wwPDB EM Validation Summary Report

Oct 19, 2026 – 10:24 PM JST

PDB ID	:	9XSB / pdb_00009xsb
EMDB ID	:	EMD-67169
Title	:	CCHFV-FL-RNA-bound state
Authors	:	Zhu, H.; Gao, X.P.
Deposited on	:	2025-11-20
Resolution	:	3.76 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:

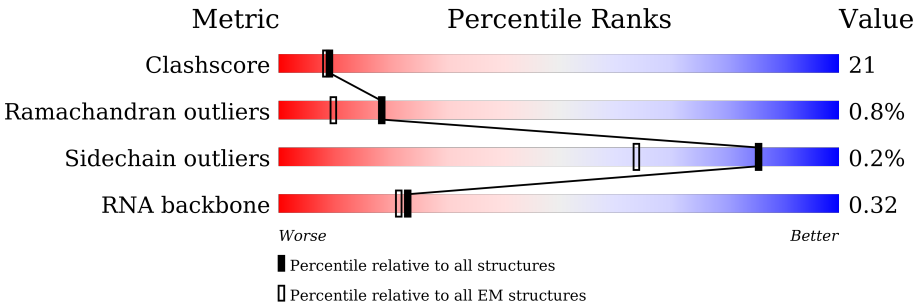
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

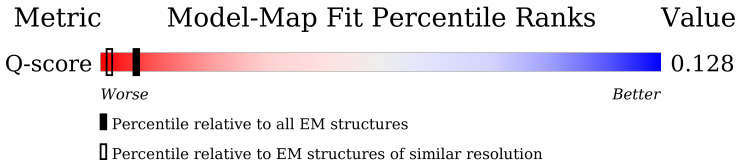
1 Overall quality at a glance

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

The reported resolution of this entry is 3.76 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10214 (3.26 - 4.26)

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	3982	14% 32% 21% 47%
2	C	18	17% 11% 28% 11% 6% 44%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 17243 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2128	17029	10795	2918	3205	111	0	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP A0A1S6XXC8
A	-7	HIS	-	expression tag	UNP A0A1S6XXC8
A	-6	HIS	-	expression tag	UNP A0A1S6XXC8
A	-5	HIS	-	expression tag	UNP A0A1S6XXC8
A	-4	HIS	-	expression tag	UNP A0A1S6XXC8
A	-3	HIS	-	expression tag	UNP A0A1S6XXC8
A	-2	HIS	-	expression tag	UNP A0A1S6XXC8
A	-1	GLY	-	expression tag	UNP A0A1S6XXC8
A	0	THR	-	expression tag	UNP A0A1S6XXC8
A	3946	TRP	-	expression tag	UNP A0A1S6XXC8
A	3947	SER	-	expression tag	UNP A0A1S6XXC8
A	3948	HIS	-	expression tag	UNP A0A1S6XXC8
A	3949	PRO	-	expression tag	UNP A0A1S6XXC8
A	3950	GLN	-	expression tag	UNP A0A1S6XXC8
A	3951	PHE	-	expression tag	UNP A0A1S6XXC8
A	3952	GLU	-	expression tag	UNP A0A1S6XXC8
A	3953	LYS	-	expression tag	UNP A0A1S6XXC8
A	3954	GLY	-	expression tag	UNP A0A1S6XXC8
A	3955	GLY	-	expression tag	UNP A0A1S6XXC8
A	3956	GLY	-	expression tag	UNP A0A1S6XXC8
A	3957	SER	-	expression tag	UNP A0A1S6XXC8
A	3958	GLY	-	expression tag	UNP A0A1S6XXC8
A	3959	GLY	-	expression tag	UNP A0A1S6XXC8
A	3960	GLY	-	expression tag	UNP A0A1S6XXC8
A	3961	SER	-	expression tag	UNP A0A1S6XXC8
A	3962	GLY	-	expression tag	UNP A0A1S6XXC8
A	3963	GLY	-	expression tag	UNP A0A1S6XXC8
A	3964	SER	-	expression tag	UNP A0A1S6XXC8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	3965	ALA	-	expression tag	UNP A0A1S6XXC8
A	3966	TRP	-	expression tag	UNP A0A1S6XXC8
A	3967	SER	-	expression tag	UNP A0A1S6XXC8
A	3968	HIS	-	expression tag	UNP A0A1S6XXC8
A	3969	PRO	-	expression tag	UNP A0A1S6XXC8
A	3970	GLN	-	expression tag	UNP A0A1S6XXC8
A	3971	PHE	-	expression tag	UNP A0A1S6XXC8
A	3972	GLU	-	expression tag	UNP A0A1S6XXC8
A	3973	LYS	-	expression tag	UNP A0A1S6XXC8

- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*CP*UP*CP*AP*AP*AP*GP*AP*AP *AP*UP*CP*GP*UP*UP*CP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	10	Total	C	N	O	P	0	0
			214	96	40	68	10		

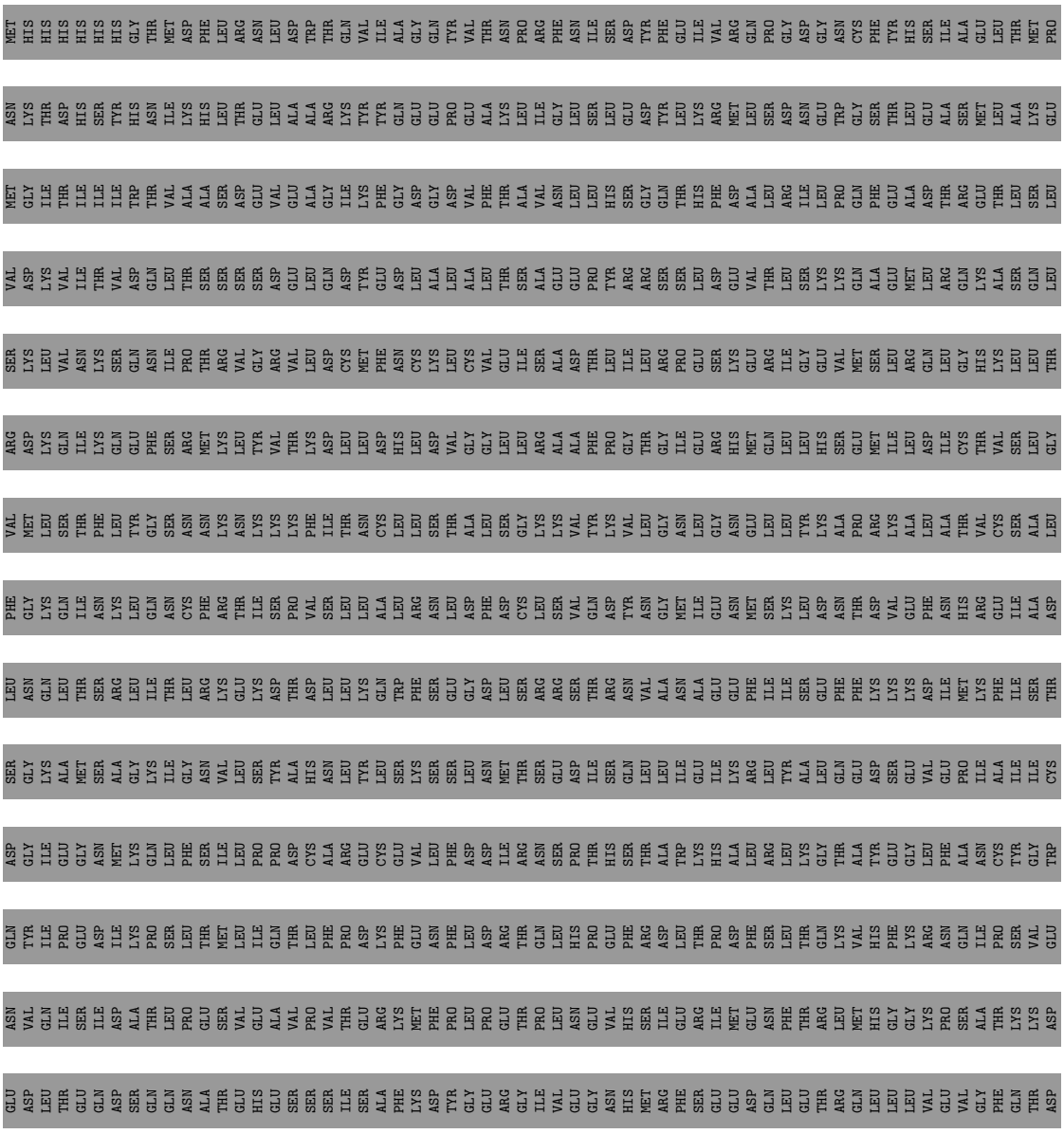
3 Residue-property plots (i)

