wwPDB EM Validation Summary Report ⓘ

Dec 17, 2022 – 02:21 pm GMT

PDB ID	:	7A7D
EMDB ID	:	EMD-11678
Title	:	Cadherin fit into cryo-ET map
Authors	:	Sikora, M.; Ermel, U.H.; Seybold, A.; Kunz, M.; Calloni, G.; Reitz, J.; Vabulas, R.M.; Hummer, G.; Frangakis, A.S.
Deposited on	:	2020-08-28
Resolution	:	26.00 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:

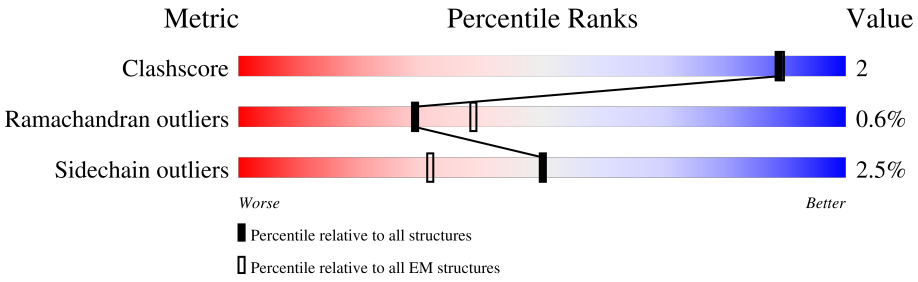
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 26.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	554	42% 77% 21% •
1	B	554	70% 81% 17% •
1	C	554	77% 79% 19% •
1	D	554	66% 78% 21% •
1	E	554	60% 77% 18% • •
1	F	554	68% 79% 18% •
1	G	554	64% 78% 20% •
2	a	544	61% 77% 21% •

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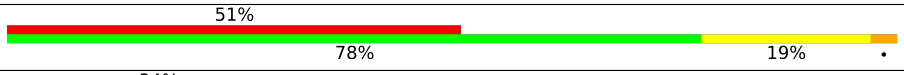
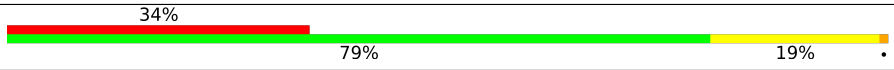
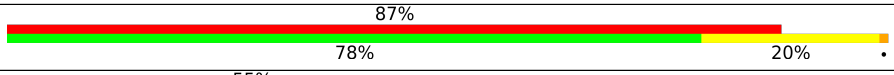
Mol	Chain	Length	Quality of chain
2	b	544	
2	c	544	
2	d	544	
2	e	544	
2	f	544	
2	g	544	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 119497 atoms, of which 59136 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 Desmoglein-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	554	Total	C	H	N	O	S	0	0
			8649	2749	4294	725	870	11		
1	B	554	Total	C	H	N	O	S	0	0
			8649	2749	4294	725	870	11		
1	C	554	Total	C	H	N	O	S	0	0
			8649	2749	4294	725	870	11		
1	D	554	Total	C	H	N	O	S	0	0
			8649	2749	4294	725	870	11		
1	E	554	Total	C	H	N	O	S	0	0
			8649	2749	4294	725	870	11		
1	F	554	Total	C	H	N	O	S	0	0
			8649	2749	4294	725	870	11		
1	G	554	Total	C	H	N	O	S	0	0
			8649	2749	4294	725	870	11		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	554	HIS	GLN	conflict	UNP Q14126
B	2252	HIS	GLN	conflict	UNP Q14126
C	1120	HIS	GLN	conflict	UNP Q14126
D	1686	HIS	GLN	conflict	UNP Q14126
E	2252	HIS	GLN	conflict	UNP Q14126
F	1686	HIS	GLN	conflict	UNP Q14126
G	1120	HIS	GLN	conflict	UNP Q14126

- Molecule 2 is a protein called Desmocollin-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	a	544	Total	C	H	N	O	S	0	0
			8422	2670	4154	708	868	22		
2	b	544	Total	C	H	N	O	S	0	0
			8422	2670	4154	708	868	22		

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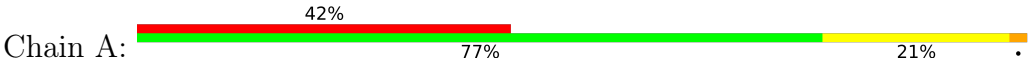
Mol	Chain	Residues	Atoms						AltConf	Trace
2	c	544	Total	C	H	N	O	S	0	0
			8422	2670	4154	708	868	22		
2	d	544	Total	C	H	N	O	S	0	0
			8422	2670	4154	708	868	22		
2	e	544	Total	C	H	N	O	S	0	0
			8422	2670	4154	708	868	22		
2	f	544	Total	C	H	N	O	S	0	0
			8422	2670	4154	708	868	22		
2	g	544	Total	C	H	N	O	S	0	0
			8422	2670	4154	708	868	22		

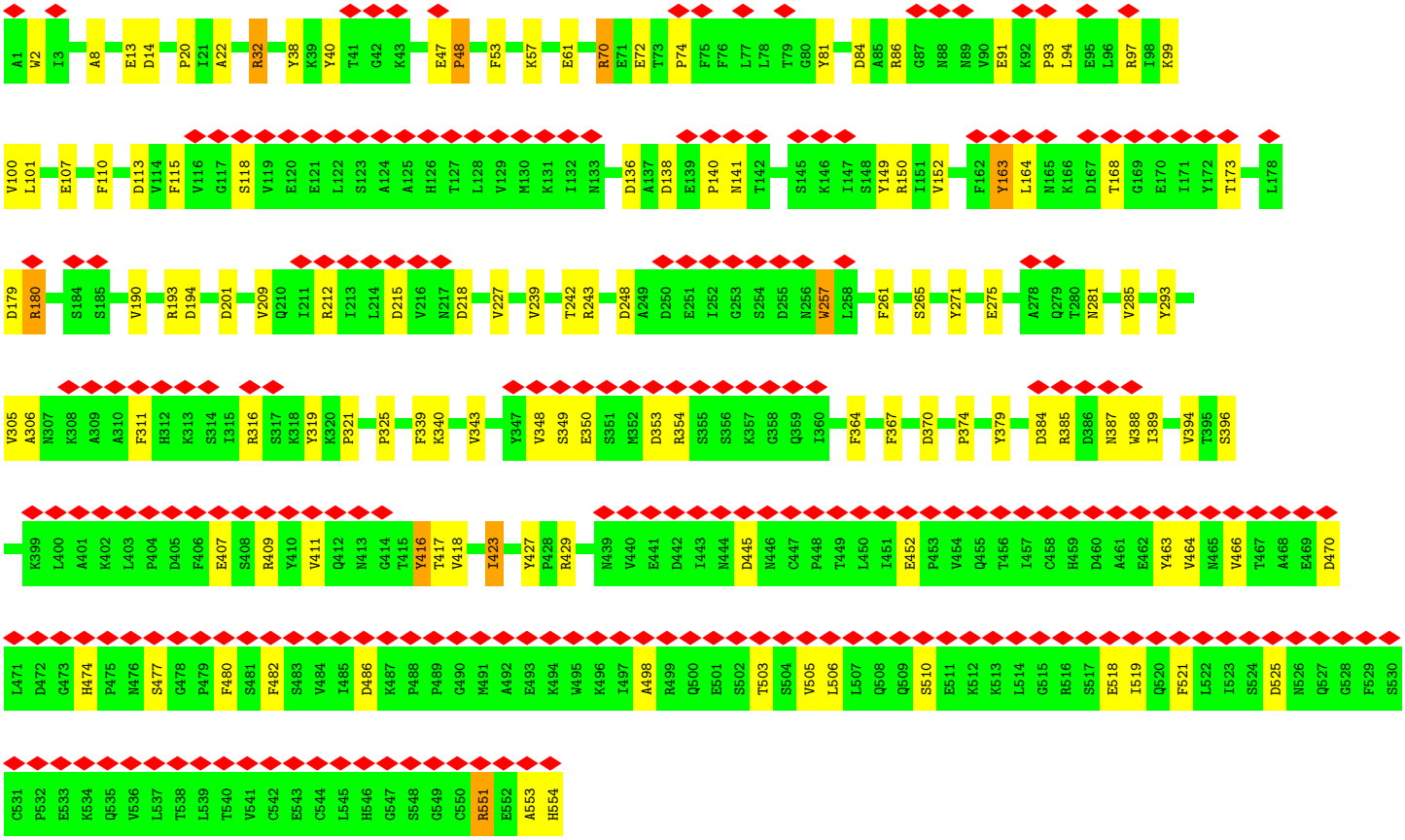
3 Residue-property plots (i)

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: Desmoglein-2

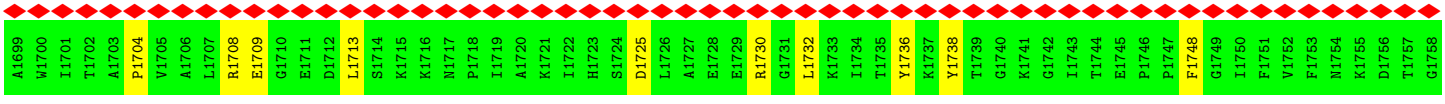
Chain A:

