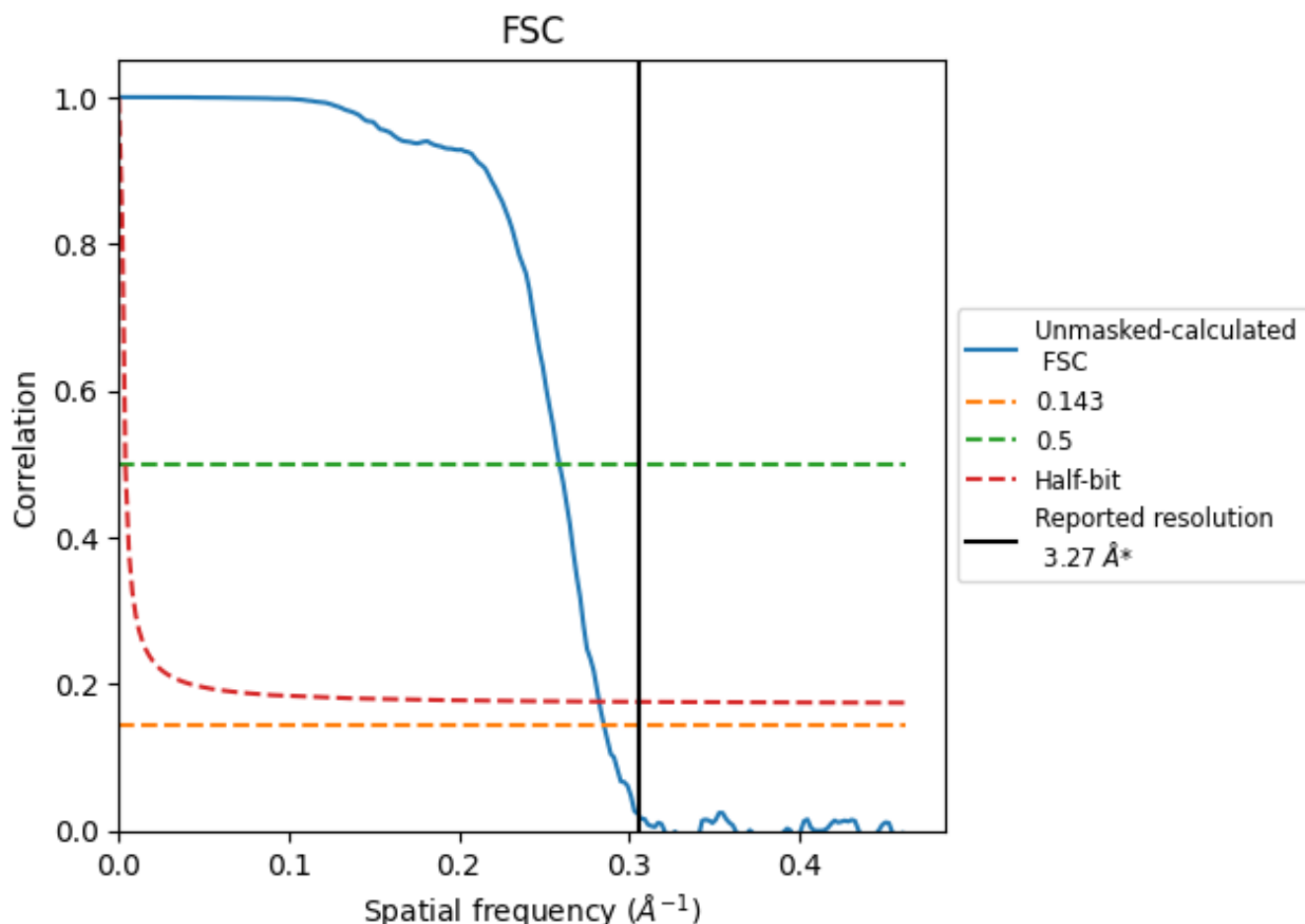


\*Reported resolution corresponds to spatial frequency of 0.306 Å<sup>-1</sup>

## 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  $0.306 \text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