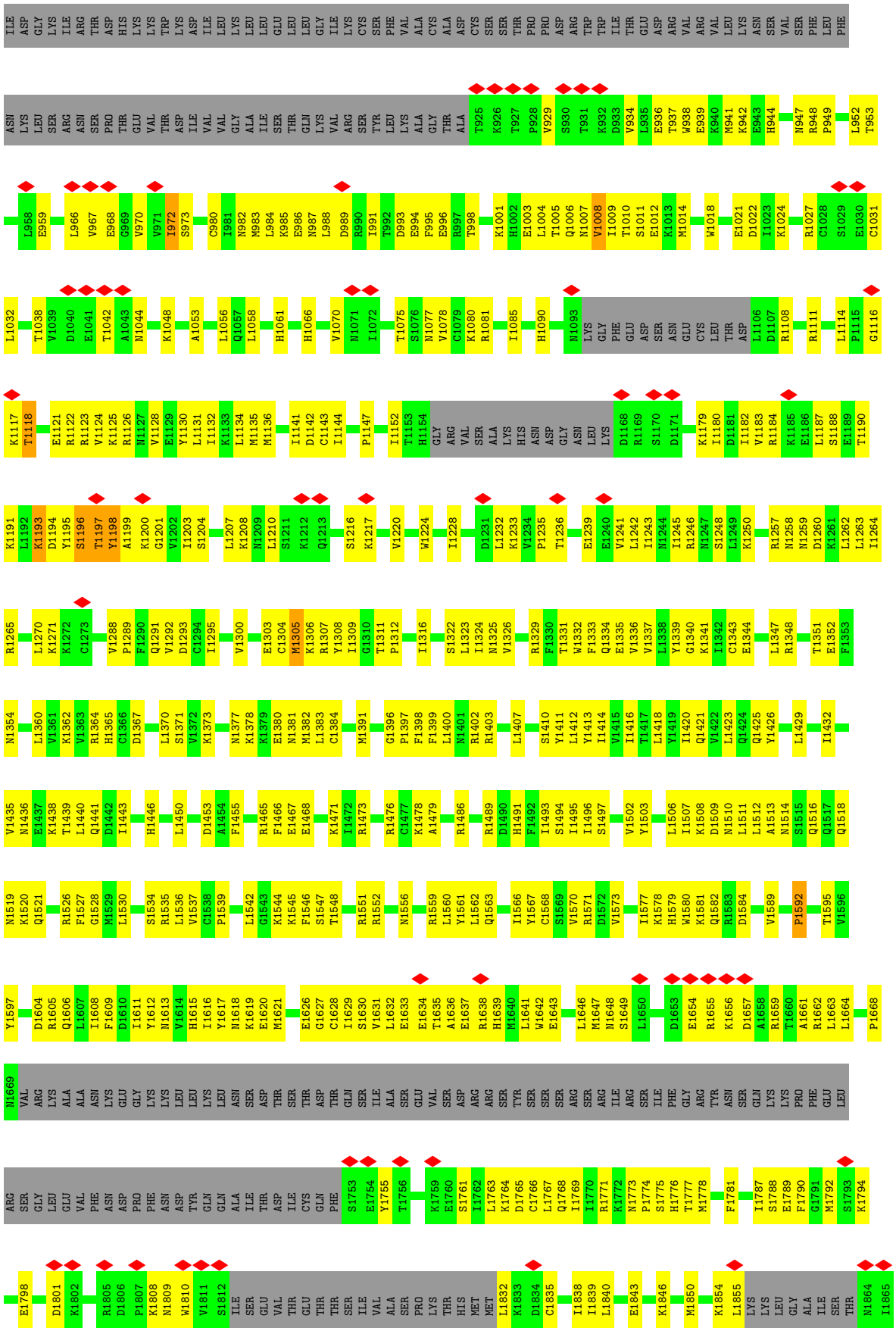
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

