wwPDB EM Validation Summary Report (i)

Dec 12, 2022 – 05:46 PM EST

PDB ID	:	3JAC
EMDB ID	:	EMD-6343
Title	:	Cryo-EM study of a channel
Authors	:	Ge, J.; Li, W.; Zhao, Q.; Li, N.; Xiao, B.; Gao, N.; Yang, M.
Deposited on	:	2015-06-05
Resolution	:	4.80 Å(reported)
Based on initial model	:	4RAX

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 (i)) were used in the production of this report:

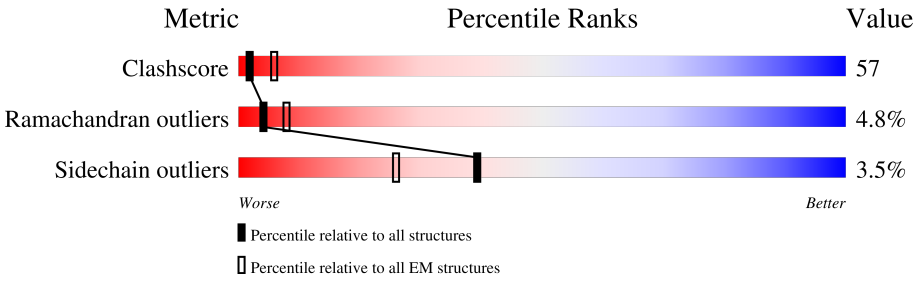
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.80 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	2553	14% 23% 9% • 64%
1	B	2553	13% 22% 10% • 64%
1	C	2553	13% 23% 9% • 64%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 15741 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 Piezo-type mechanosensitive ion channel component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	918	5247	3208	995	1038	6	0	0
1	B	918	5247	3208	995	1038	6	0	0
1	C	918	5247	3208	995	1038	6	0	0

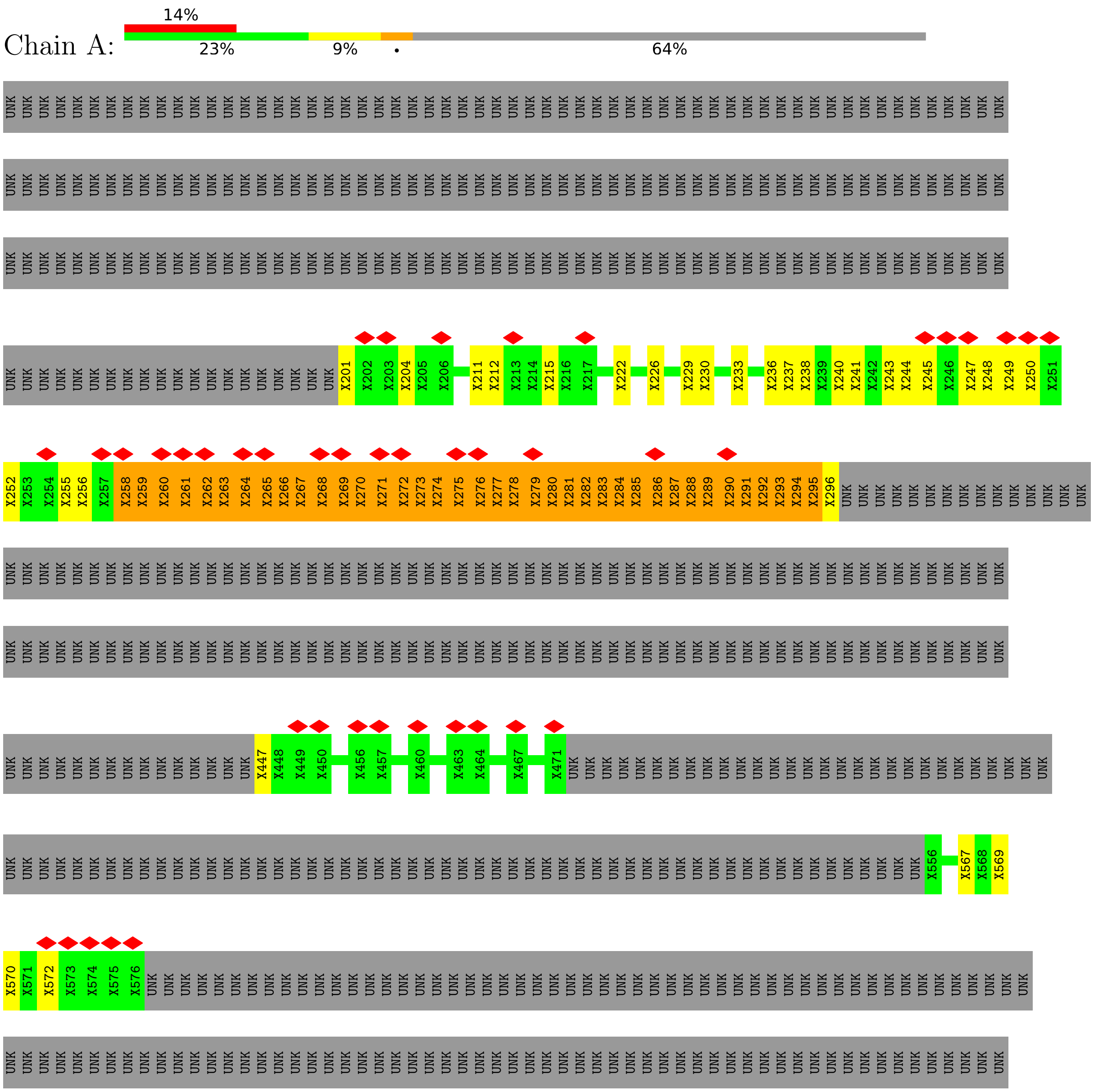
There are 18 discrepancies between the modelled and reference sequences:

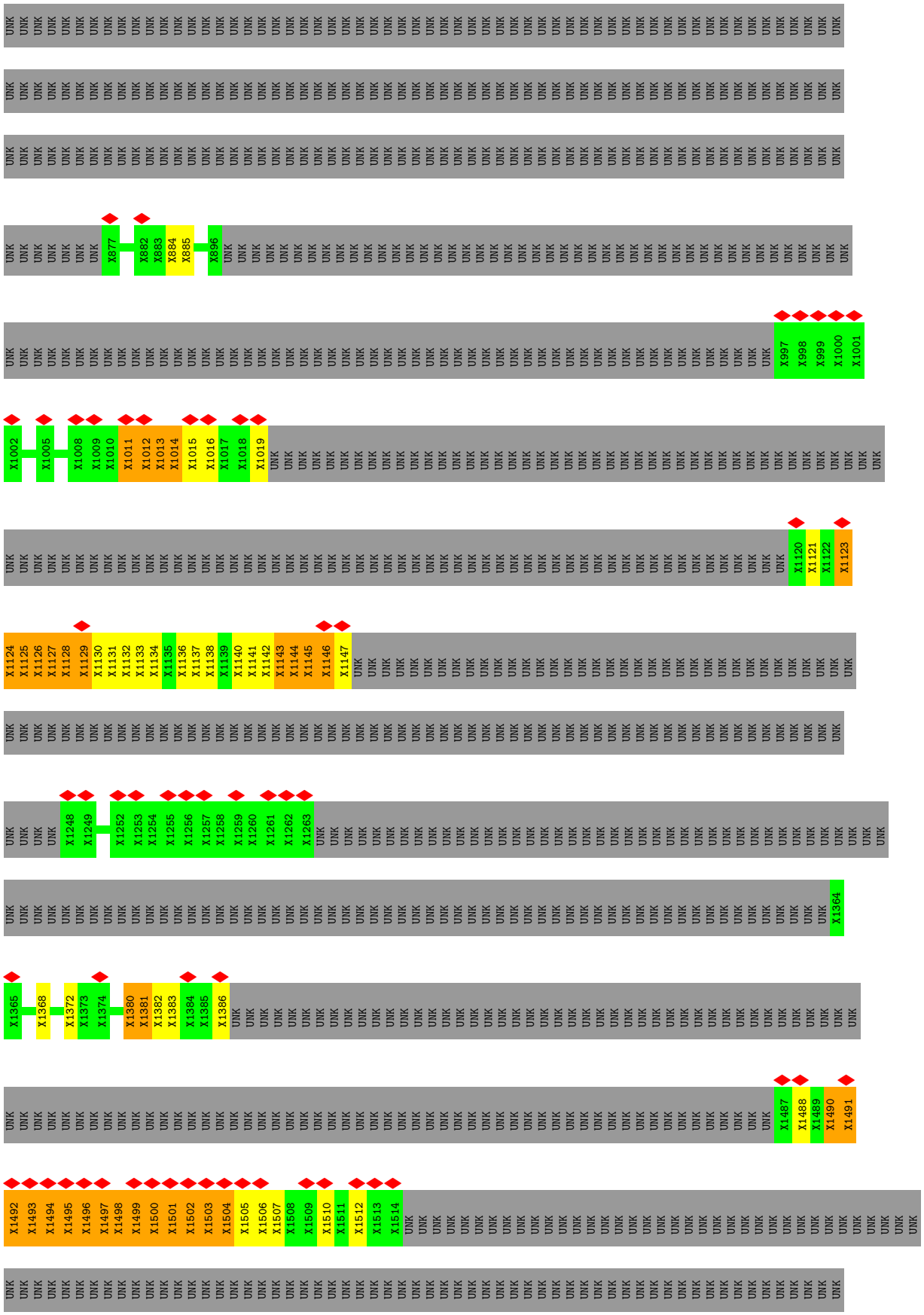
Chain	Residue	Modelled	Actual	Comment	Reference
A	2548	LEU	-	expression tag	UNP E2JF22
A	2549	GLU	-	expression tag	UNP E2JF22
A	2550	VAL	-	expression tag	UNP E2JF22
A	2551	LEU	-	expression tag	UNP E2JF22
A	2552	PHE	-	expression tag	UNP E2JF22
A	2553	GLN	-	expression tag	UNP E2JF22
B	2548	LEU	-	expression tag	UNP E2JF22
B	2549	GLU	-	expression tag	UNP E2JF22
B	2550	VAL	-	expression tag	UNP E2JF22
B	2551	LEU	-	expression tag	UNP E2JF22
B	2552	PHE	-	expression tag	UNP E2JF22
B	2553	GLN	-	expression tag	UNP E2JF22
C	2548	LEU	-	expression tag	UNP E2JF22
C	2549	GLU	-	expression tag	UNP E2JF22
C	2550	VAL	-	expression tag	UNP E2JF22
C	2551	LEU	-	expression tag	UNP E2JF22
C	2552	PHE	-	expression tag	UNP E2JF22
C	2553	GLN	-	expression tag	UNP E2JF22