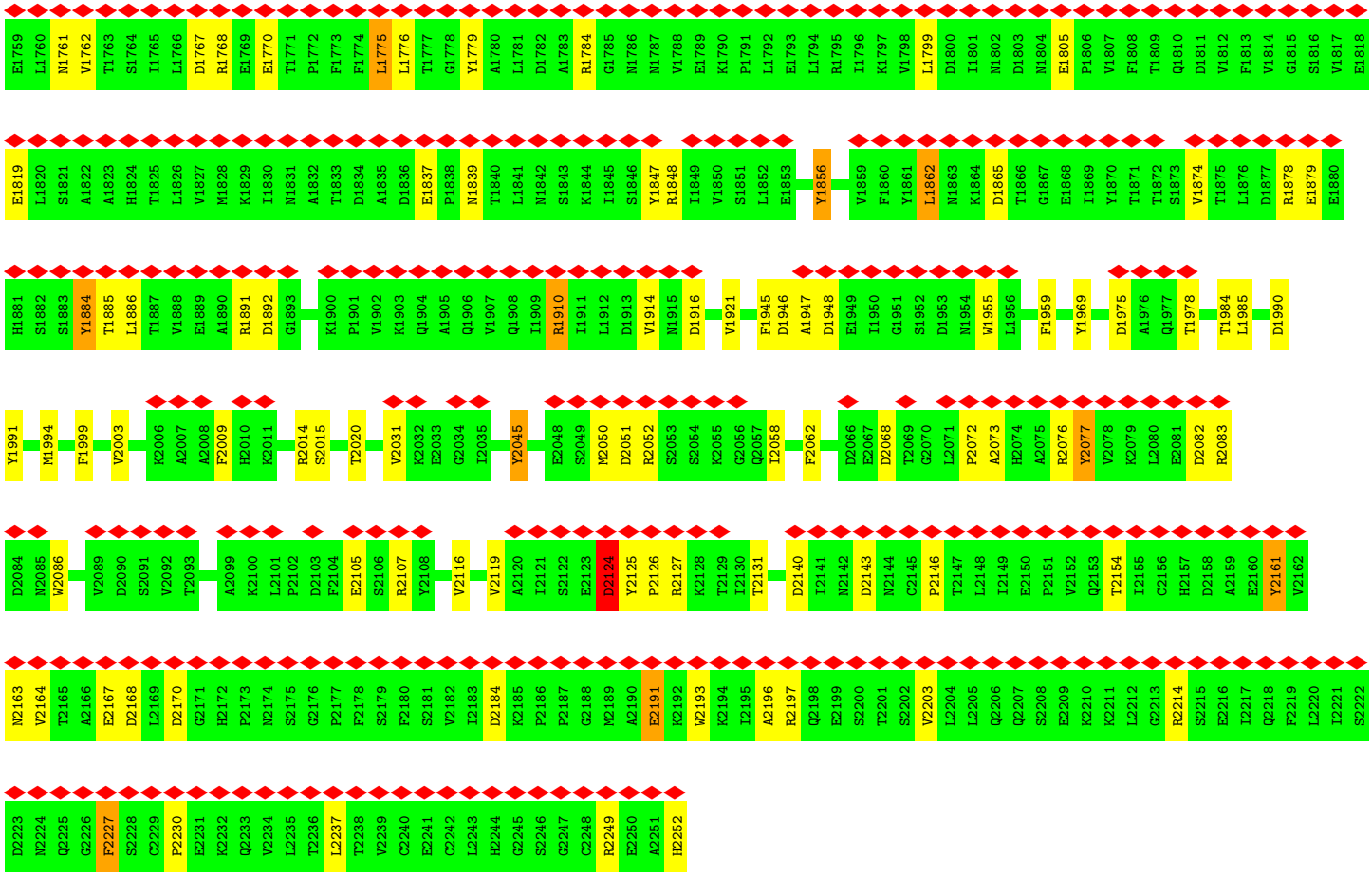




• Molecule 1: Desmoglein-2

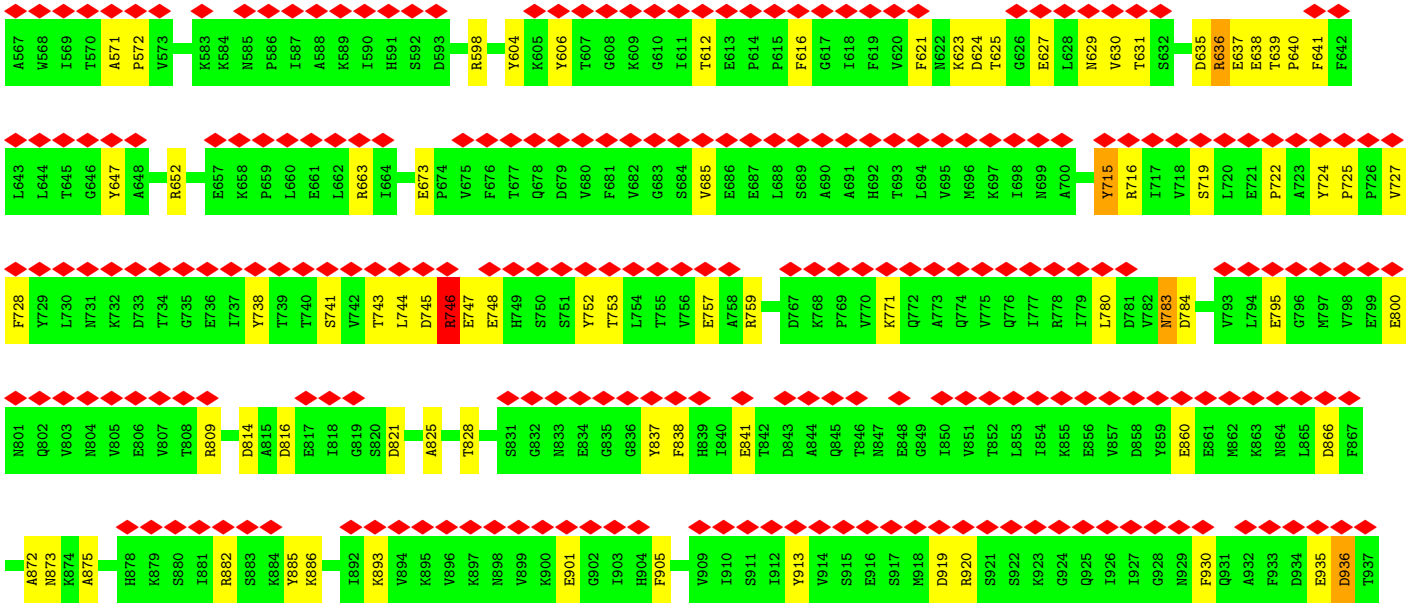
Chain B:

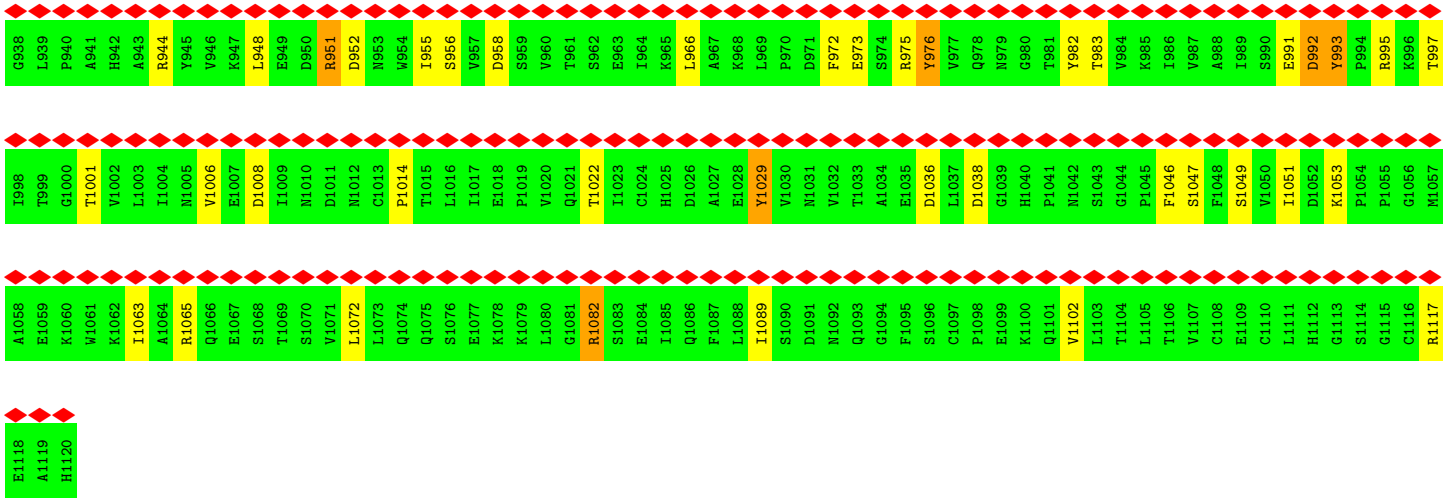




• Molecule 1: Desmoglein-2

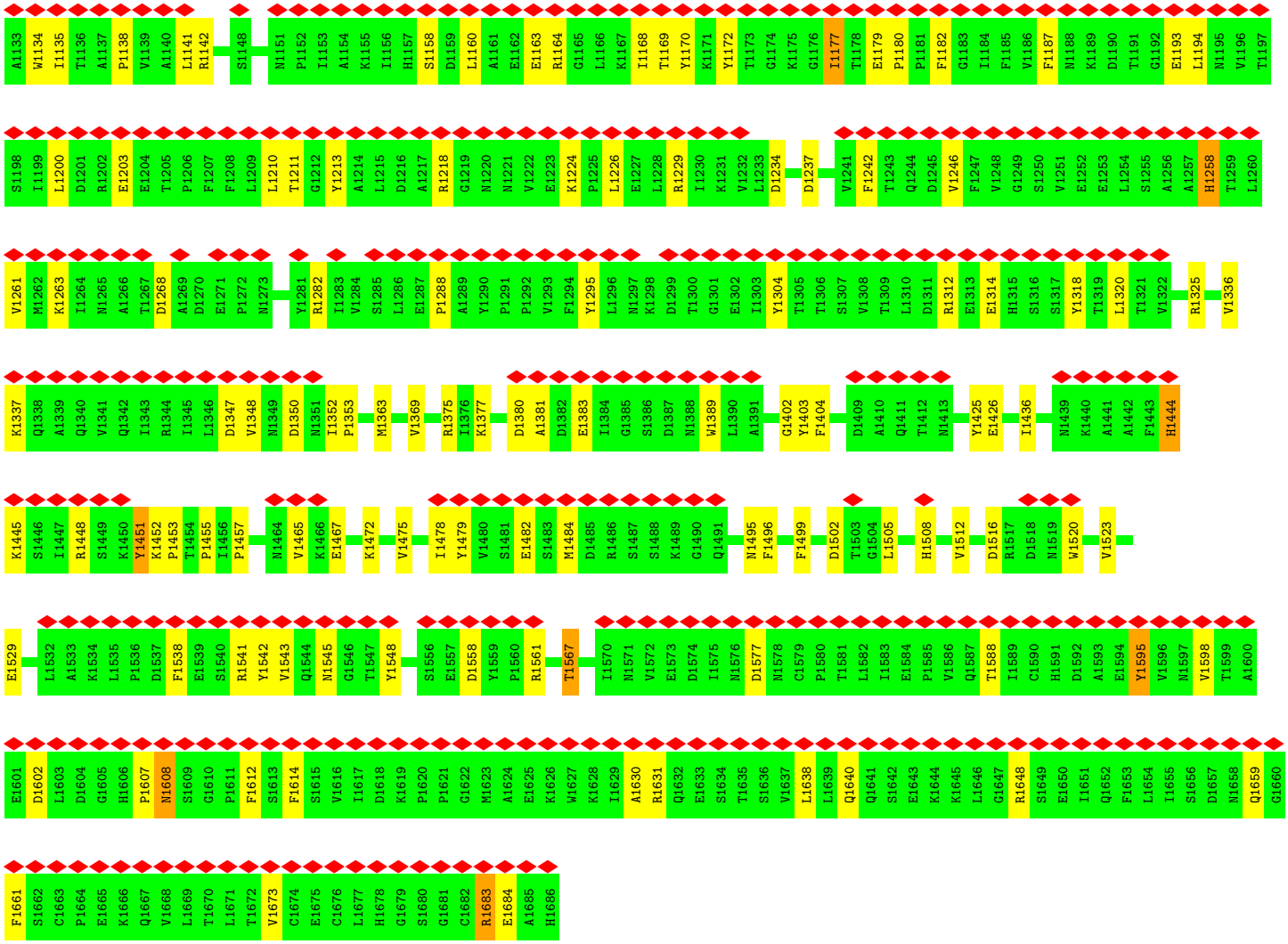
Chain C:





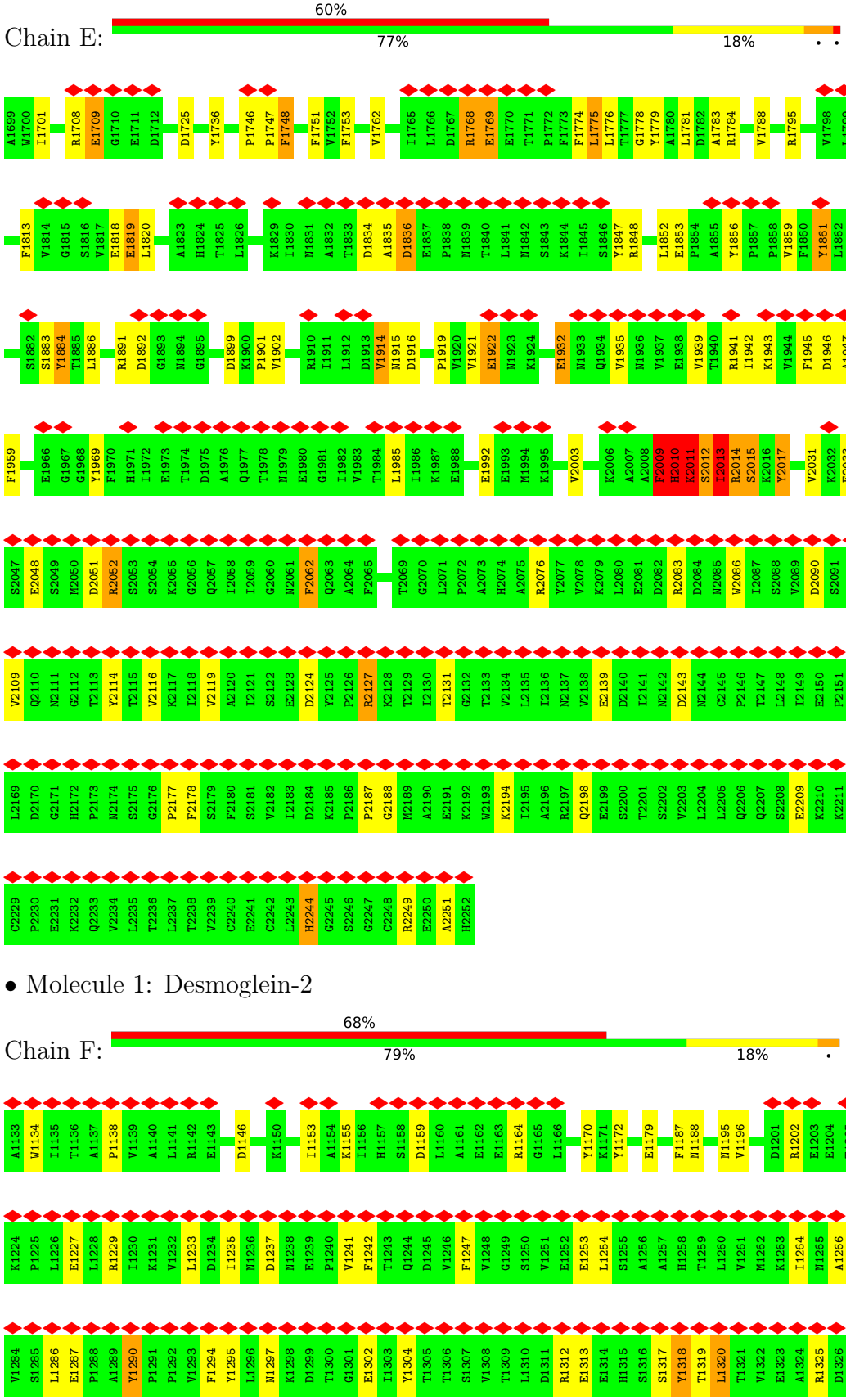
- Molecule 1: Desmoglein-2

Chain D:



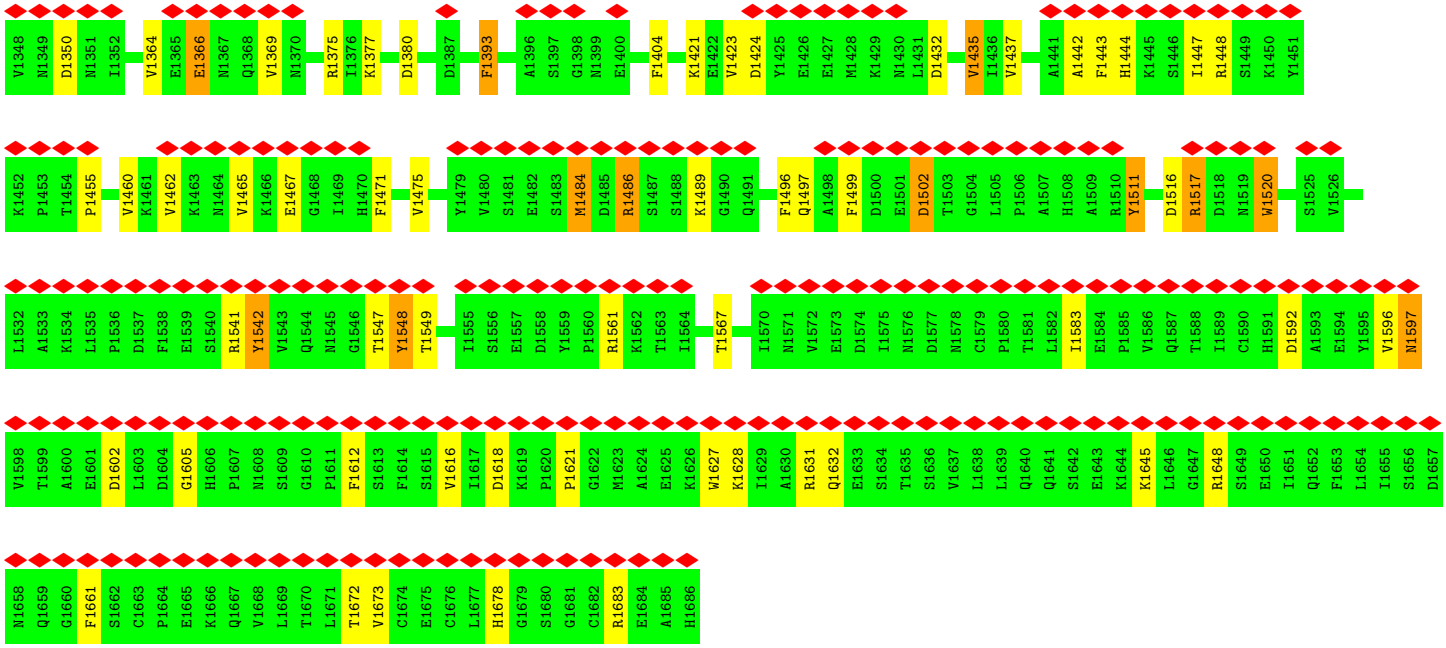
• Molecule 1: Desmoglein-2

Chain E:



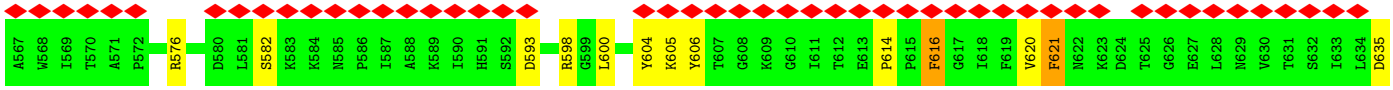
• Molecule 1: Desmoglein-2

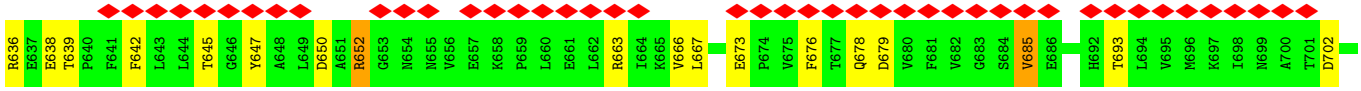
Chain F:

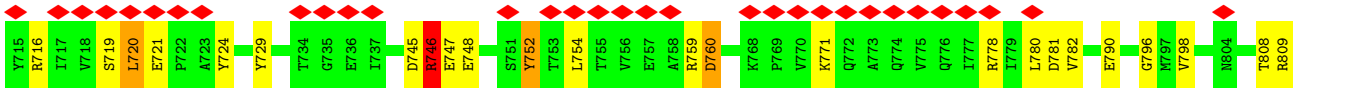


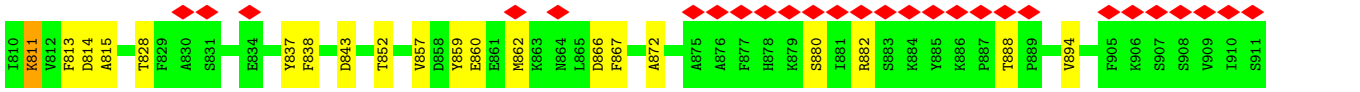
• Molecule 1: Desmoglein-2

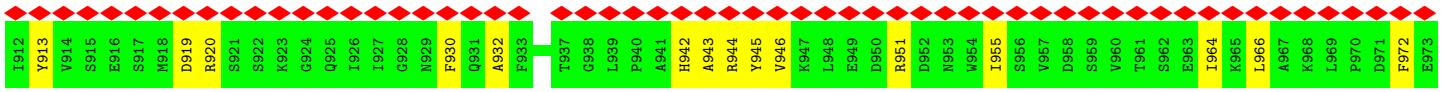
Chain G:

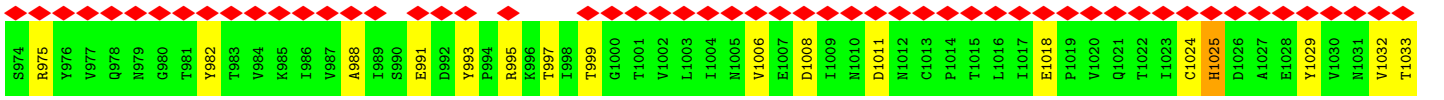


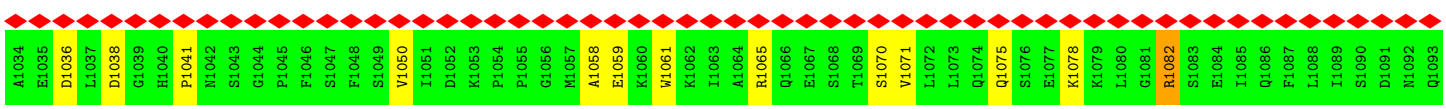


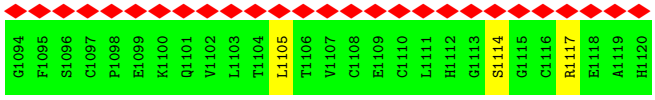






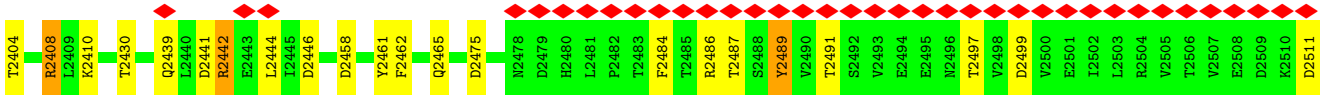


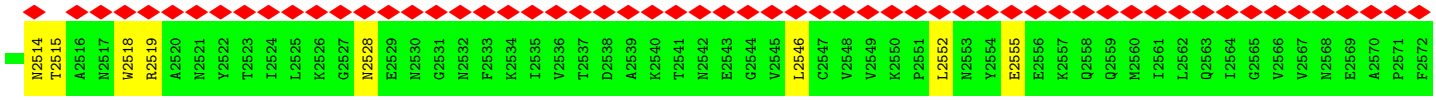


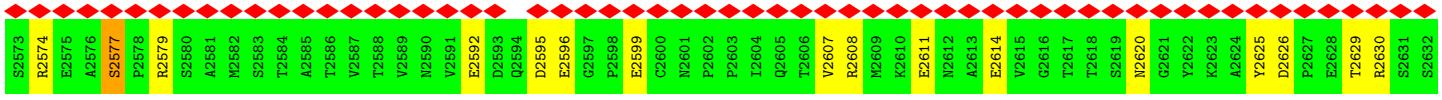


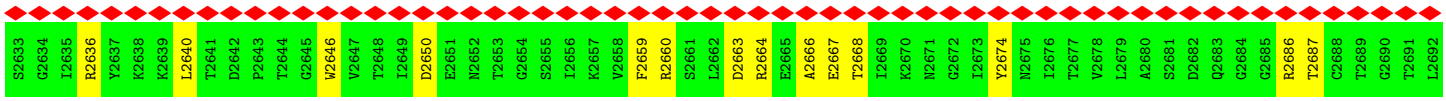
• Molecule 2: Desmocollin-2

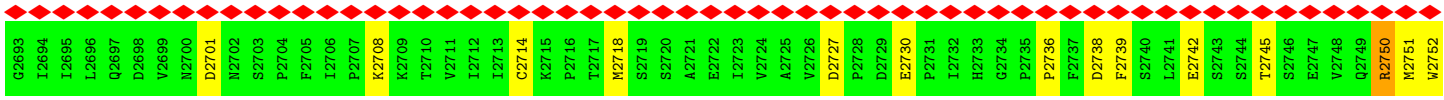
Chain a:

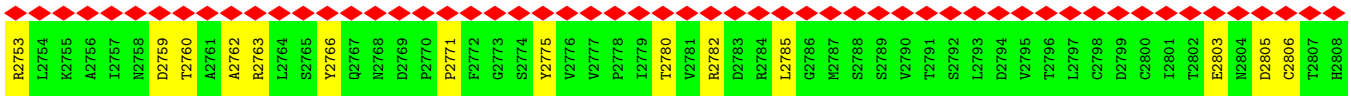






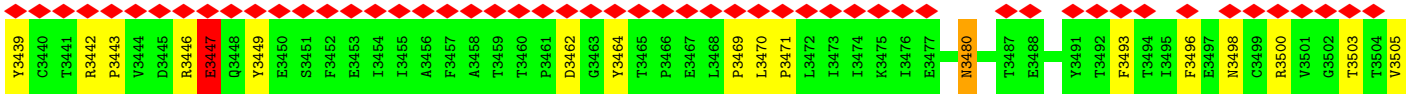


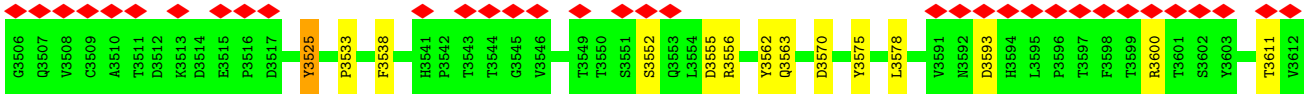


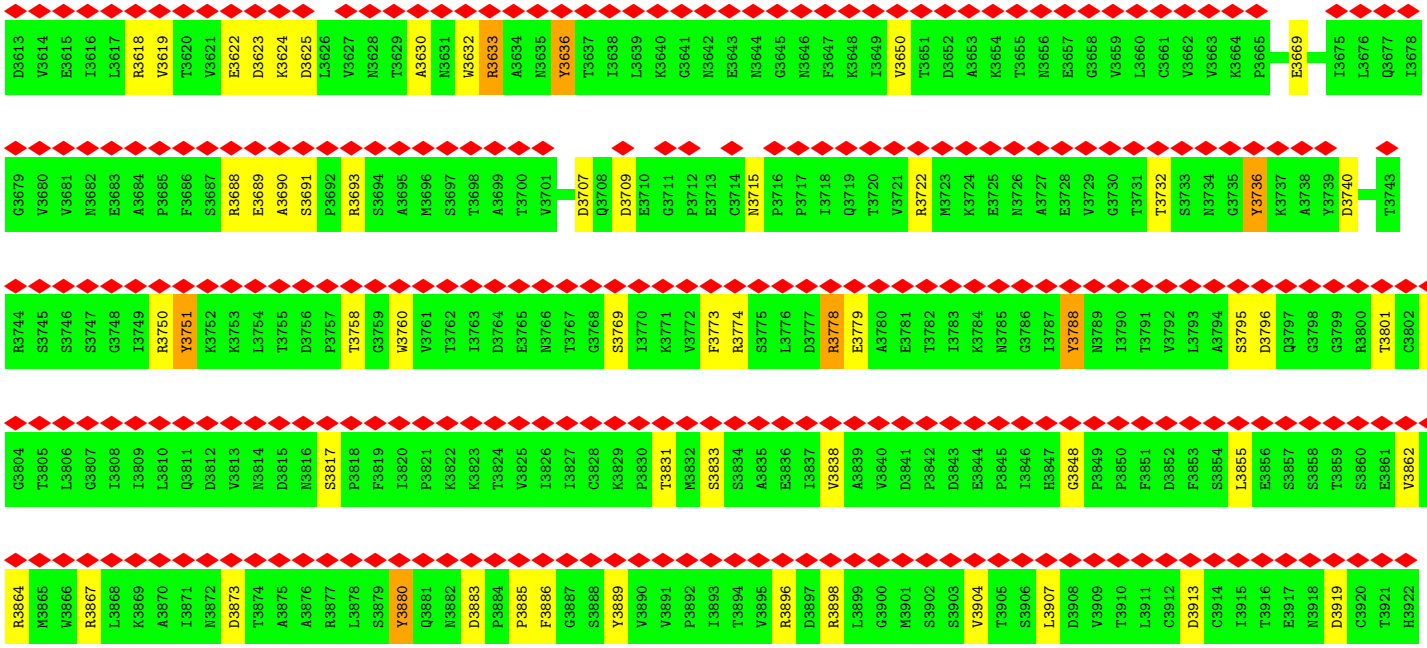


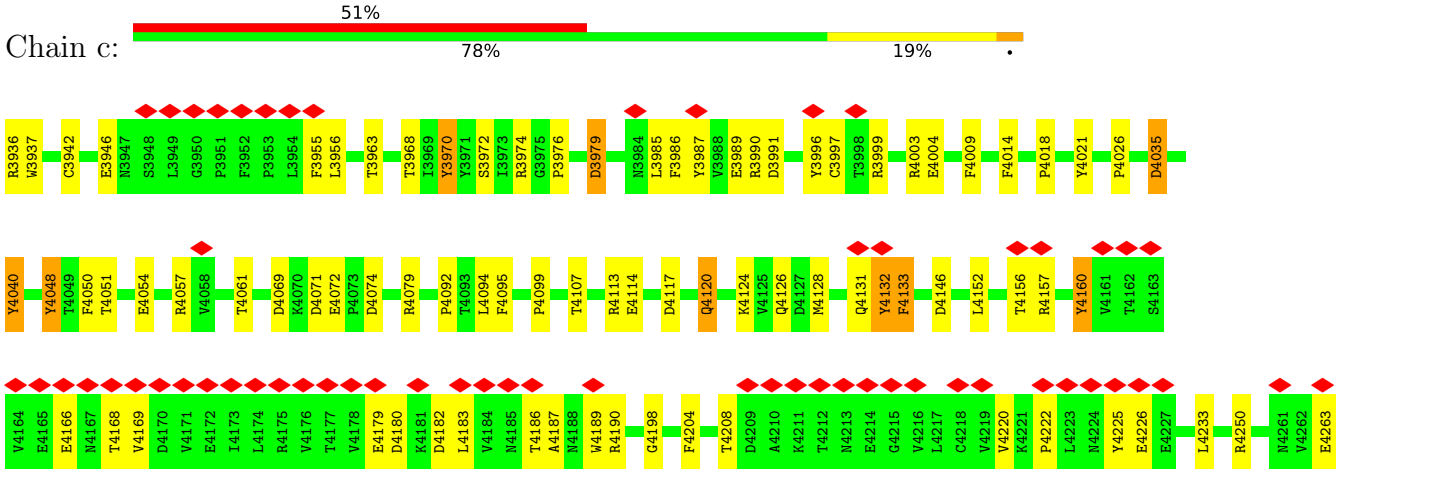
• Molecule 2: Desmocollin-2

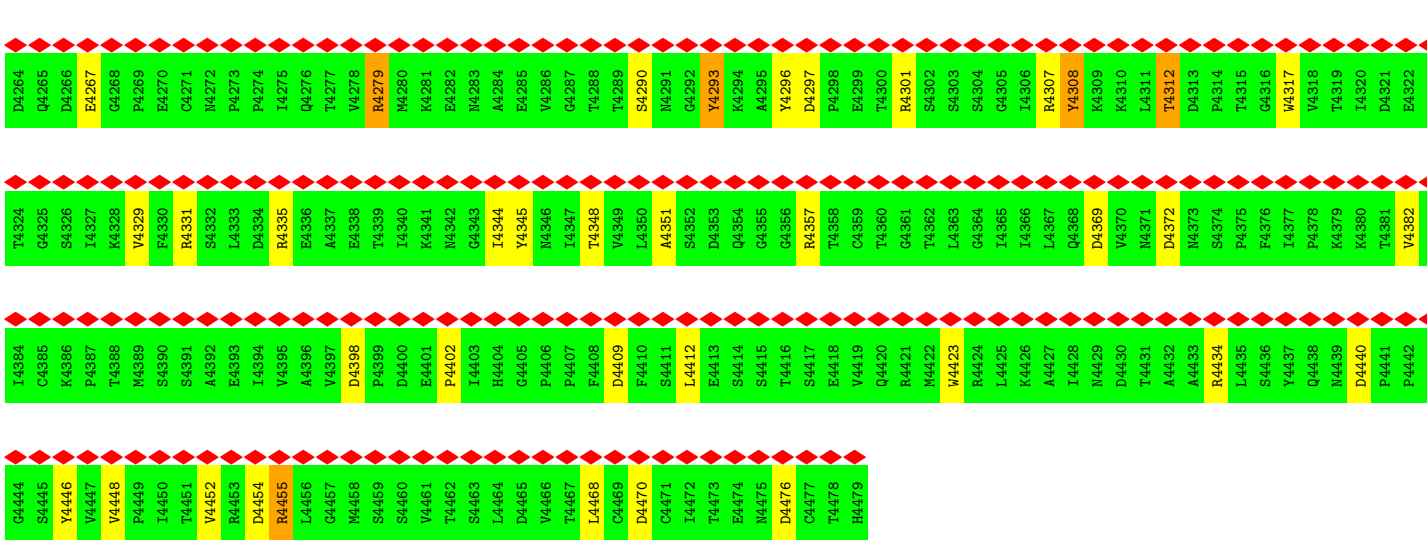
Chain b:









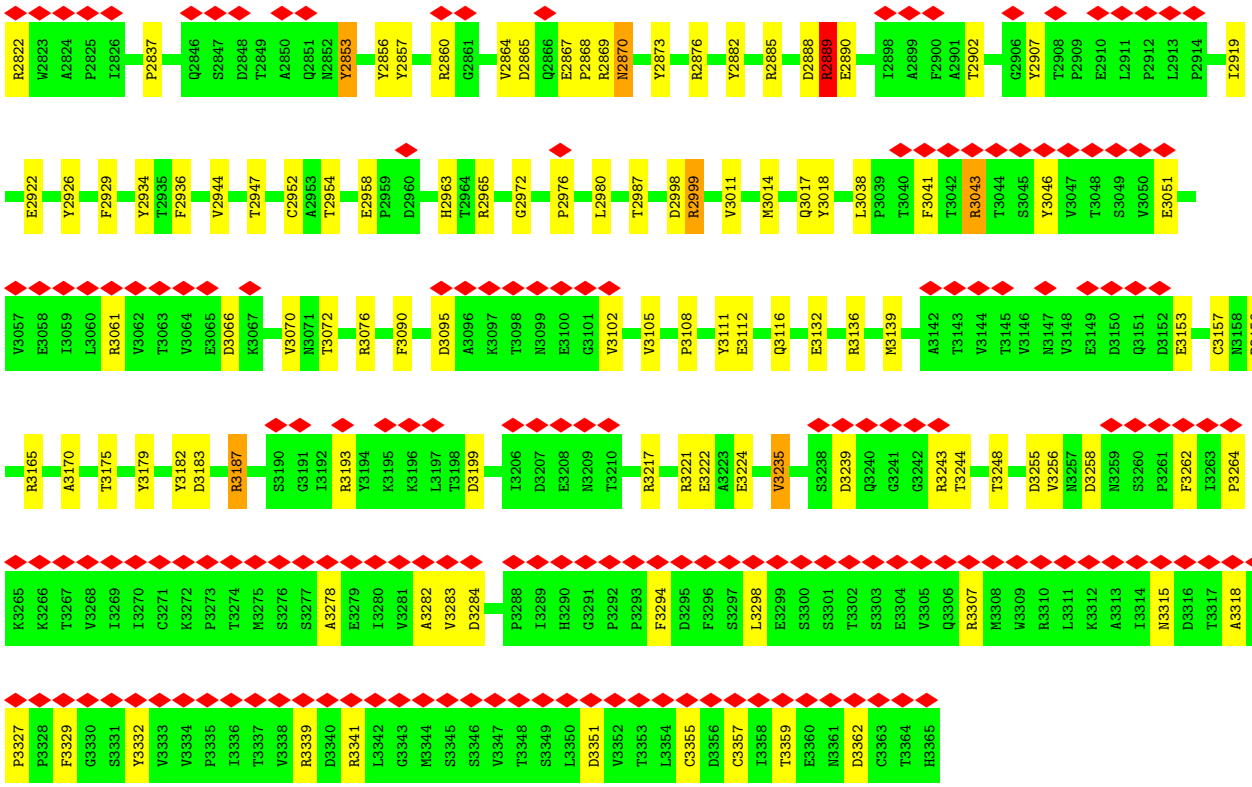


• Molecule 2: Desmocollin-2

Chain c:

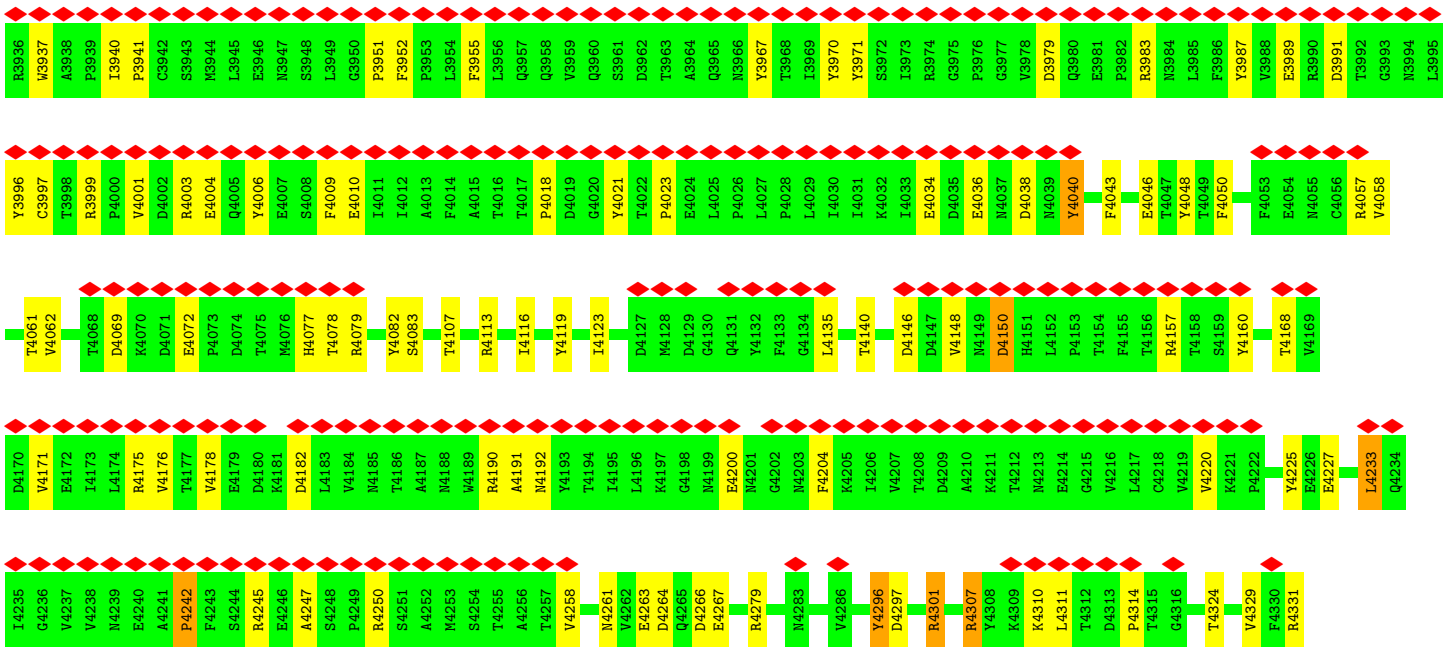
• Molecule 2: Desmocollin-2

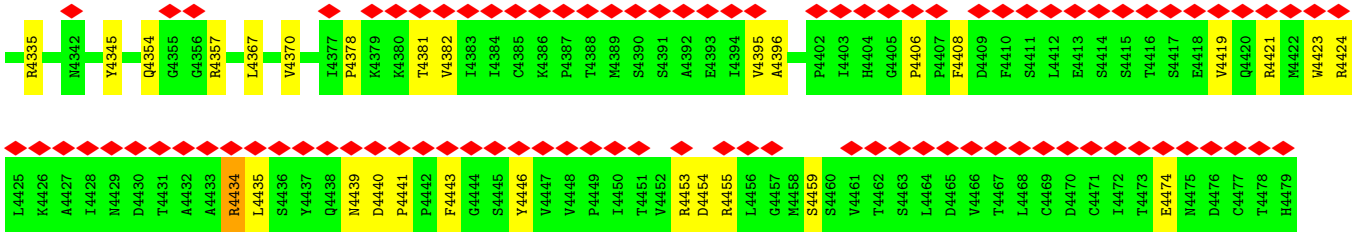
Chain d:



• Molecule 2: Desmocollin-2

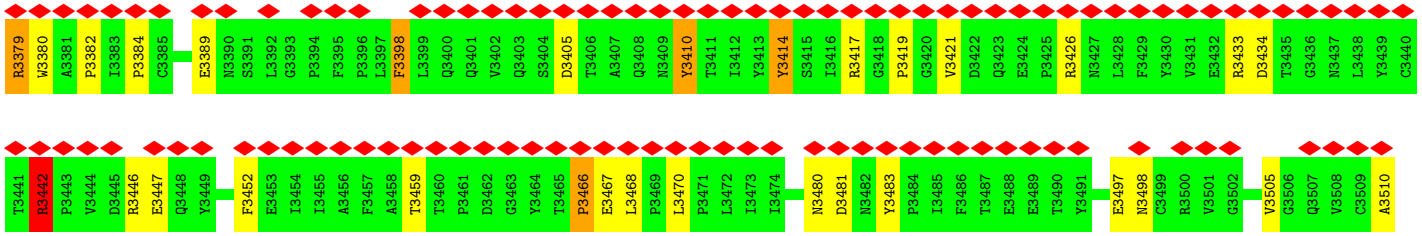
Chain e:

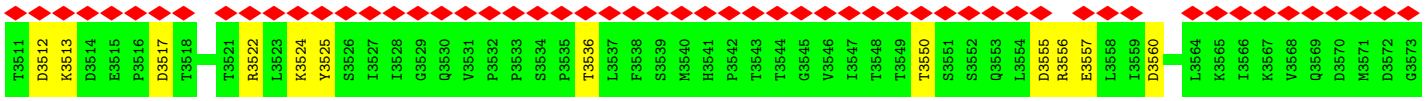


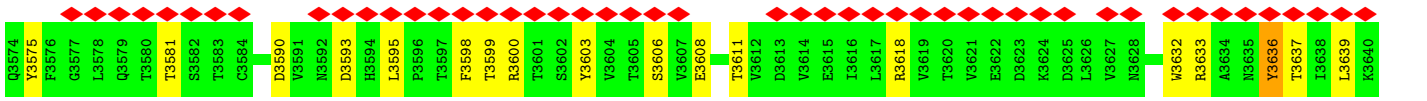


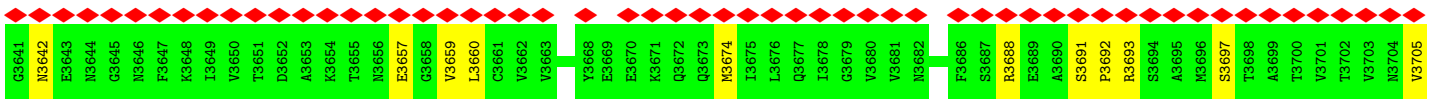
• Molecule 2: Desmocollin-2

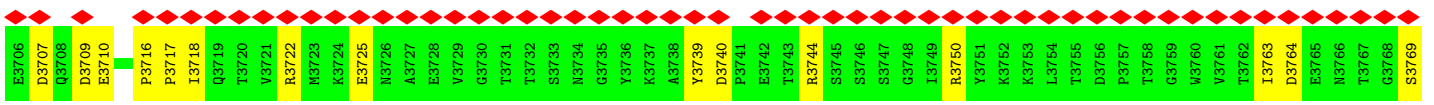
Chain f:

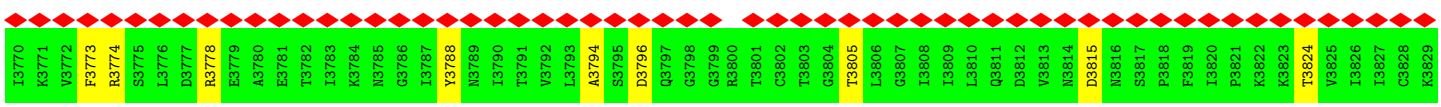


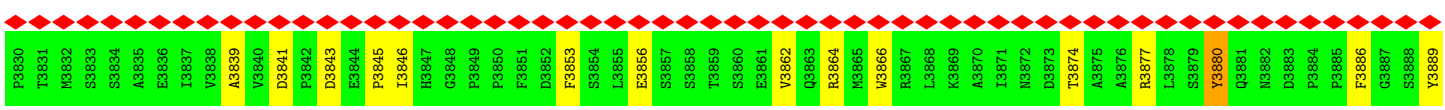


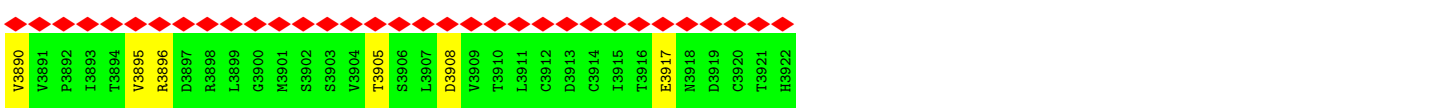






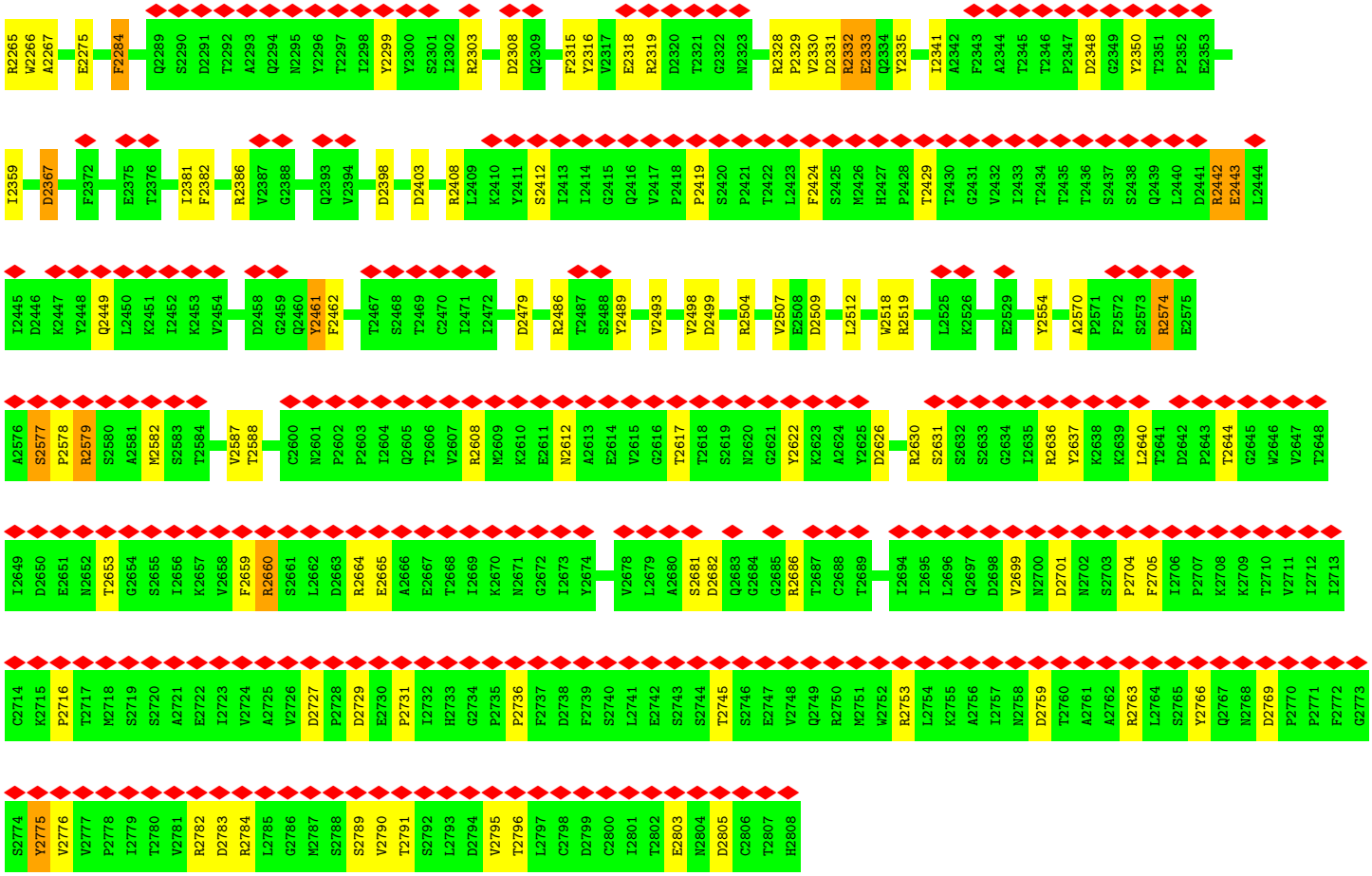






• Molecule 2: Desmocollin-2

Chain g:


R2265 W2266 A2267 E2275 F2284 Q2289 S2290 D2291 T2292 A2293 Q2294 N2295 Y2296 T2297 I2298 Y2299 Y2300 S2301 I2302 R2303 D2308 Q2309 F2315 Y2316 V2317 E2318 R2319 D2320 T2321 G2322 N2323 R2328 P2329 V2330 D2331 R2332 E2333 Q2334 Y2335 I2341 A2342 F2343 A2344 T2345 T2346 P2347 D2348 G2349 Y2350 T2351 P2352 E2353
I2359 D2367 F2372 E2375 T2376 I2381 F2382 R2386 V2387 G2388 Q2393 V2394 D2398 D2403 R2408 L2409 K2410 Y2411 S2412 I2413 I2414 G2415 Q2416 V2417 P2418 P2419 S2420 P2421 T2422 L2423 F2424 S2425 M2426 H2427 P2428 T2429 T2430 G2431 V2432 I2433 T2434 T2435 T2436 S2437 S2438 Q2439 L2440 D2441 R2442 E2443 L2444
I2445 D2446 K2447 Y2448 Q2449 L2450 K2451 I2452 K2453 V2454 D2458 G2459 Q2460 Y2461 F2462 T2467 S2468 T2469 C2470 I2471 I2472 D2479 R2486 T2487 S2488 Y2489 V2493 V2498 D2499 R2504 V2507 E2508 D2509 L2512 W2518 R2519 L2525 K2526 E2529 Y2554 A2570 P2571 F2572 S2573 R2574 E2575
A2576 S2577 P2578 R2579 S2580 A2581 M2582 S2583 T2584 V2587 T2588 C2600 N2601 P2602 P2603 I2604 Q2605 T2606 V2607 R2608 M2609 K2610 E2611 N2612 A2613 E2614 V2615 G2616 T2617 T2618 S2619 N2620 G2621 Y2622 K2623 A2624 Y2625 D2626 R2630 S2631 S2632 S2633 G2634 I2635 R2636 Y2637 K2638 K2639 L2640 T2641 D2642 P2643 T2644 G2645 W2646 V2647 T2648
I2649 D2650 E2651 N2652 T2653 G2654 S2655 I2656 K2657 V2658 F2659 R2660 S2661 L2662 D2663 R2664 E2665 A2666 E2667 T2668 I2669 K2670 N2671 G2672 I2673 Y2674 V2678 L2679 A2680 S2681 D2682 Q2683 G2684 G2685 R2686 T2687 C2688 T2689 I2694 I2695 L2696 Q2697 D2698 V2699 N2700 D2701 N2702 S2703 P2704 F2705 I2706 P2707 K2708 K2709 T2710 V2711 I2712 I2713
C2714 K2715 P2716 T2717 M2718 S2719 S2720 A2721 E2722 I2723 V2724 A2725 V2726 D2727 P2728 D2729 E2730 P2731 I2732 H2733 G2734 P2735 P2736 F2737 D2738 P2739 S2740 L2741 E2742 S2743 S2744 T2745 S2746 E2747 V2748 Q2749 R2750 M2751 W2752 R2753 L2754 K2755 A2756 I2757 N2758 D2759 T2760 A2761 A2762 R2763 L2764 S2765 Y2766 Q2767 N2768 D2769 P2770 P2771 F2772 G2773
S2774 Y2775 V2776 V2777 P2778 I2779 T2780 V2781 R2782 D2783 R2784 L2785 G2786 M2787 S2788 S2789 V2790 T2791 S2792 L2793 D2794 V2795 T2796 L2797 C2798 D2799 C2800 I2801 T2802 E2803 N2804 D2805 C2806 T2807 H2808

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	3656	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.95	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	64000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.210	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0133	Depositor
Map size (Å)	550.4, 550.4, 550.4	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	4.3, 4.3, 4.3	Depositor

5 Model quality

5.1 Standard geometry

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	0.54	0/4438	1.98	133/6026 (2.2%)
1	B	0.54	0/4438	1.96	121/6026 (2.0%)
1	C	0.53	0/4438	1.94	118/6026 (2.0%)
1	D	0.54	0/4438	1.93	107/6026 (1.8%)
1	E	0.87	10/4438 (0.2%)	2.21	150/6026 (2.5%)
1	F	0.54	0/4438	1.98	125/6026 (2.1%)
1	G	0.54	0/4438	1.96	120/6026 (2.0%)
2	a	0.64	1/4355 (0.0%)	2.02	132/5943 (2.2%)
2	b	0.56	0/4355	1.97	116/5943 (2.0%)
2	c	0.55	0/4355	2.02	150/5943 (2.5%)
2	d	0.55	0/4355	2.01	146/5943 (2.5%)
2	e	0.56	0/4355	2.02	140/5943 (2.4%)
2	f	0.56	0/4355	1.95	119/5943 (2.0%)
2	g	0.61	2/4355 (0.0%)	2.05	137/5943 (2.3%)
All	All	0.59	13/61551 (0.0%)	2.00	1814/83783 (2.2%)

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	8
1	B	0	15
1	C	0	13
1	D	0	15
1	E	0	18
1	F	0	12
1	G	0	9
2	a	0	15
2	b	0	11
2	c	0	11
2	d	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	e	0	12
2	f	0	11
2	g	0	13
All	All	0	168

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	2010	HIS	ND1-CE1	25.77	1.99	1.34
2	a	2333	GLU	CD-OE1	-19.74	1.03	1.25
1	E	2012	SER	CB-OG	-17.47	1.19	1.42
1	E	2010	HIS	CG-ND1	17.03	1.76	1.38
1	E	2011	LYS	C-N	15.63	1.70	1.34

The worst 5 of 1814 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	2010	HIS	CG-ND1-CE1	-44.79	45.49	108.20
1	E	2010	HIS	CA-CB-CG	-28.51	65.14	113.60
1	E	2012	SER	N-CA-CB	27.63	151.94	110.50
2	a	2486	ARG	NE-CZ-NH2	20.05	130.33	120.30
1	B	2076	ARG	NE-CZ-NH1	18.93	129.77	120.30

There are no chirality outliers.

5 of 168 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	ARG	Sidechain
1	A	32	ARG	Sidechain
1	A	40	TYR	Sidechain
1	A	416	TYR	Sidechain
1	A	429	ARG	Sidechain

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	4355	4294	4294	10	0
1	B	4355	4294	4291	8	0
1	C	4355	4294	4291	6	0
1	D	4355	4294	4291	15	0
1	E	4355	4294	4291	55	0
1	F	4355	4294	4291	11	0
1	G	4355	4294	4291	7	0
2	a	4268	4154	4151	0	0
2	b	4268	4154	4150	0	0
2	c	4268	4154	4151	0	0
2	d	4268	4154	4151	0	0
2	e	4268	4154	4151	0	0
2	f	4268	4154	4151	0	0
2	g	4268	4154	4151	0	0
All	All	60361	59136	59096	110	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 2.

The worst 5 of 110 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:E:2010:HIS:CG	1:E:2010:HIS:ND1	1.76	1.54
1:E:2010:HIS:N	1:E:2010:HIS:CA	1.73	1.51
1:E:2011:LYS:C	1:E:2012:SER:N	1.70	1.42
1:E:1769:GLU:CG	1:E:1835:ALA:HB1	1.51	1.38
1:E:1769:GLU:HG2	1:E:1835:ALA:CB	1.60	1.31

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	552/554 (100%)	513 (93%)	39 (7%)	0	100	100
1	B	552/554 (100%)	512 (93%)	38 (7%)	2 (0%)	34	72
1	C	552/554 (100%)	516 (94%)	32 (6%)	4 (1%)	22	63
1	D	552/554 (100%)	516 (94%)	34 (6%)	2 (0%)	34	72
1	E	552/554 (100%)	510 (92%)	32 (6%)	10 (2%)	8	40
1	F	552/554 (100%)	516 (94%)	33 (6%)	3 (0%)	29	69
1	G	552/554 (100%)	517 (94%)	33 (6%)	2 (0%)	34	72
2	a	542/544 (100%)	505 (93%)	33 (6%)	4 (1%)	22	63
2	b	542/544 (100%)	505 (93%)	31 (6%)	6 (1%)	14	52
2	c	542/544 (100%)	499 (92%)	42 (8%)	1 (0%)	47	81
2	d	542/544 (100%)	493 (91%)	47 (9%)	2 (0%)	34	72
2	e	542/544 (100%)	501 (92%)	38 (7%)	3 (1%)	25	66
2	f	542/544 (100%)	498 (92%)	39 (7%)	5 (1%)	17	57
2	g	542/544 (100%)	499 (92%)	40 (7%)	3 (1%)	25	66
All	All	7658/7686 (100%)	7100 (93%)	511 (7%)	47 (1%)	29	66

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	992	ASP
1	E	1783	ALA
1	E	2010	HIS
1	E	2011	LYS
1	E	2013	ILE

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	492/492 (100%)	481 (98%)	11 (2%)	52	71
1	B	492/492 (100%)	484 (98%)	8 (2%)	62	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	492/492 (100%)	480 (98%)	12 (2%)	49	69
1	D	492/492 (100%)	481 (98%)	11 (2%)	52	71
1	E	492/492 (100%)	478 (97%)	14 (3%)	43	65
1	F	492/492 (100%)	483 (98%)	9 (2%)	59	77
1	G	492/492 (100%)	477 (97%)	15 (3%)	41	63
2	a	494/494 (100%)	479 (97%)	15 (3%)	41	63
2	b	494/494 (100%)	483 (98%)	11 (2%)	52	71
2	c	494/494 (100%)	479 (97%)	15 (3%)	41	63
2	d	494/494 (100%)	483 (98%)	11 (2%)	52	71
2	e	494/494 (100%)	479 (97%)	15 (3%)	41	63
2	f	494/494 (100%)	478 (97%)	16 (3%)	39	61
2	g	494/494 (100%)	483 (98%)	11 (2%)	52	71
All	All	6902/6902 (100%)	6728 (98%)	174 (2%)	50	68

5 of 174 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	c	4156	THR
2	e	4233	LEU
2	c	4308	TYR
2	d	3351	ASP
2	f	3468	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	a	2568	ASN
2	g	2568	ASN
2	c	4039	ASN
2	f	3592	ASN
2	c	3994	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	2011:LYS	C	2012:SER	N	1.70

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11678. 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: 64

Y Index: 64

Z Index: 64

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: 62

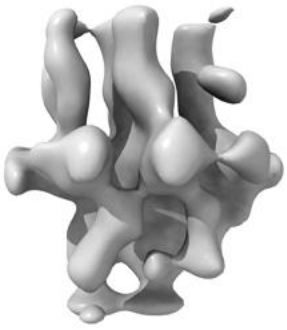
Y Index: 66

Z Index: 66

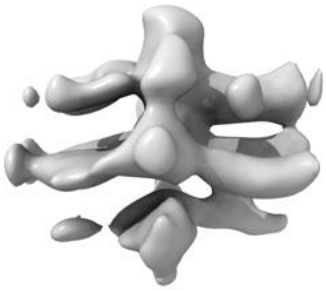
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

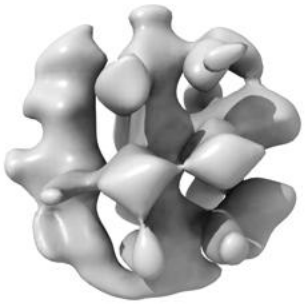
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0133. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