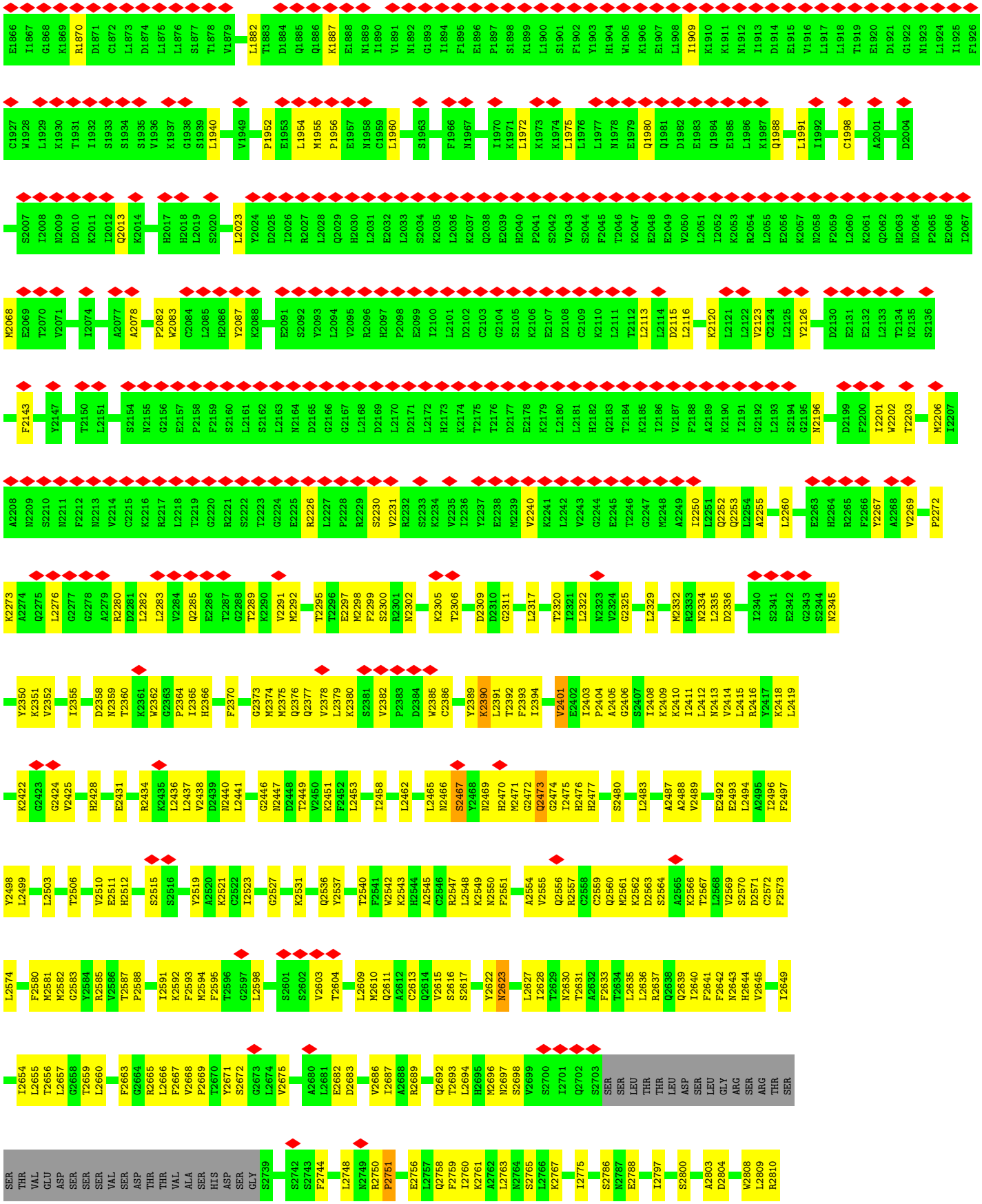
- Molecule 1: RNA-directed RNA polymerase L