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: Piezo-type mechanosensitive ion channel component 1

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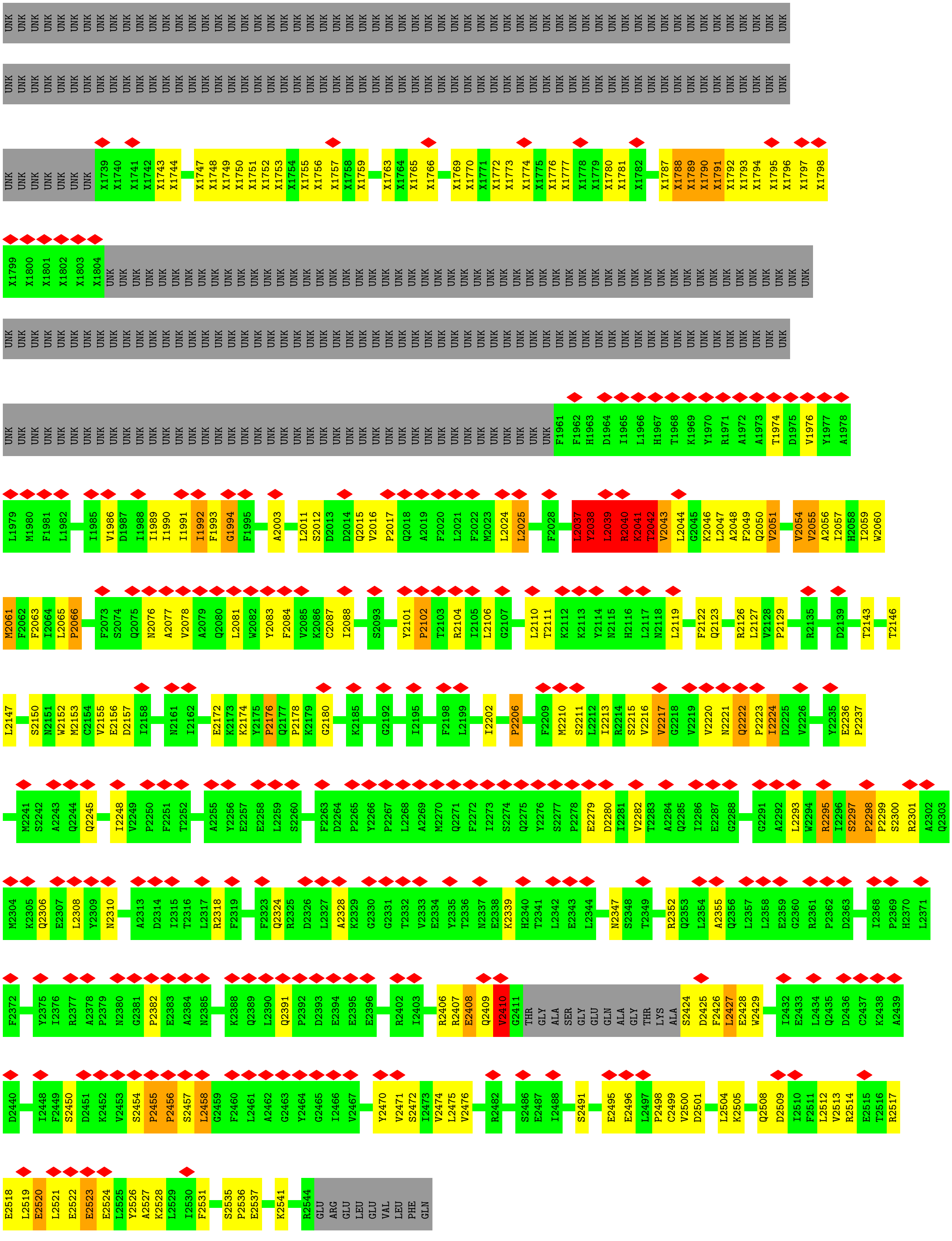
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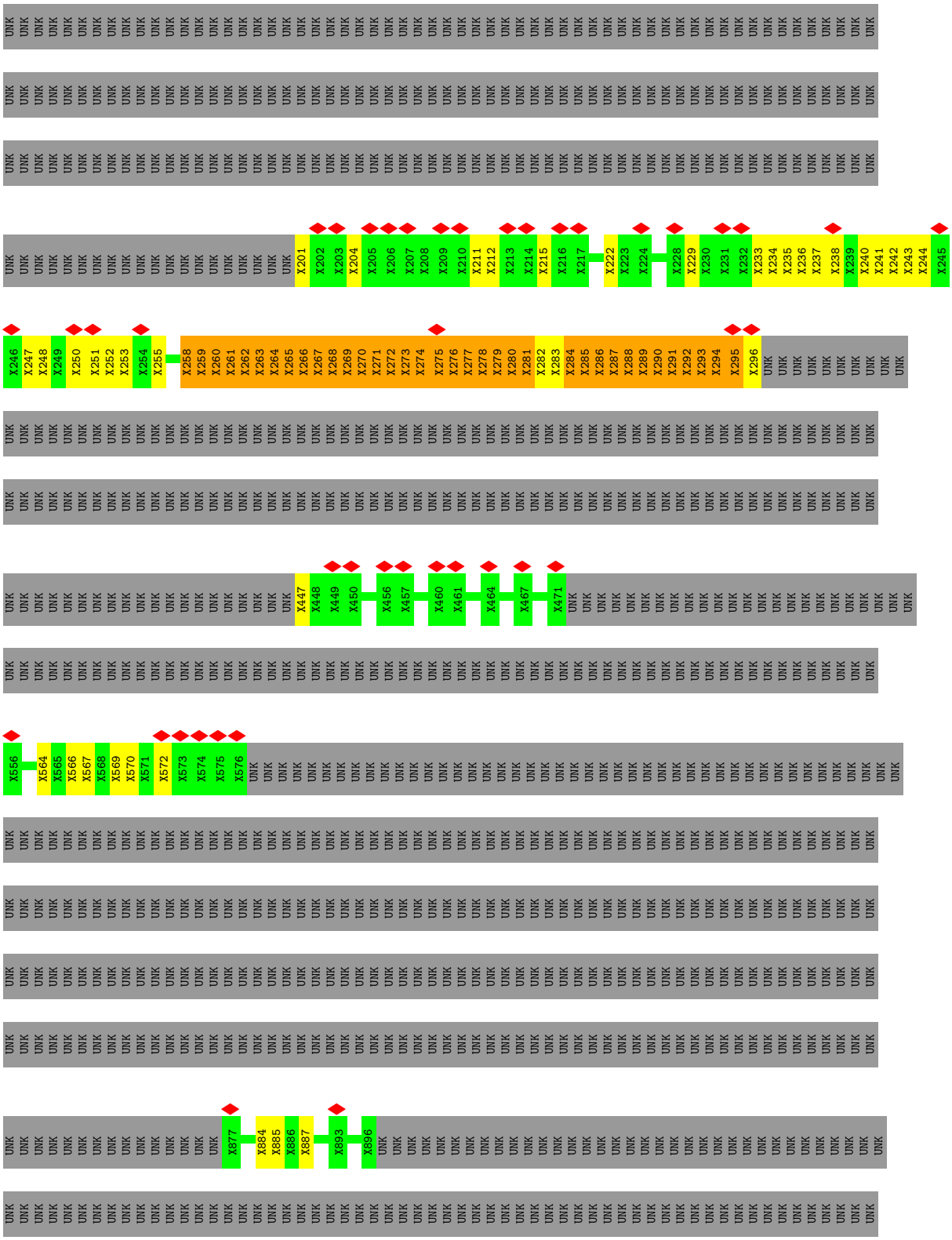
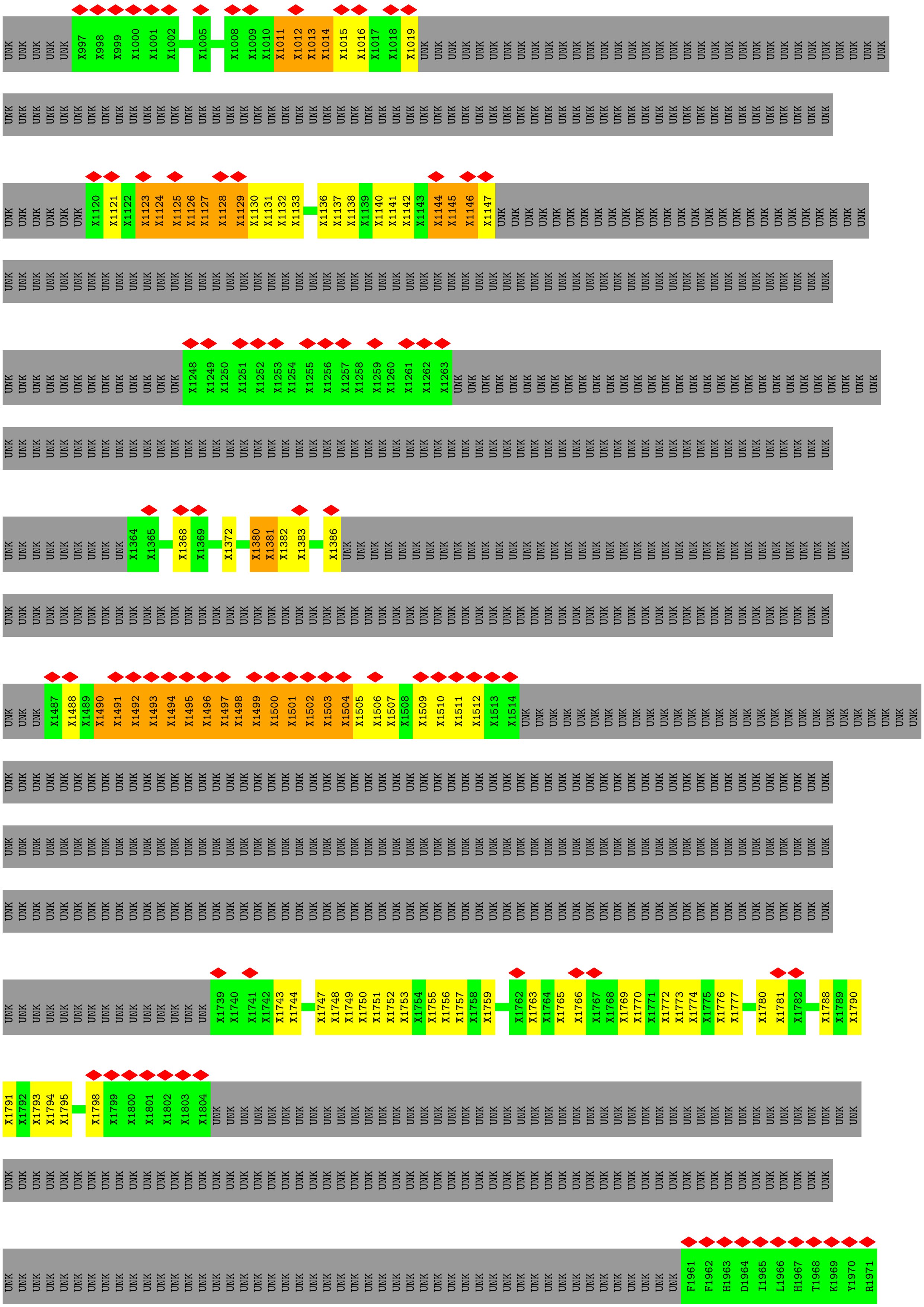
L1979 M1980 F1981 L1982 I1985 V1986 D1987 I1988 I1989 I1990 I1991 I1992 F1993 G1994 F1995 A2003 L2011 S2012 D2013 D2014 Q2015 V2016 P2017 Q2018 A2019 F2020 L2021 F2022 M2023 L2024 L2025 F2028 L2037 Y2038 L2039 R2040 K2041 T2042 V2043 L2044 G2045 K2046 L2047 A2048 F2049 Q2050 V2051 V2054 V2055 A2056 I2057 H2058 I2059 W2060
M2061 F2062 F2063 I2064 L2065 P2066 F2073 S2074 Q2075 N2076 A2077 V2078 A2079 Q2080 L2081 W2082 Y2083 F2084 V2085 K2086 C2087 I2088 S2093 Y2101 P2102 T2103 R2104 I2105 L2106 G2107 L2110 T2111 K2112 K2113 Y2114 N2115 H2116 L2117 N2118 L2119 F2122 Q2123 R2126 L2127 V2128 P2129 R2135 D2139 T2143 T2146
L2147 S2150 N2151 W2152 M2153 C2154 V2155 E2156 D2157 I2158 N2161 I2162 E2172 K2173 K2174 Y2175 P2176 Q2177 P2178 K2179 G2180 K2185 G2192 I2195 F2198 L2199 I2202 P2206 F2209 M2210 S2211 L2212 I2213 R2214 S2215 V2216 V2217 G2218 V2219 V2220 N2221 Q2222 P2223 I2224 D2225 V2226 Y2235 E2236 P2237