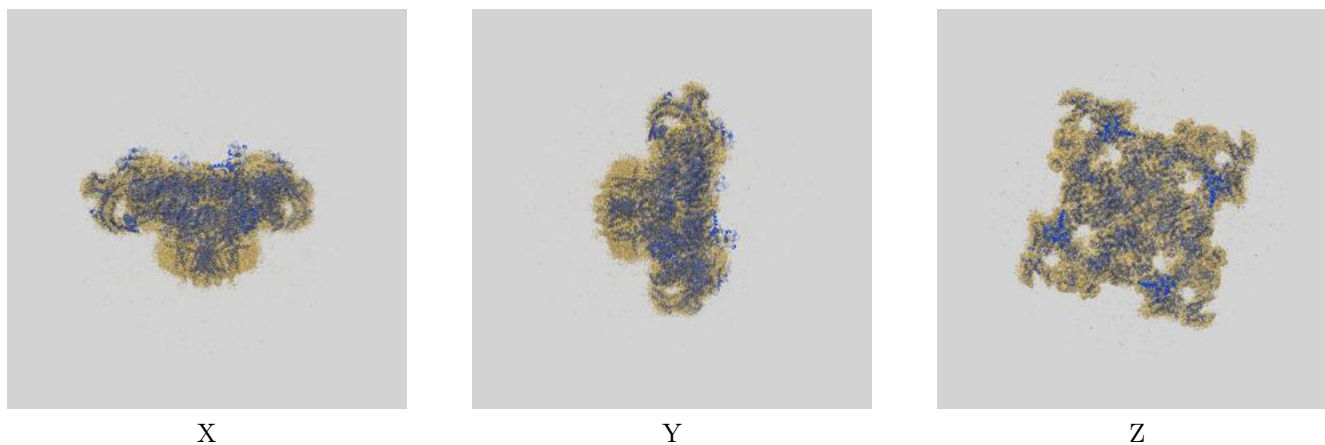
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.27	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.50	3.86	3.54

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

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

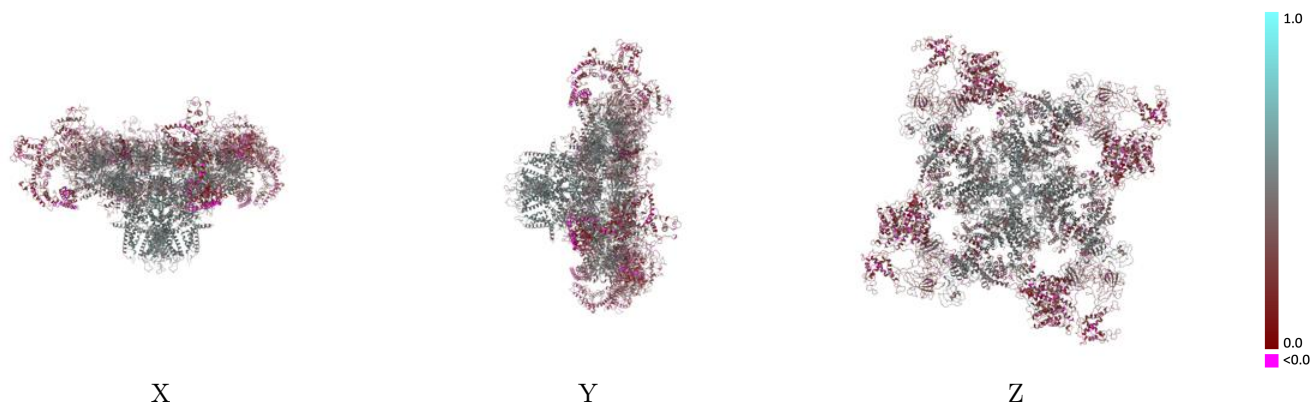
This section contains information regarding the fit between EMDB map EMD-21861 and PDB model 6WOU. Per-residue inclusion information can be found in section 3 on page 5.

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



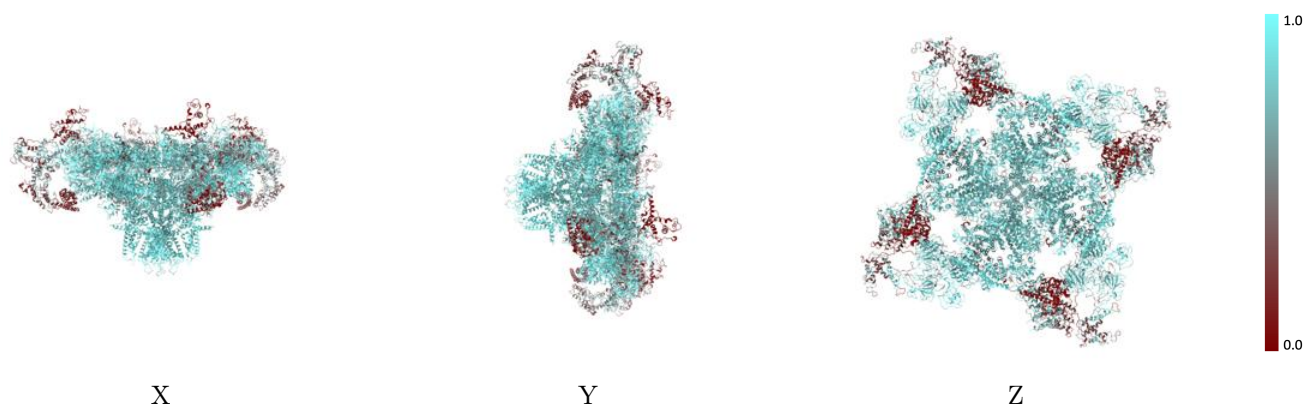
The images above show the 3D surface view of the map at the recommended contour level 0.132 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