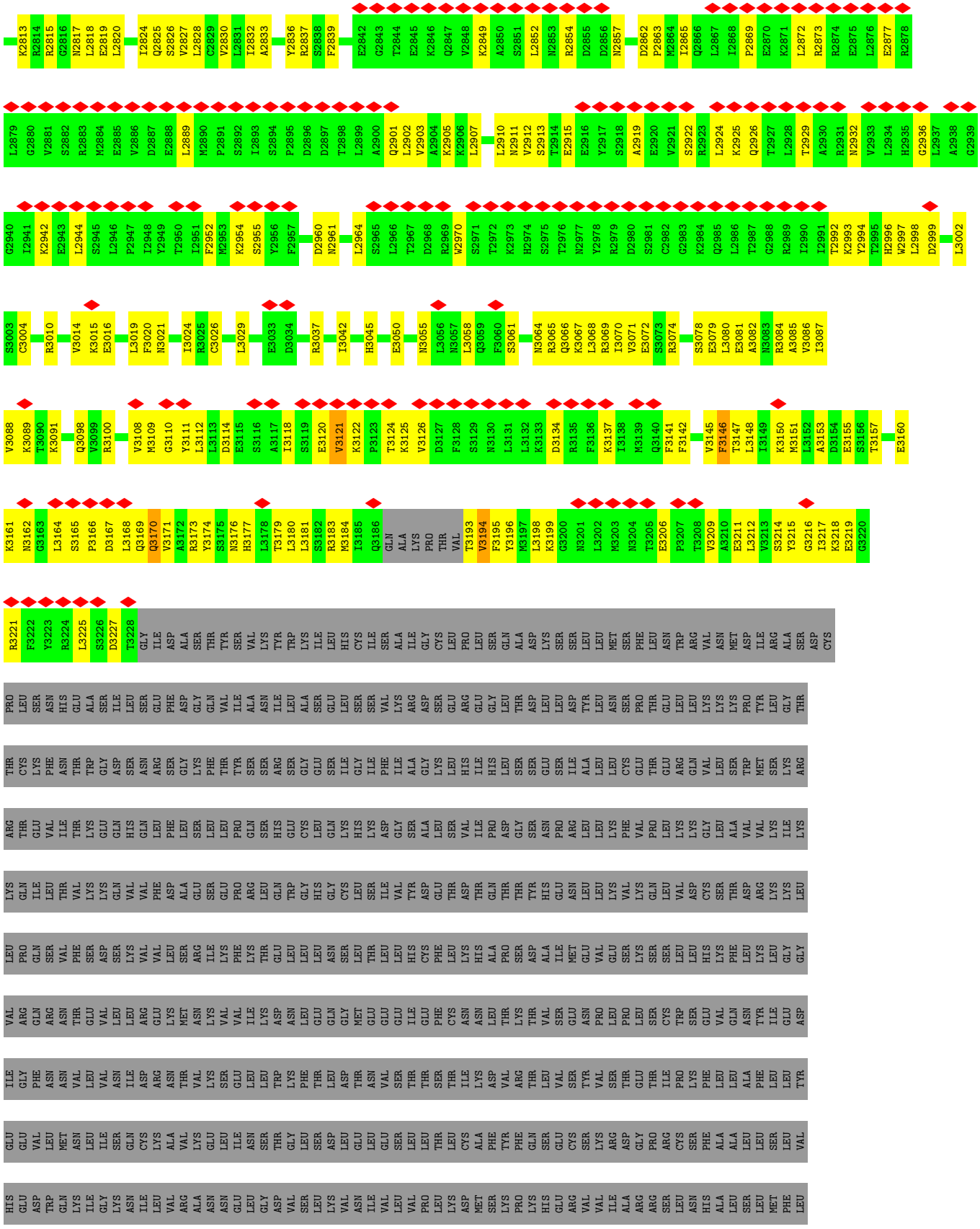
Chain A:

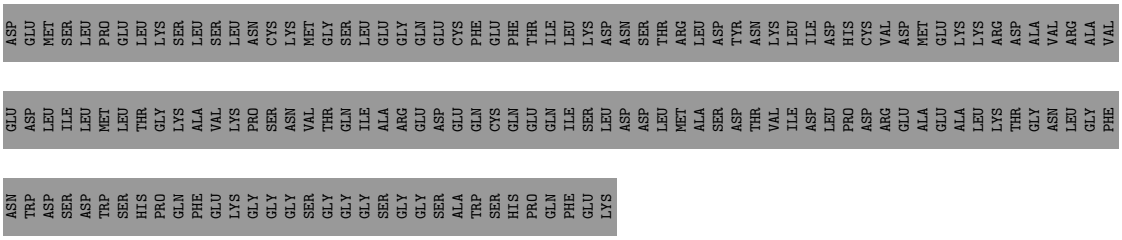




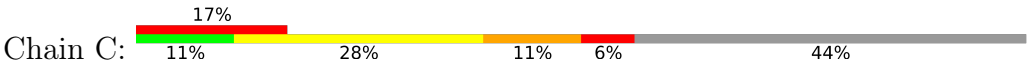


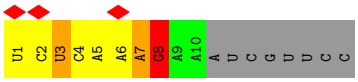

E1866 I1867 G1868 K1869 R1870 D1871 C1872 L1873 D1874 L1875 L1876 S1877 T1878 V1879 L1882 T1883 D1884 Q1885 Q1886 K1887 E1888 N1889 I1890 V1891 N1892 G1893 I1894 F1895 E1896 P1897 S1898 K1899 L1900 S1901 F1902 Y1903 H1904 W1905 K1906 E1907 L1908 I1909 K1910 K1911 N1912 I1913 D1914 E1915 V1916 L1917 L1918 T1919 E1920 D1921 G1922 N1923 L1924 I1925 F1926
G1927 W1928 L1929 K1930 T1931 I1932 S1933 S1934 S1935 V1936 K1937 G1938 S1939 L1940 V1949 P1952 E1953 L1954 M1955 P1956 E1957 N1958 C1959 L1960 S1963 F1966 N1967 I1970 K1971 L1972 K1973 K1974 L1975 L1976 L1977 N1978 E1979 Q1980 Q1981 D1982 E1983 Q1984 E1985 L1986 K1987 Q1988 L1991 I1992 C1998 A2001 D2004
S2007 I2008 N2009 D2010 K2011 I2012 Q2013 K2014 H2017 H2018 L2019 S2020 L2023 Y2024 D2025 I2026 R2027 L2028 Q2029 H2030 L2031 E2032 L2033 S2034 K2035 L2036 K2037 Q2038 E2039 H2040 P2041 S2042 V2043 S2044 F2045 T2046 K2047 E2048 E2049 V2050 L2051 I2052 K2053 R2054 L2055 E2056 K2057 N2058 F2059 L2060 K2061 Q2062 H2063 N2064 P2065 E2066 I2067
M2068 E2069 T2070 V2071 I2074 A2077 A2078 P2082 W2083 C2084 L2085 H2086 Y2087 K2088 E2091 S2092 Y2093 L2094 V2095 R2096 H2097 P2098 E2099 I2100 L2101 D2102 C2103 G2104 S2105 K2106 E2107 D2108 C2109 K2110 L2111 T2112 L2113 L2114 D2115 L2116 K2120 L2121 L2122 V2123 C2124 L2125 Y2126 D2130 E2131 E2132 L2133 T2134 N2135 S2136
F2143 Y2147 T2150 L2151 S2154 N2155 G2156 E2157 P2158 F2159 S2160 L2161 S2162 L2163 N2164 D2165 G2166 G2167 L2168 D2169 L2170 D2171 L2172 H2173 K2174 T2175 T2176 D2177 E2178 K2179 L2180 L2181 H2182 Q2183 T2184 K2185 I2186 V2187 F2188 A2189 K2190 I2191 G2192 L2193 S2194 G2195 N2196 D2199 F2200 I2201 W2202 T2203 M2206 I2207
A2208 N2209 S2210 N2211 F2212 N2213 V2214 C2215 K2216 R2217 L2218 T2219 G2220 R2221 S2222 T2223 G2224 E2225 R2226 L2227 P2228 R2229 S2230 V2231 R2232 S2233 K2234 V2235 I2236 Y2237 E2238 M2239 V2240 K2241 L2242 V2243 G2244 E2245 T2246 G2247 M2248 A2249 I2250 L2251 Q2252 Q2253 L2254 A2255 L2260 E2263 H2264 R2265 F2266 Y2267 A2268 V2269 P2272