M2241 S2242 A2243 Q2244 Q2245 I2248 V2249 P2250 F2251 T2252 A2255 Y2256 E2257 E2258 L2259 S2260 F2263 D2264 P2265 Y2266 P2267 L2268 A2269 M2270 Q2271 F2272 L2273 S2274 Q2275 Y2276 S2277 P2278 E2279 D2280 I2281 V2282 T2283 A2284 Q2285 I2286 E2287 G2288 G2291 A2292 L2293 W2294 R2295 I2296 S2297 P2298 P2299 S2300 R2301 A2302 Q2303
M2304 K2305 Q2306 E2307 L2308 Y2309 N2310 A2313 D2314 I2315 T2316 L2317 R2318 F2319 F2323 Q2324 R2325 D2326 L2327 A2328 K2329 G2330 G2331 T2332 V2333 E2334 Y2335 T2336 N2337 E2338 K2339 H2340 T2341 L2342 E2343 L2344 N2347 S2348 T2349 R2352 Q2353 L2354 A2355 Q2356 L2357 L2358 E2359 G2360 R2361 P2362 D2363 I2368 P2369 H2370 L2371
F2372 Y2375 I2376 R2377 A2378 P2379 N2380 G2381 P2382 E2383 A2384 N2385 K2388 Q2389 L2390 Q2391 P2392 D2393 E2394 E2395 E2396 R2402 I2403 R2406 R2407 E2408 Q2409 V2410 G2411 THR GLY ALA SER GLY GLU GLN ALA GLY THR LYS ALA S2424 D2425 F2426 L2427 E2428 W2429 I2432 E2433 L2434 Q2435 D2436 C2437 K2438 A2439
D2440 I2448 F2449 S2450 D2451 K2452 V2453 S2454 P2455 P2456 S2457 L2458 G2459 F2460 L2461 A2462 G2463 Y2464 G2465 I2466 V2467 Y2470 V2471 S2472 I2473 V2474 L2475 V2476 R2482 S2486 E2487 I2488 S2491 E2495 E2496 L2497 P2498 C2499 V2500 D2501 L2504 K2505 Q2508 D2509 I2510 F2511 L2512 V2513 R2514 E2515 T2516 R2517
E2518 L2519 E2520 L2521 E2522 E2523 E2524 L2525 Y2526 A2527 K2528 L2529 I2530 F2531 S2535 P2536 E2537 K2541 R2544 GLU ARG GLU LEU GLU VAL LEU PHE GLN

- Molecule 1: Piezo-type mechanosensitive ion channel component 1

Chain B:

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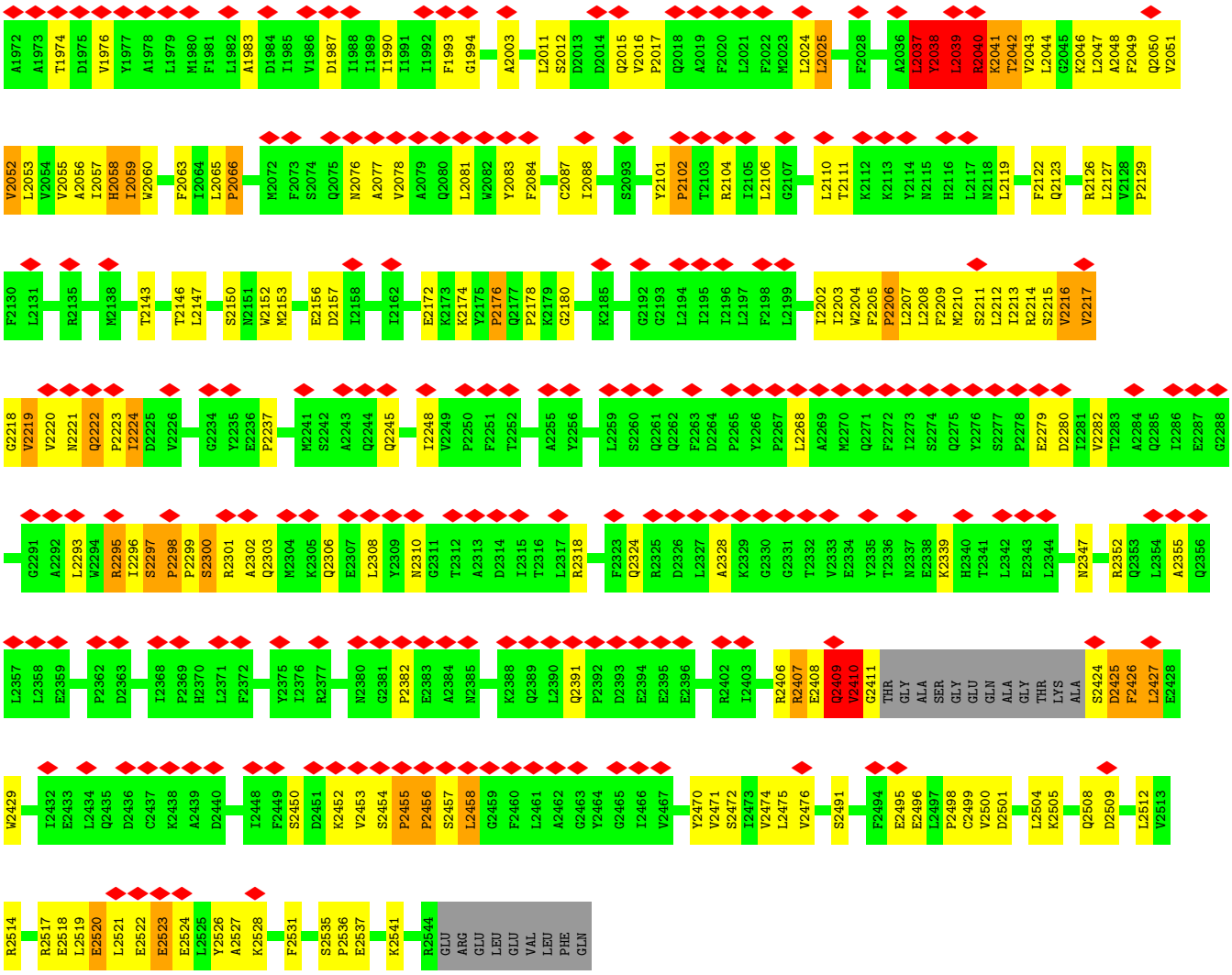
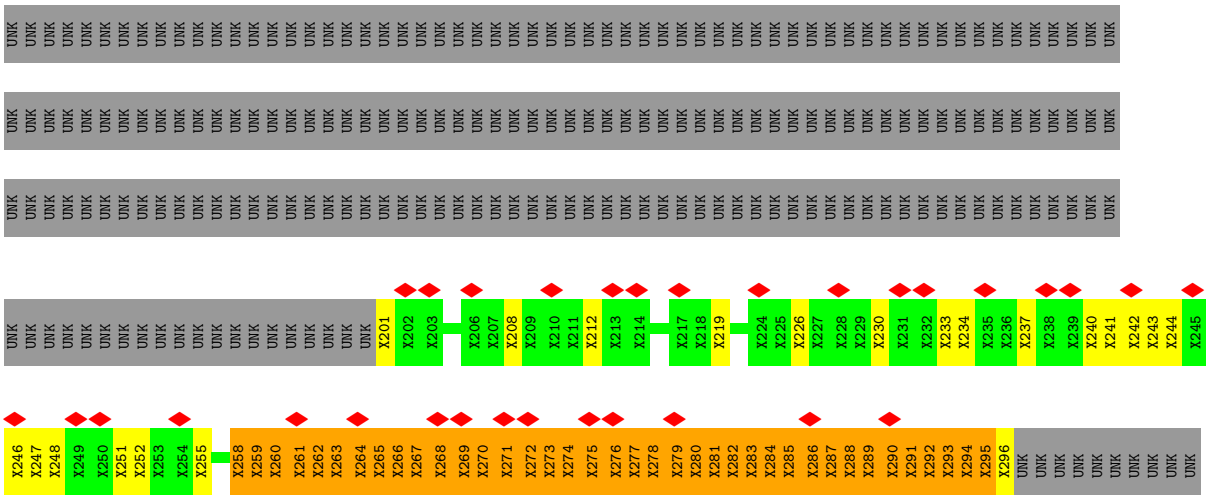
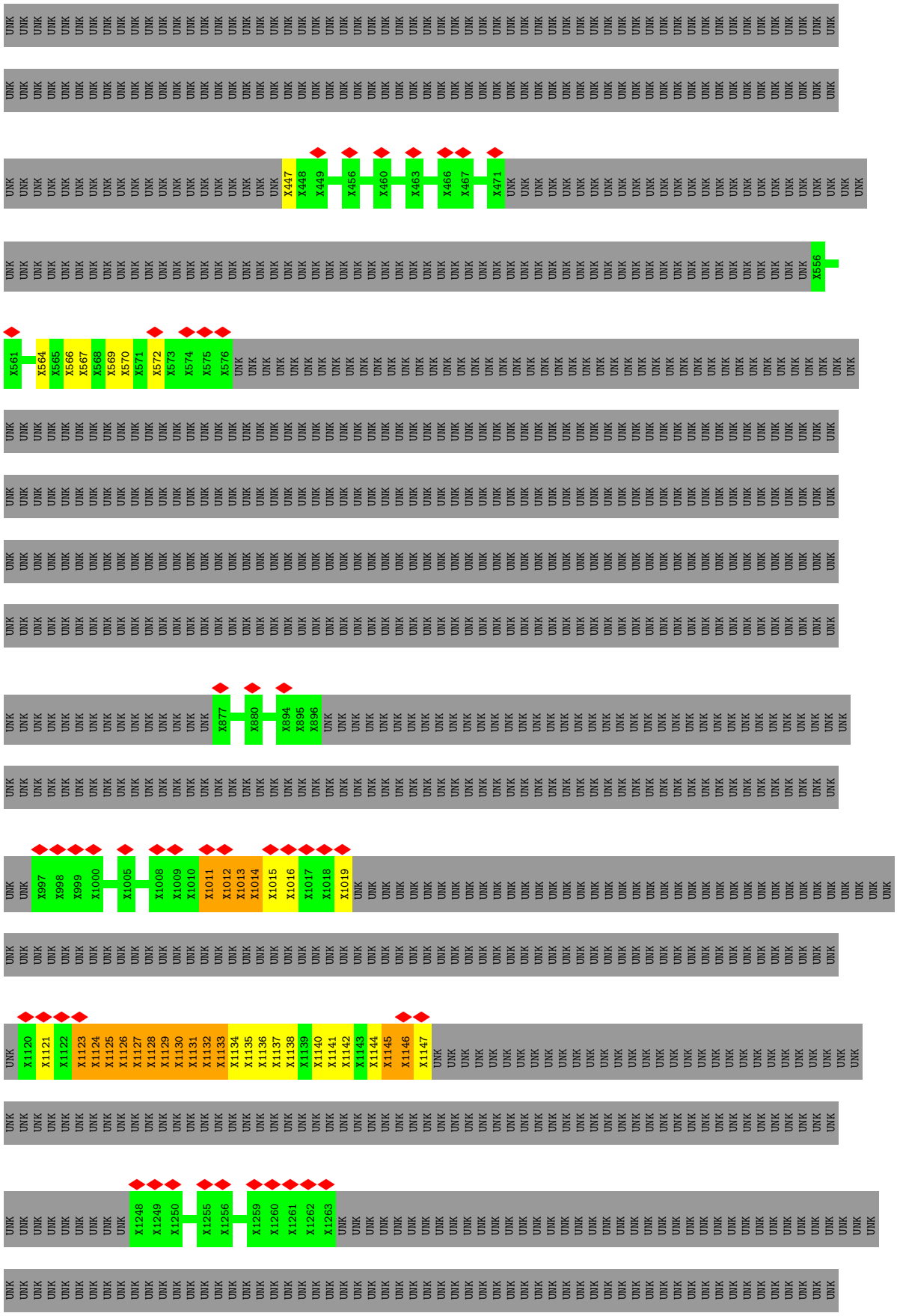