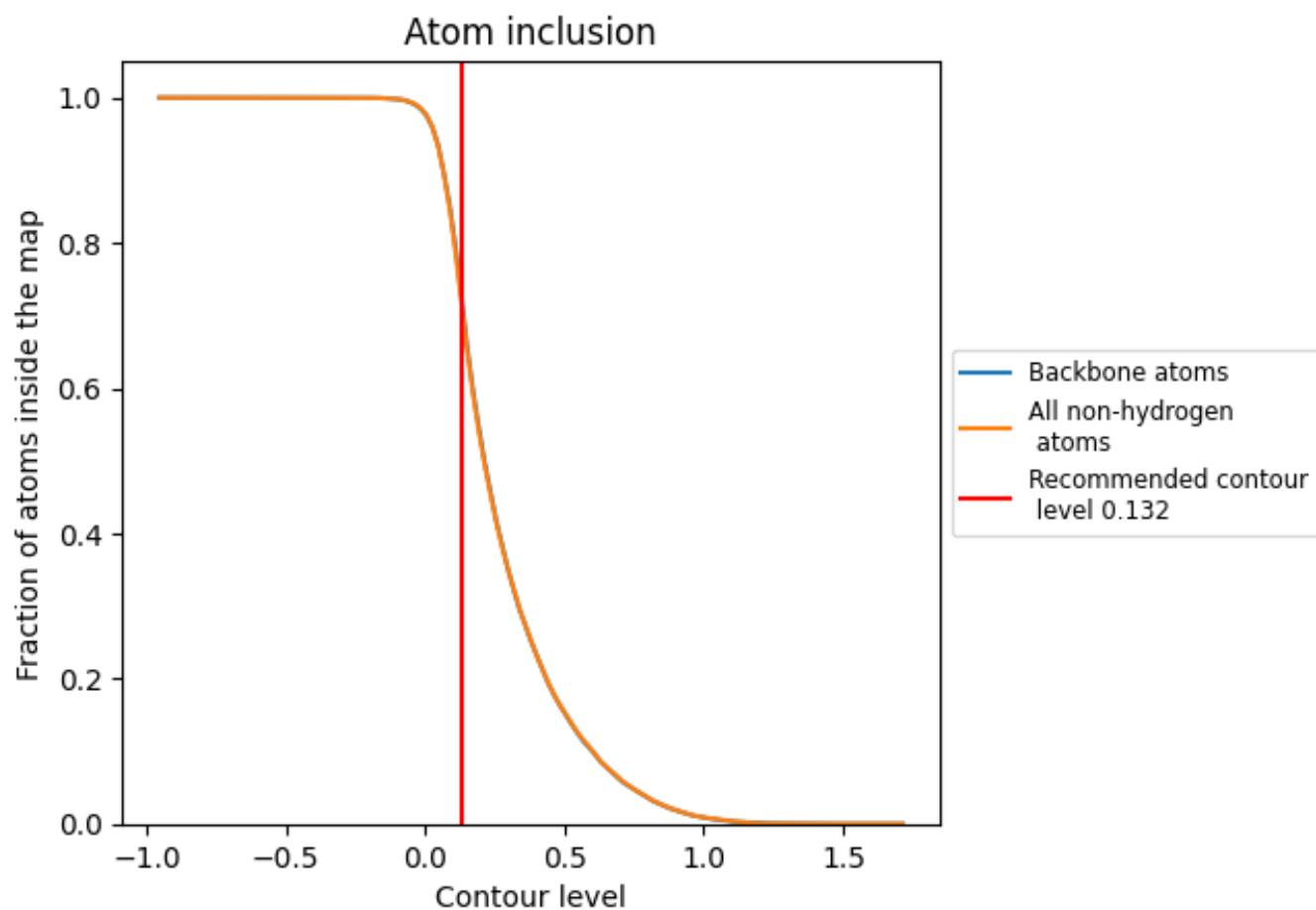
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.132).



















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 71% 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 (0.132) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7117	 0.3760
A	 0.7107	 0.3740
B	 0.7107	 0.3730
C	 0.7110	 0.3740
D	 0.7109	 0.3740
E	 0.8710	 0.4550
F	 0.8722	 0.4560
G	 0.8672	 0.4560
H	 0.8685	 0.4580