K2273 A2274 Q2275 L2276 G2277 G2278 A2279 R2280 D2281 L2282 L2283 V2284 Q2285 E2286 T2287 G2288 T2289 K2290 V2291 M2292 T2295 T2296 E2297 M2298 F2299 S2300 R2301 N2302 K2305 T2306 D2309 D2310 G2311 L2317 T2320 I2321 L2322 N2323 V2324 G2325 L2329 M2332 R2333 N2334 L2335 D2336 I2340 S2341 E2342 G2343 S2344 N2345
Y2350 K2351 V2352 I2355 D2358 N2359 T2360 K2361 W2362 G2363 P2364 I2365 H2366 F2370 G2373 M2374 M2375 Q2376 Q2377 V2378 L2379 K2380 S2381 V2382 P2383 D2384 W2385 C2386 Y2389 K2390 L2391 T2392 F2393 I2394 V2401 F2402 I2403 P2404 A2405 G2406 S2407 I2408 K2409 K2410 I2411 L2412 N2413 V2414 L2415 R2416 Y2417 K2418 L2419
K2422 G2423 G2424 V2425 H2428 E2431 R2434 K2435 L2436 L2437 V2438 D2439 N2440 L2441 G2446 N2447 D2448 T2449 K2450 K2451 F2452 L2453 I2458 L2462 L2465 N2466 S2467 Y2468 N2469 H2470 M2471 G2472 Q2473 G2474 I2475 H2476 H2477 S2480 L2483 A2487 A2488 V2489 E2492 E2493 L2494 A2495 I2496 F2497
Y2498 L2499 L2503 T2506 V2510 E2511 H2512 S2515 S2516 Y2519 A2520 K2521 C2522 I2523 G2527 K2531 Q2536 Y2537 T2540 F2541 W2542 K2543 H2544 A2545 C2546 R2547 L2548 K2549 N2550 F2551 A2554 V2555 Q2556 R2557 C2558 C2559 Q2560 M2561 K2562 D2563 S2564 A2565 K2566 T2567 L2568 V2569 S2570 D2571 C2572 F2573
L2574 F2580 M2581 M2582 G2583 Y2584 R2585 V2586 T2587 P2588 I2591 K2592 F2593 M2594 F2595 T2596 G2597 L2598 S2601 S2602 V2603 T2604 L2609 M2610 Q2611 A2612 C2613 Q2614 V2615 S2616 S2617 Y2622 N2623 L2627 I2628 T2629 N2630 T2631 A2632 F2633 T2634 L2635 L2636 R2637 Q2638 Q2639 I2640 F2641 F2642 N2643 H2644 V2645 I2649
I2654 L2655 T2656 L2657 G2658 T2659 L2660 F2663 G2664 R2665 L2666 F2667 V2668 P2669 T2670 Y2671 S2672 G2673 L2674 V2675 A2680 L2681 E2682 D2683 V2686 I2687 A2688 R2689 Q2692 T2693 L2694 H2695 M2696 N2697 S2698 V2699 S2700 I2701 Q2702 S2703 SER SER LEU THR THR LEU ASP SER LEU GLY ARG SER ARG THR SER
SER THR VAL GLU ASP SER SER SER VAL SER ASP THR THR VAL ALA SER HIS ASP SER GLY S2739 S2742 S2743 F2744 L2748 W2749 R2750 P2751 E2756 L2757 Q2758 F2759 I2760 K2761 A2762 L2763 W2764 S2765 L2766 K2767 I2775 S2786 W2787 E2788 I2797 S2800 A2803 D2804 W2808 L2809 R2810