- Molecule 1: Piezo-type mechanosensitive ion channel component 1

Chain C: 13% 23% 9% 64%

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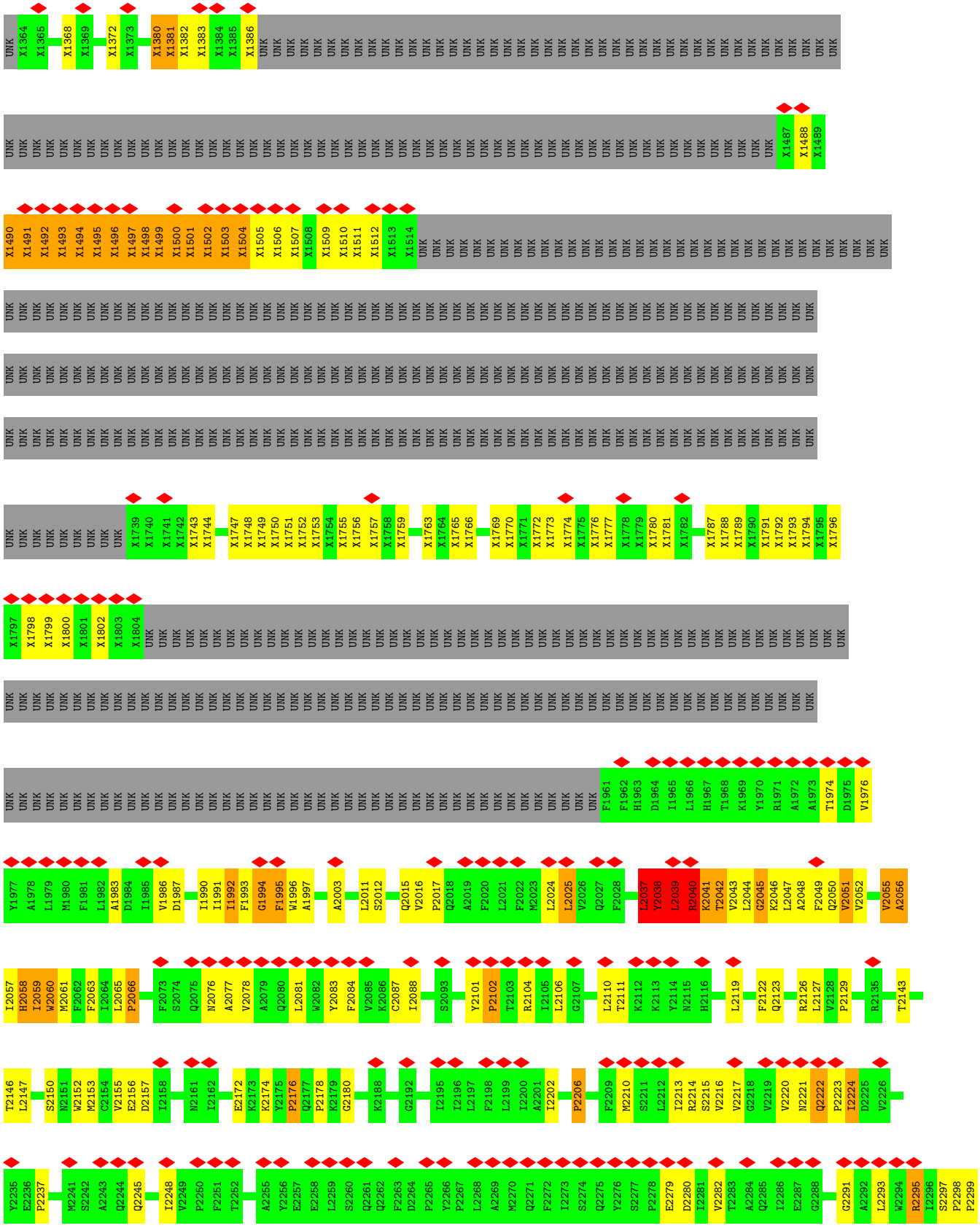
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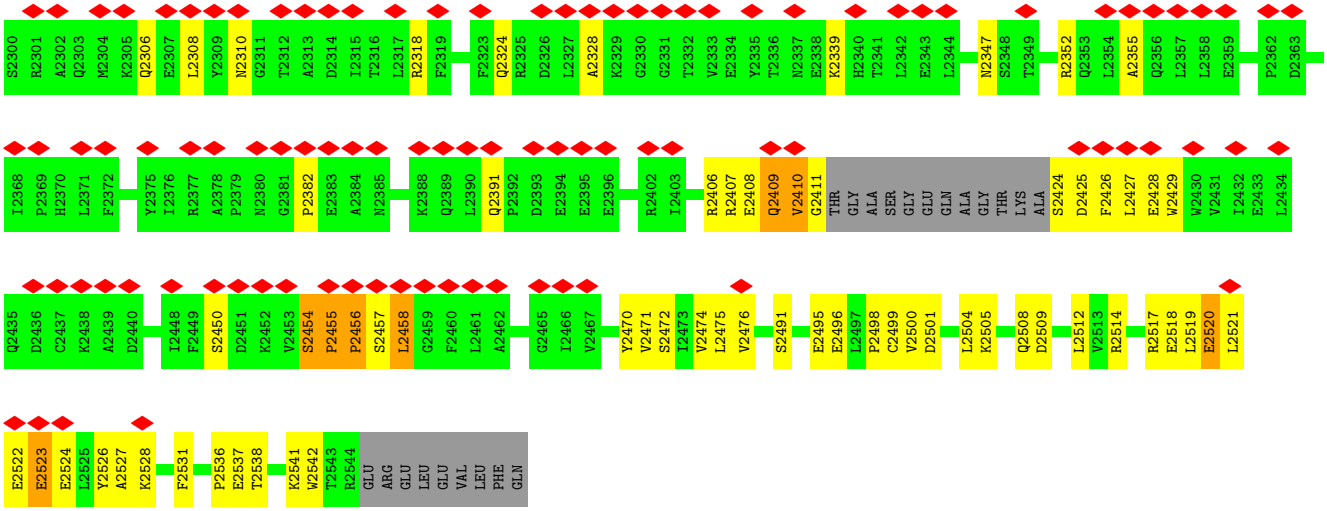
Y2235 E2236 P2237 M2241 S2242 A2243 Q2244 Q2245 I2248 V2249 P2250 F2251 T2252 A2255 Y2256 E2257 E2258 L2259 S2260 Q2261 Q2262 F2263 D2264 P2265 Y2266 P2267 L2268 A2269 M2270 Q2271 F2272 I2273 S2274 Q2275 Y2276 S2277 P2278 E2279 D2280 I2281 V2282 T2283 A2284 Q2285 I2286 E2287 G2288 G2291 A2292 L2293 W2294 R2295 I2296 S2297 P2298 P2299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N2347 S2348 T2349
R2352 Q2353 L2354 A2355 Q2356 L2357 L2358 E2359
P2362 D2363
I2368 P2369 H2370 L2371 F2372
Y2375 I2376 R2377 A2378 P2379 N2380 G2381 P2382 E2383 A2384 N2385
K2388 Q2389 L2390 Q2391 P2392 D2393 E2394 E2395 E2396
R2402 I2403
R2406 R2407 E2408 Q2409 V2410 G2411 THR GLY ALA SER GLY GLU GLN ALA GLY THR LYS ALA S2424 D2425 F2426 L2427 E2428 W2429 W2430 V2431 I2432 E2433 L2434

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G2465 I2466 V2467
Y2470 V2471 S2472 I2473 V2474 L2475 V2476
S2491
E2495 E2496 L2497 P2498 C2499 V2500 D2501
L2504 K2505
Q2508 D2509
L2512 V2513 R2514
R2517 E2518 L2519 E2520 L2521

E2522 E2523 E2524 L2525 Y2526 A2527 K2528
F2531
P2536 E2537 T2538
K2541 W2542 T2543 R2544 GLU ARG GLU LEU GLU VAL LEU PHE GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30021	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	CTFFIND	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	16	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	22500	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0273	Depositor
Map size (Å)	316.80002, 316.80002, 316.80002	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.42	2/3562 (0.1%)	0.67	19/4908 (0.4%)
1	B	0.43	2/3562 (0.1%)	0.66	19/4908 (0.4%)
1	C	0.40	1/3562 (0.0%)	0.61	16/4908 (0.3%)
All	All	0.41	5/10686 (0.0%)	0.65	54/14724 (0.4%)

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	80
1	B	0	72
1	C	0	76
All	All	0	228

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2298	PRO	N-CD	5.23	1.55	1.47
1	B	2410	VAL	CA-CB	5.17	1.65	1.54
1	C	2455	PRO	N-CD	5.02	1.54	1.47
1	B	2455	PRO	N-CD	5.02	1.54	1.47
1	A	2455	PRO	N-CD	5.01	1.54	1.47

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2410	VAL	CB-CA-C	8.86	128.24	111.40
1	B	2410	VAL	CG1-CB-CG2	-8.19	97.79	110.90
1	B	2037	LEU	O-C-N	-8.16	109.65	122.70
1	C	2037	LEU	O-C-N	-8.15	109.65	122.70
1	A	2037	LEU	O-C-N	-8.14	109.67	122.70

There are no chirality outliers.

5 of 228 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	258	UNK	Mainchain
1	A	259	UNK	Mainchain
1	A	260	UNK	Mainchain
1	A	261	UNK	Mainchain
1	A	262	UNK	Mainchain

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	5247	0	2895	498	0
1	B	5247	0	2893	538	0
1	C	5247	0	2898	527	0
All	All	15741	0	8686	1389	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 57.