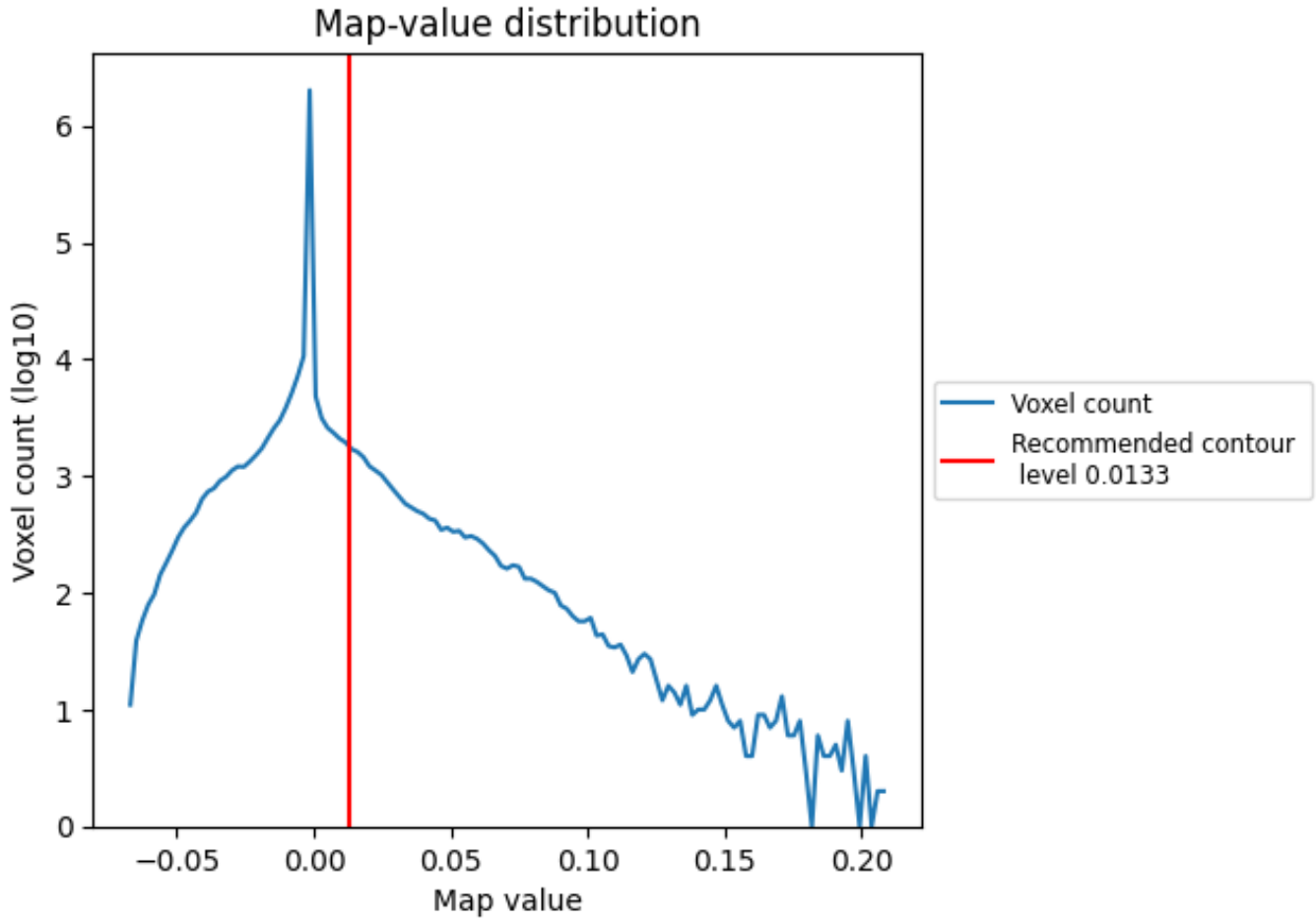
6.5 Mask visualisation (i)

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

7 Map analysis

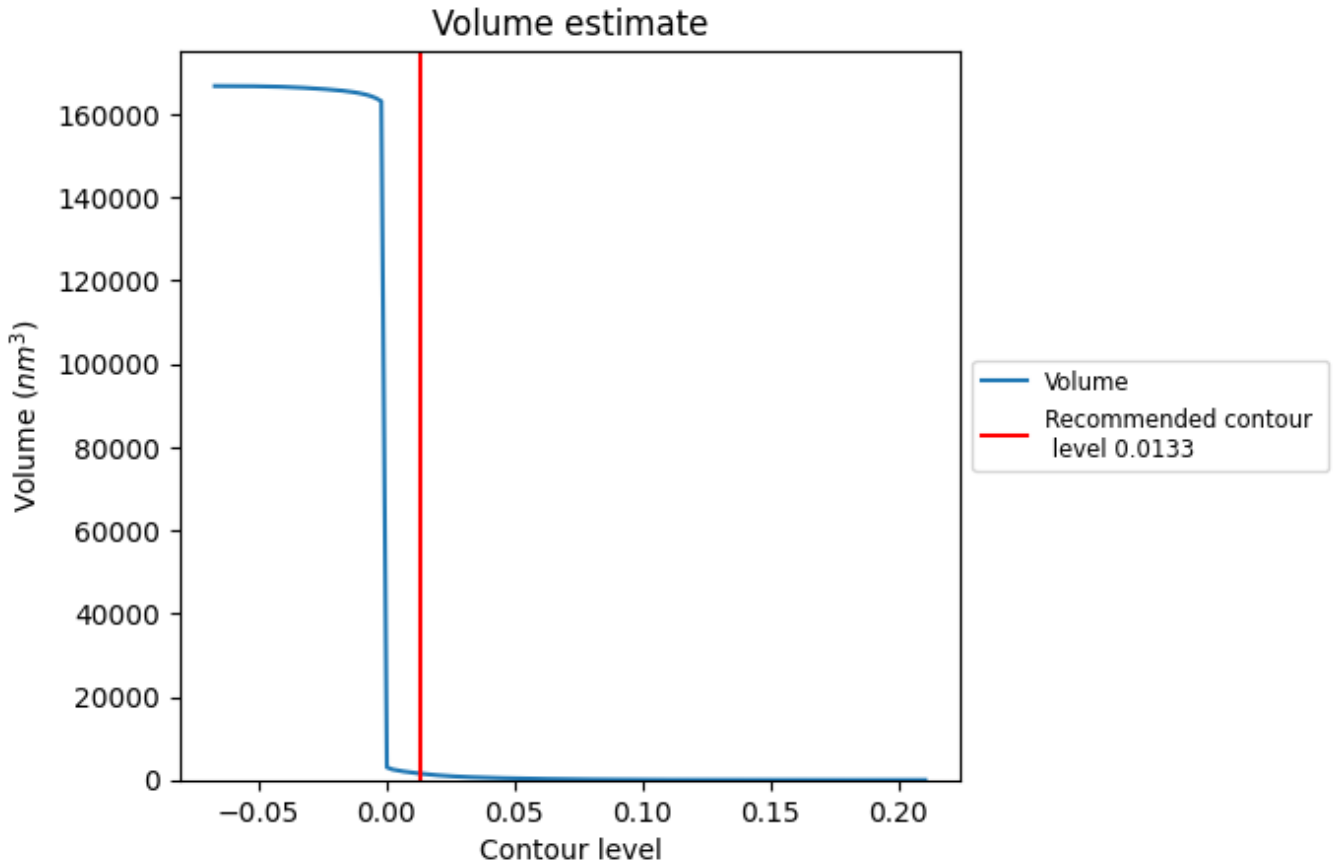
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

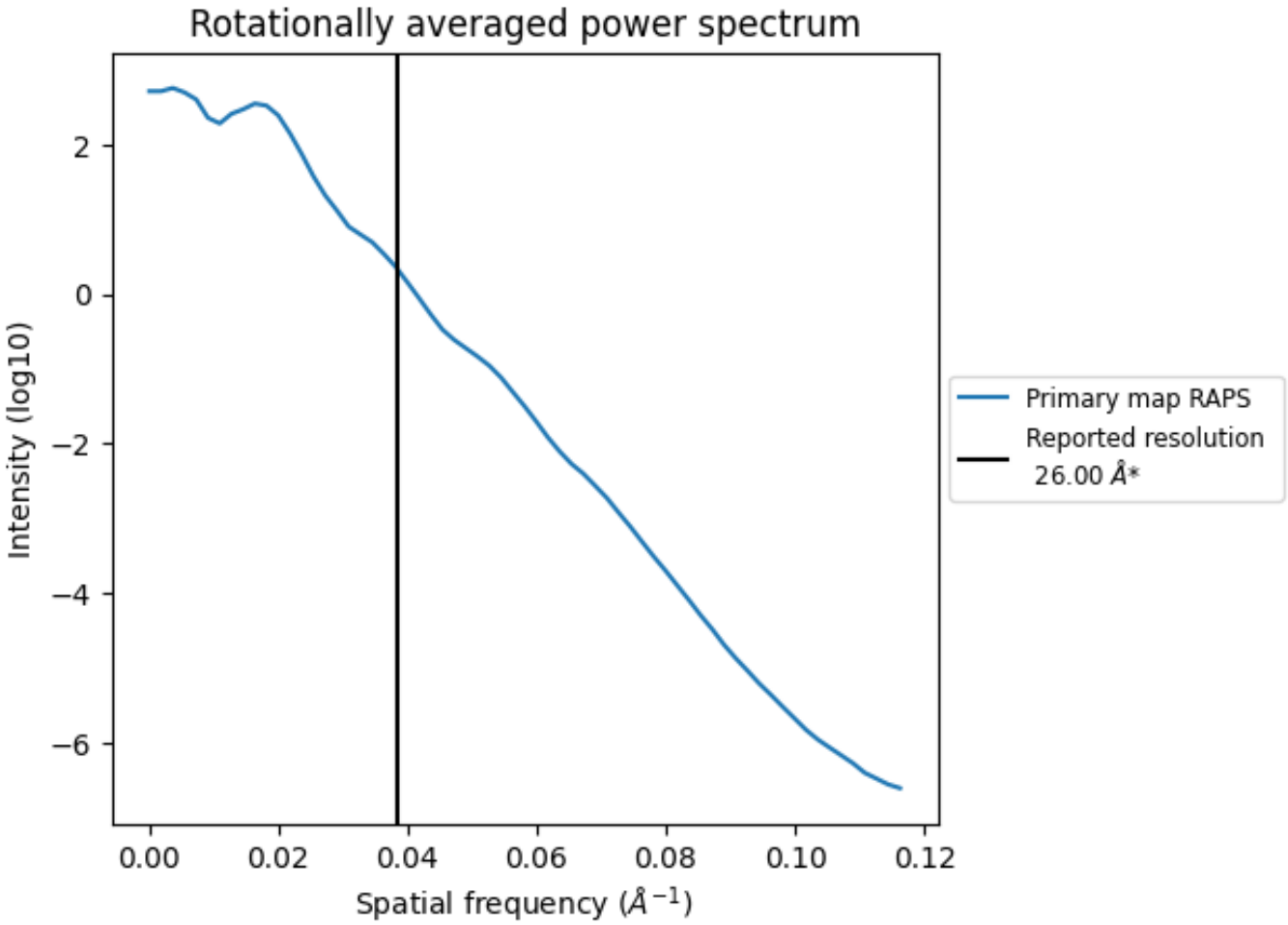
7.2 Volume estimate (i)



The volume at the recommended contour level is 1526 nm^3; this corresponds to an approximate mass of 1378 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)

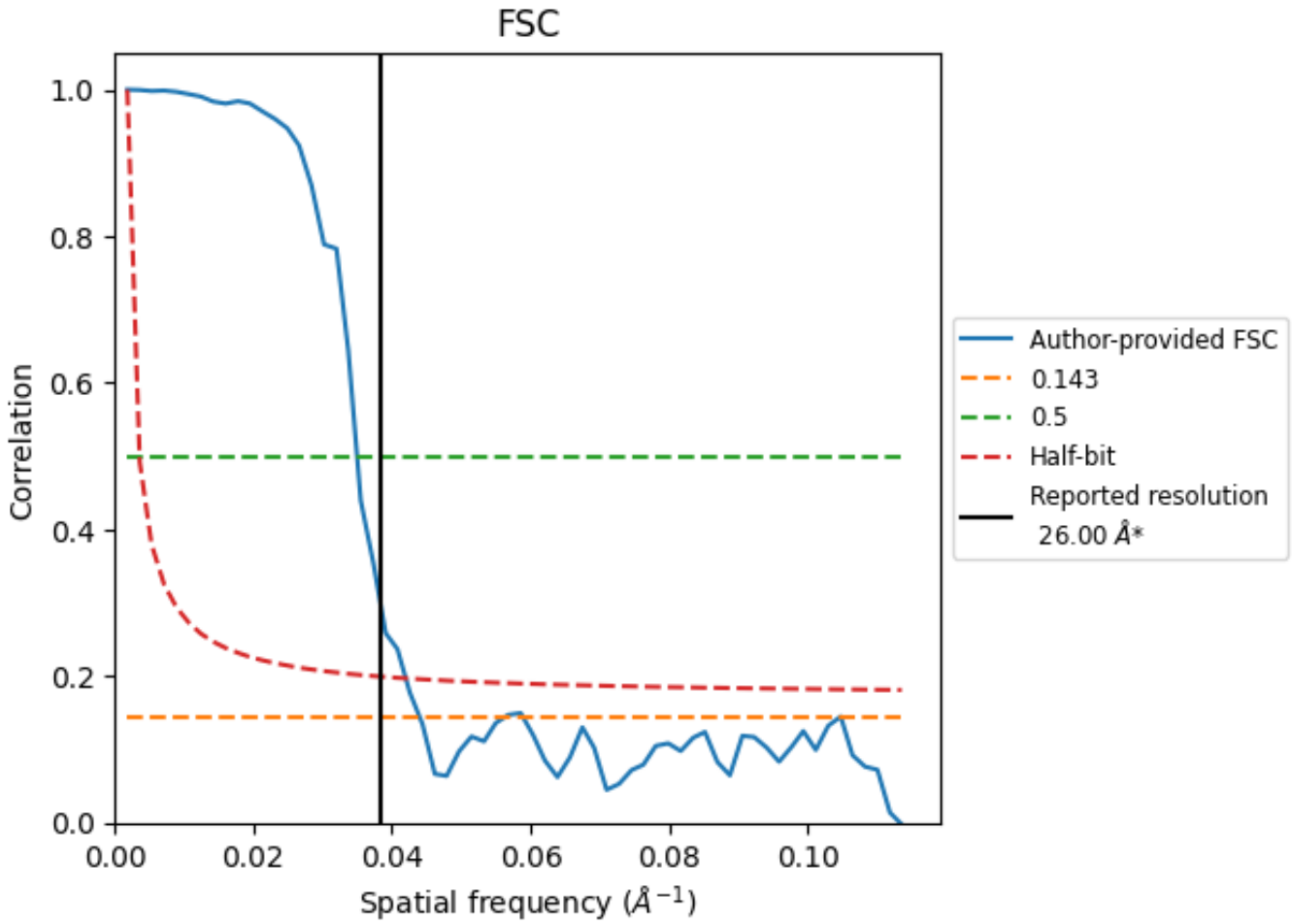


*Reported resolution corresponds to spatial frequency of 0.038 Å^{-1}

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 0.038 Å^{-1}

8.2 Resolution estimates (i)

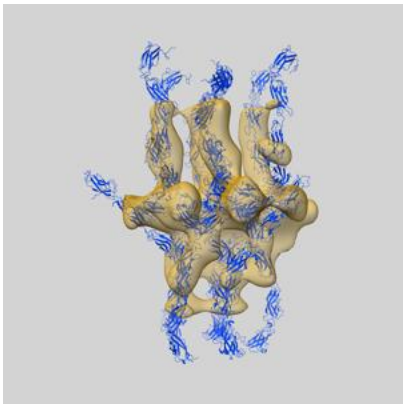
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	26.00	-
Author-provided FSC curve	22.73	28.57	23.81
Unmasked-calculated*	-	-	-

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

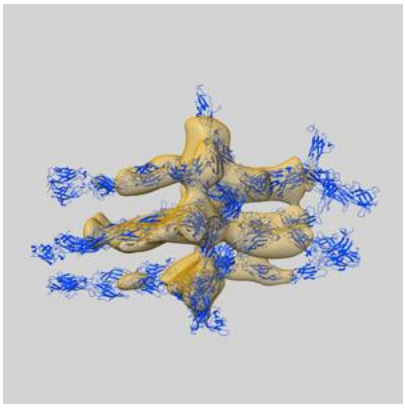
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11678 and PDB model 7A7D. Per-residue inclusion information can be found in section 3 on page 6.

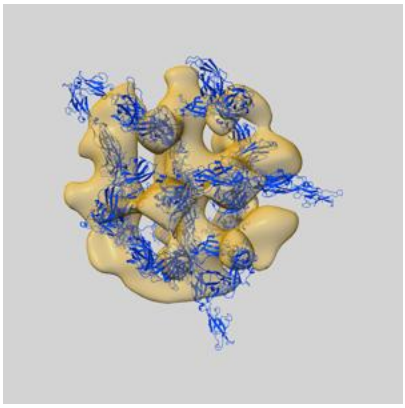
9.1 Map-model overlay



X



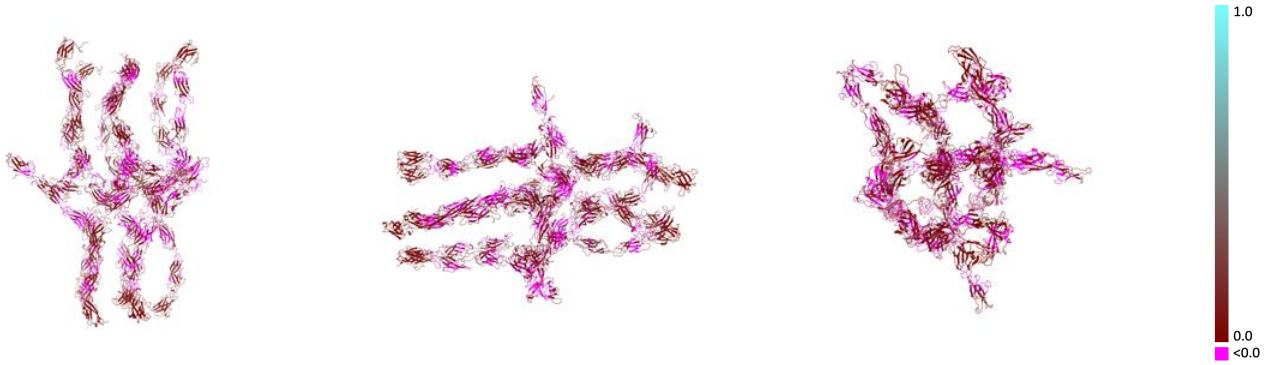
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0133 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.

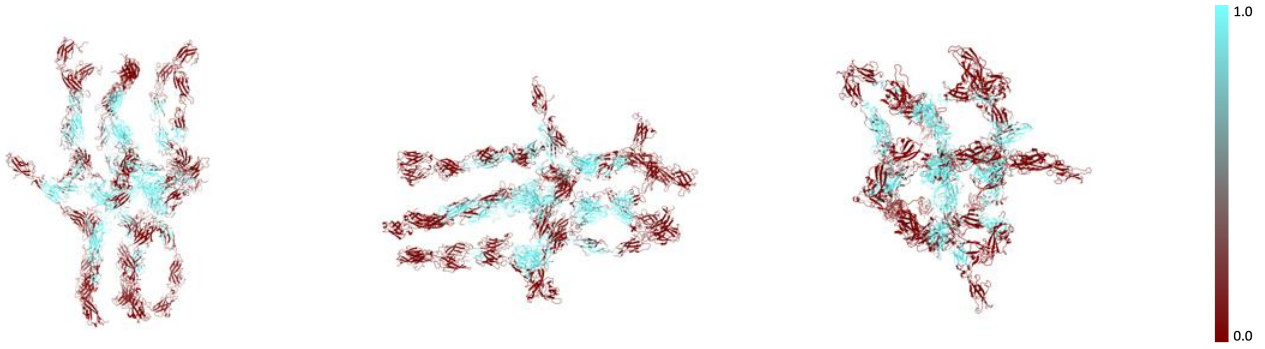
9.2 Q-score mapped to coordinate model (i)



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.

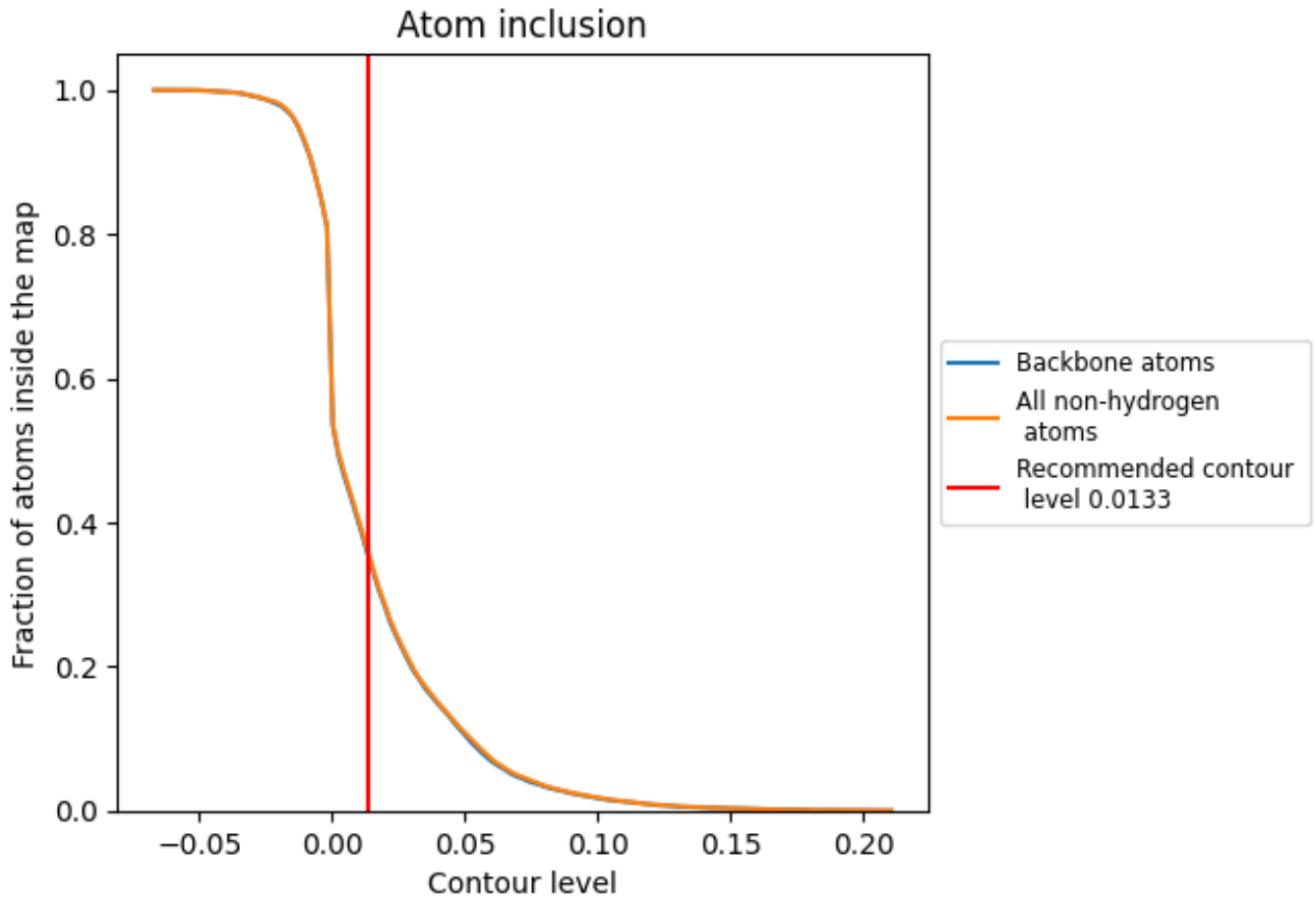
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0133).

9.4 Atom inclusion (i)



At the recommended contour level, 36% of all backbone atoms, 36% 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 (0.0133) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3615	0.0190
A	0.5617	0.0360
B	0.2968	0.0080
C	0.2207	0.0050
D	0.3273	0.0090
E	0.3843	0.0380
F	0.2945	0.0190
G	0.3454	0.0280
a	0.4007	0.0340
b	0.1989	0.0090
c	0.4870	0.0250
d	0.6420	0.0160
e	0.3782	0.0050
f	0.1095	0.0080
g	0.4446	0.0270