The worst 5 of 1389 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:C:2410:VAL:HG21	1:C:2426:PHE:CD2	1.22	1.67
1:C:2410:VAL:HG21	1:C:2426:PHE:CE2	1.16	1.62
1:C:2409:GLN:CA	1:C:2410:VAL:HG22	1.28	1.60
1:C:230:UNK:HA	1:C:259:UNK:CB	1.19	1.58
1:B:201:UNK:HA	1:B:288:UNK:CB	1.18	1.57

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	568/2553 (22%)	512 (90%)	31 (6%)	25 (4%)	2	24
1	B	568/2553 (22%)	513 (90%)	27 (5%)	28 (5%)	2	22
1	C	568/2553 (22%)	513 (90%)	27 (5%)	28 (5%)	2	22
All	All	1704/7659 (22%)	1538 (90%)	85 (5%)	81 (5%)	4	23

5 of 81 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1992	ILE
1	A	1993	PHE
1	A	2025	LEU
1	A	2043	VAL
1	A	2051	VAL

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	200/522 (38%)	194 (97%)	6 (3%)	41	63
1	B	200/522 (38%)	190 (95%)	10 (5%)	24	50
1	C	200/522 (38%)	195 (98%)	5 (2%)	47	68
All	All	600/1566 (38%)	579 (96%)	21 (4%)	39	60

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2425	ASP
1	C	2295	ARG
1	C	2454	SER
1	C	2391	GLN
1	C	2224	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2245	GLN
1	A	2409	GLN
1	B	2245	GLN
1	B	2409	GLN
1	C	2245	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)

There are no ligands in this entry.

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.

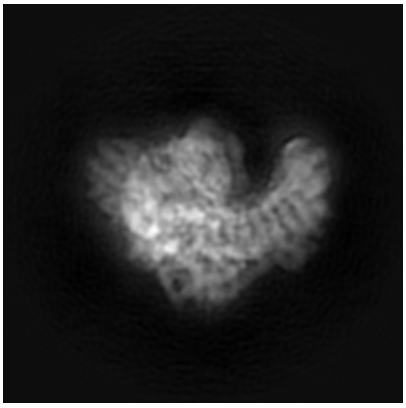
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-6343. These allow visual inspection of the internal detail of the map and identification of artifacts.

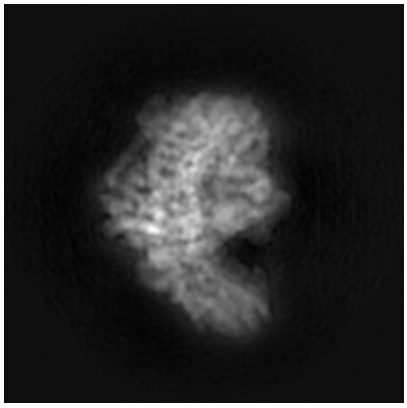
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

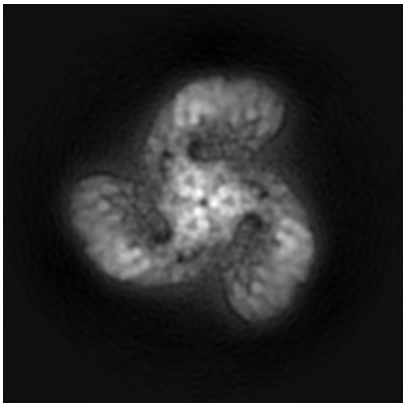
6.1.1 Primary map



X



Y

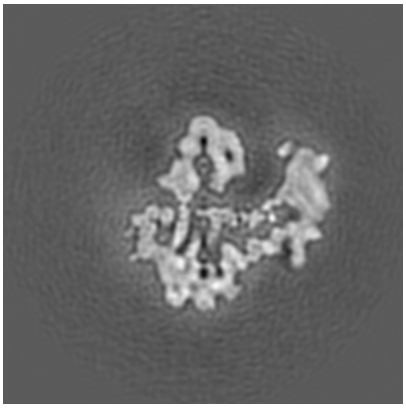


Z

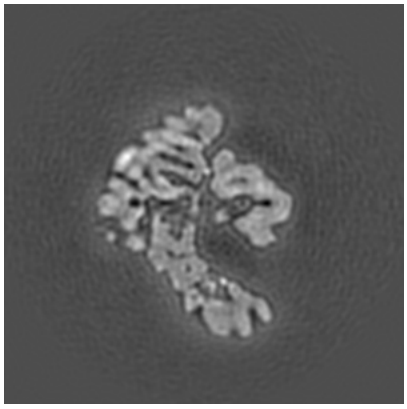
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

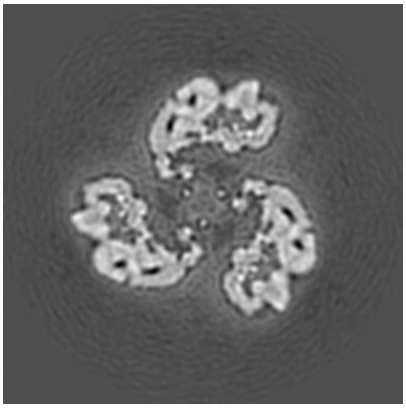
6.2.1 Primary map



X Index: 120



Y Index: 120



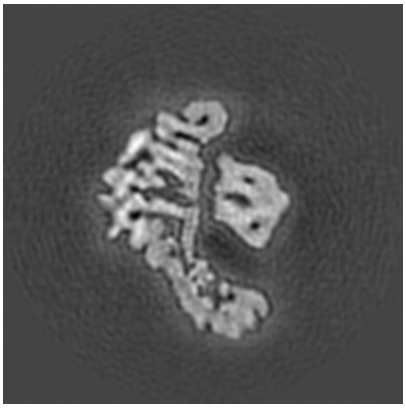
Z Index: 120

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

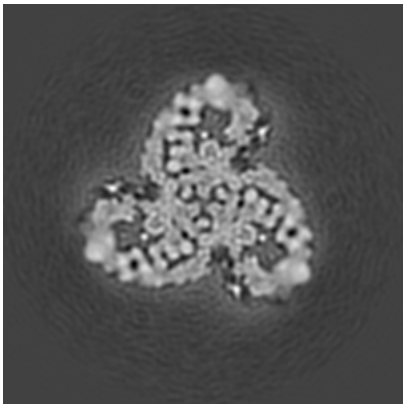
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 107



Y Index: 115

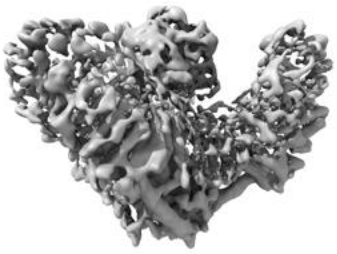


Z Index: 112

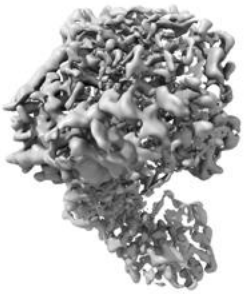
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

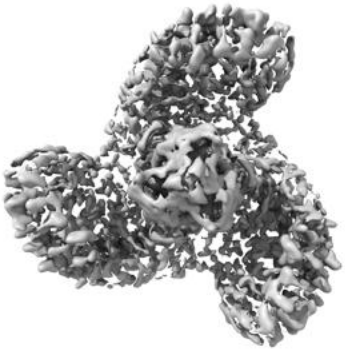
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0273. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

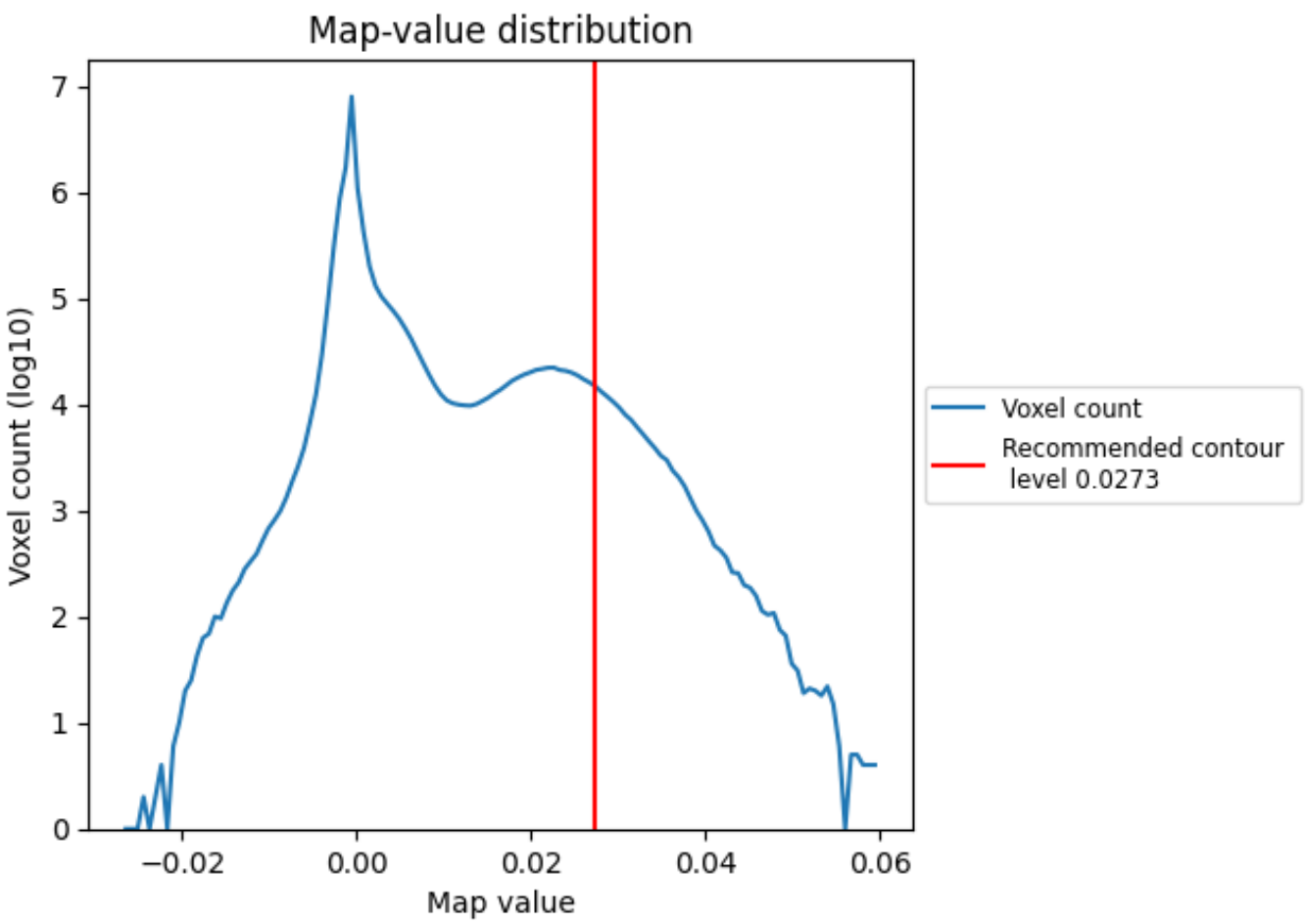
6.5 Mask visualisation (i)

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

7 Map analysis (i)

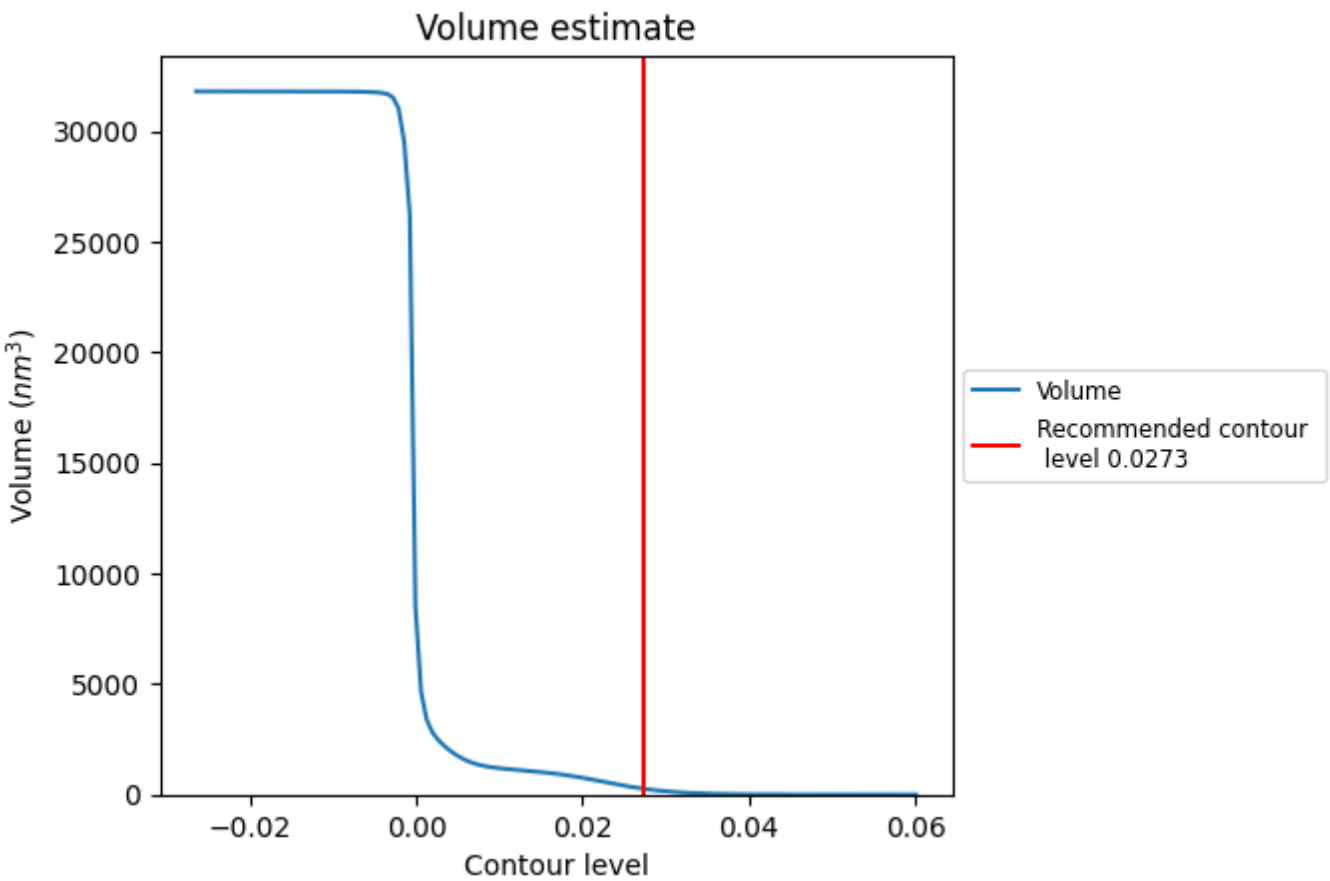
This section contains the results of statistical analysis of the map.

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.

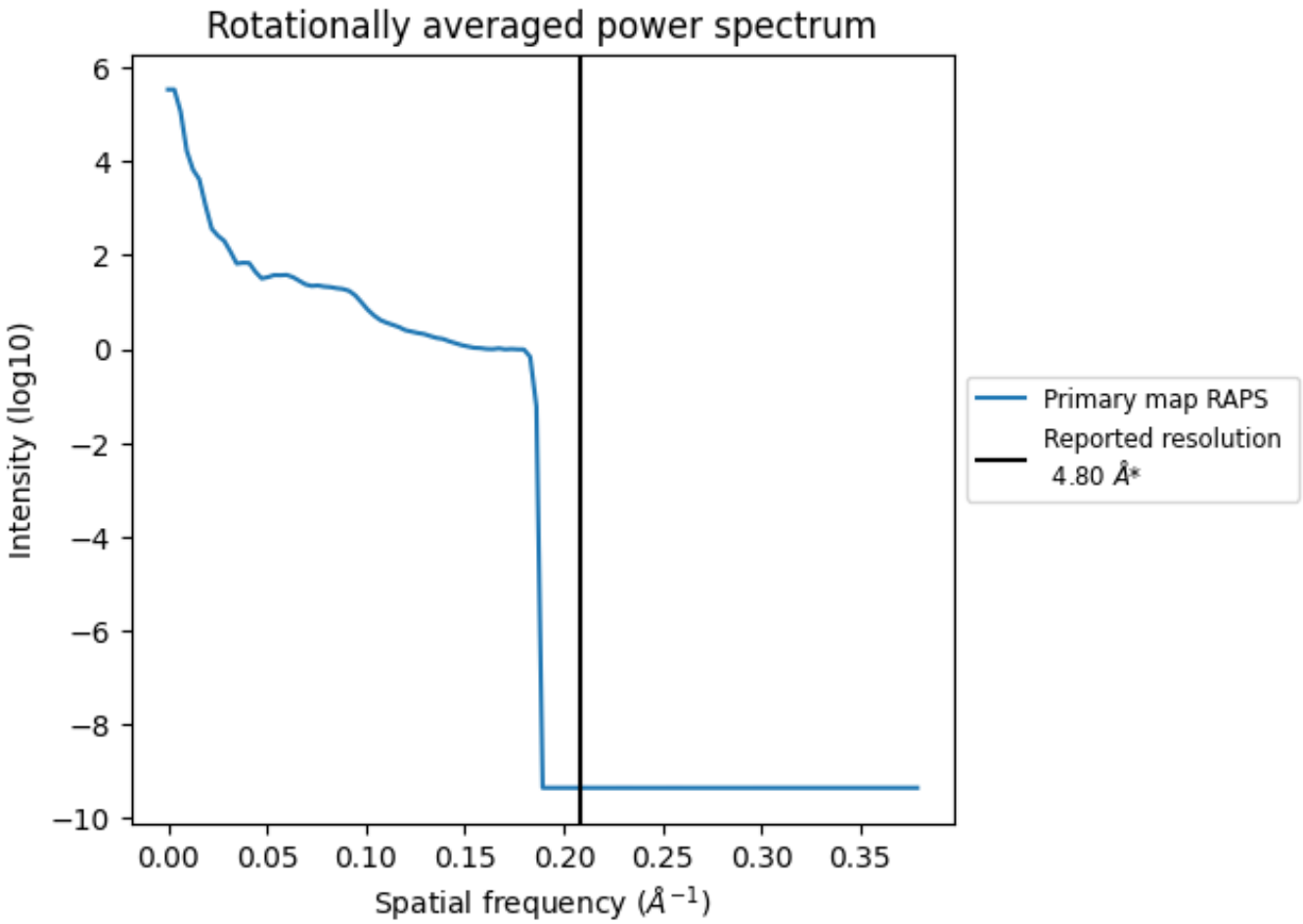
7.2 Volume estimate (i)



The volume at the recommended contour level is 265 nm^3; this corresponds to an approximate mass of 240 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 0.208 Å^{-1}

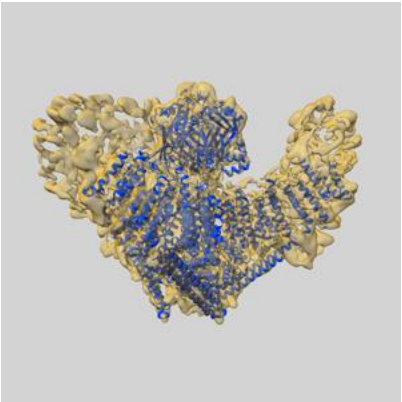
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

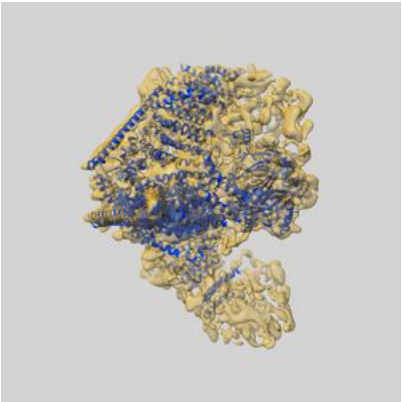
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6343 and PDB model 3JAC. Per-residue inclusion information can be found in section 3 on page 4.

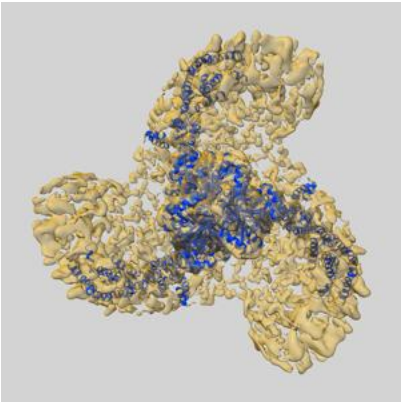
9.1 Map-model overlay (i)



X



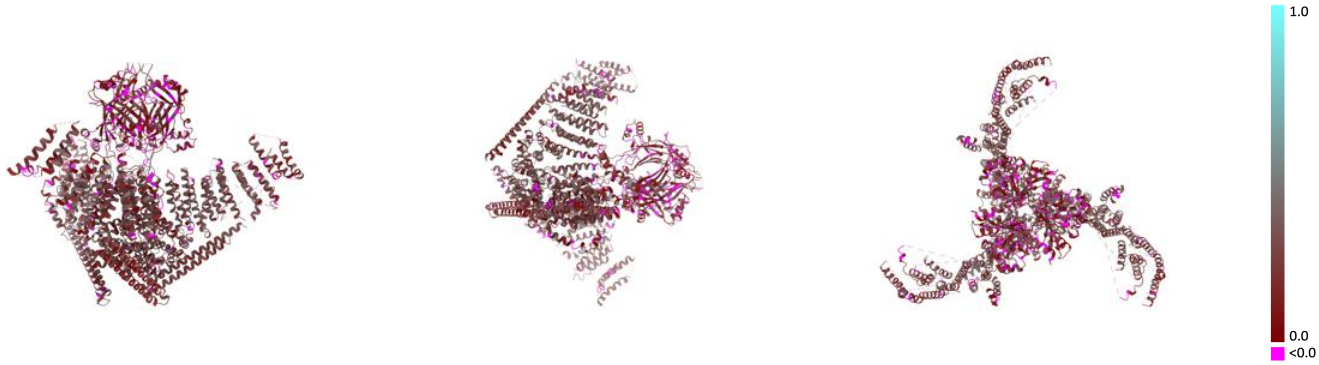
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0273 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.

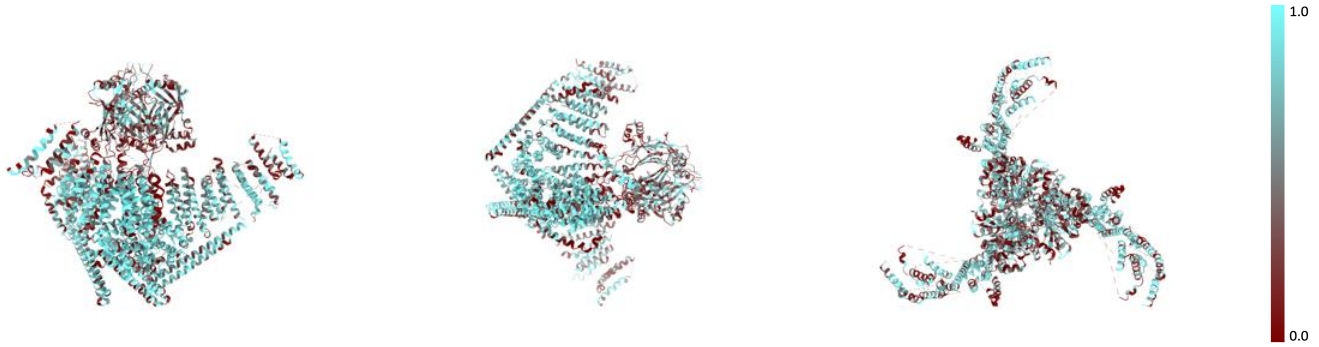
9.2 Q-score mapped to coordinate model (i)



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.

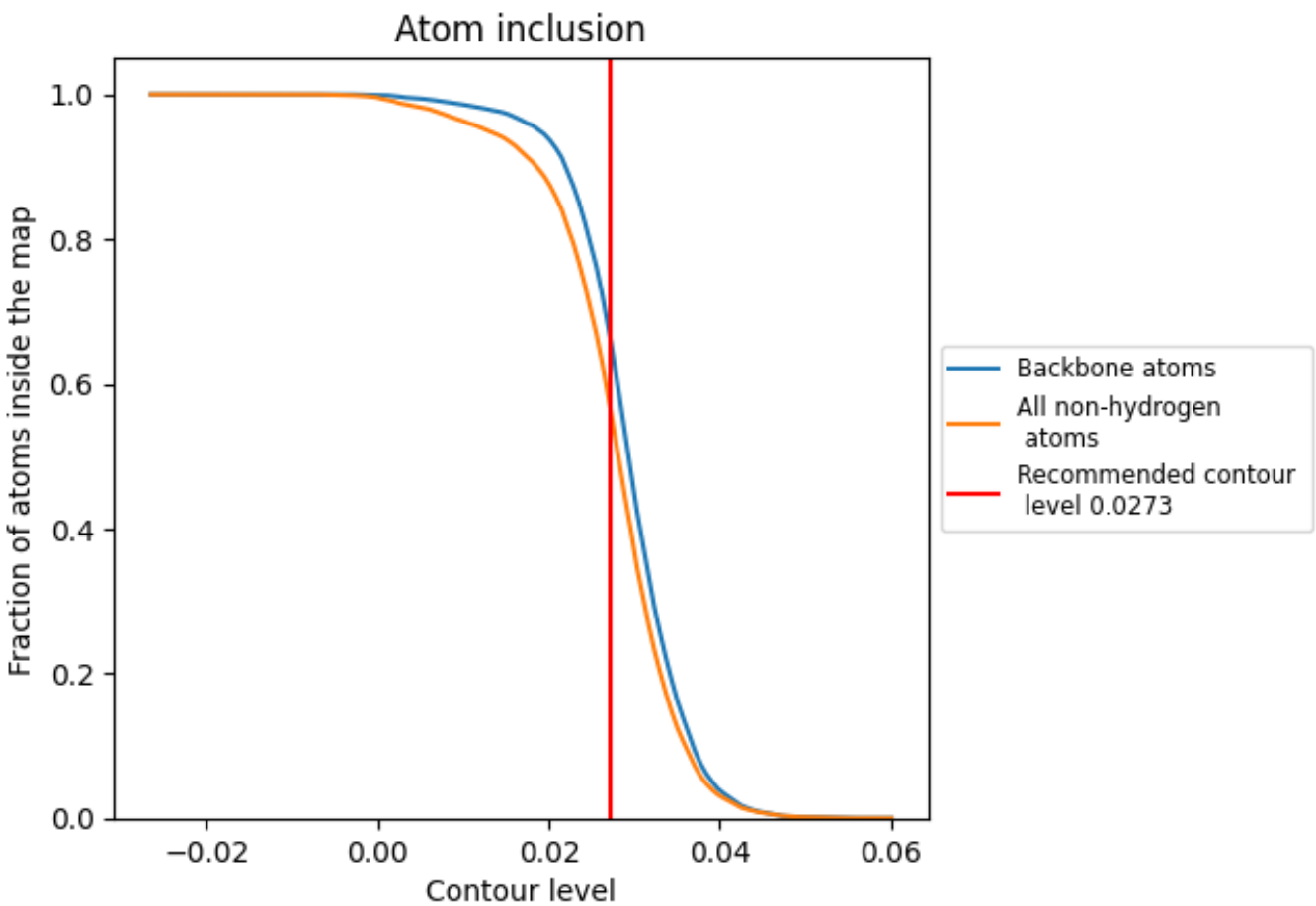
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0273).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0273) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5610	0.1900
A	0.5615	0.1890
B	0.5617	0.1880
C	0.5598	0.1920