K2813 R2814 R2815 G2816 N2817 L2818 E2819 L2820 I2824 Q2825 S2826 V2827 L2828 C2829 V2830 L2831 I2832 A2833 Y2836 R2837 S2838 F2839 E2842 G2843 T2844 E2845 K2846 Q2847 V2848 K2849 A2850 S2851 L2852 N2853 R2854 D2855 D2856 N2857 D2862 P2863 M2864 I2865 Q2866 L2867 I2868 P2869 E2870 K2871 L2872 R2873 R2874 E2875 L2876 E2877 R2878
L2879 G2880 V2881 S2882 R2883 M2884 E2885 V2886 D2887 E2888 L2889 M2890 P2891 S2892 I2893 S2894 P2895 D2896 D2897 T2898 L2899 A2900 Q2901 L2902 V2903 A2904 K2905 K2906 L2907 L2910 N2911 V2912 S2913 T2914 E2915 E2916 Y2917 S2918 A2919 E2920 V2921 S2922 R2923 L2924 K2925 Q2926 T2927 L2928 T2929 A2930 R2931 N2932 V2933 L2934 H2935 G2936 L2937 A2938 G2939
G2940 I2941 K2942 E2943 L2944 S2945 L2946 P2947 I2948 Y2949 T2950 I2951 F2952 M2953 K2954 S2955 Y2956 F2957 D2960 N2961 L2964 S2965 L2966 T2967 D2968 R2969 W2970 S2971 T2972 K2973 H2974 S2975 T2976 N2977 Y2978 R2979 D2980 S2981 C2982 G2983 K2984 Q2985 L2986 T2987 G2988 R2989 I2990 I2991 T2992 K2993 Y2994 T2995 H2996 W2997 L2998 D2999 L3002
S3003 C3004 R3010 V3014 K3015 E3016 L3019 F3020 N3021 I3024 R3025 C3026 L3029 E3033 D3034 R3037 I3042 H3045 E3050 N3055 L3056 N3057 L3058 Q3059 F3060 S3061 N3064 R3065 Q3066 K3067 L3068 R3069 I3070 V3071 E3072 S3073 R3074 S3078 E3079 L3080 E3081 A3082 N3083 R3084 A3085 V3086 I3087
V3088 K3089 T3090 K3091 Q3098 V3099 R3100 V3108 M3109 G3110 Y3111 L3112 L3113 D3114 E3115 S3116 A3117 I3118 S3119 E3120 V3121 K3122 P3123 T3124 K3125 V3126 D3127 F3128 S3129 N3130 L3131 L3132 K3133 D3134 R3135 F3136 K3137 I3138 M3139 Q3140 F3141 F3142 V3145 F3146 T3147 L3148 I3149 K3150 M3151 L3152 A3153 D3154 E3155 S3156 T3157 E3160
K3161 N3162 G3163 L3164 S3165 P3166 D3167 L3168 Q3169 Q3170 V3171 A3172 R3173 Y3174 S3175 N3176 H3177 L3178 T3179 L3180 L3181 S3182 R3183 M3184 I3185 Q3186 GLN ALA LYS PRO THR VAL T3193 V3194 F3195 Y3196 M3197 L3198 K3199 G3200 N3201 L3202 M3203 N3204 T3205 E3206 P3207 T3208 V3209 A3210 E3211 L3212 V3213 S3214 Y3215 G3216 I3217 K3218 E3219 G3220
R3221 F3222 Y3223 R3224 L3225 S3226 D3227 T3228 GLY ILE ASP ALA SER THR TYR SER VAL LYS TYR TRP LYS ILE LEU HIS CYS ILE SER ALA ILE GLY CYS LEU PRO LEU SER GLN ALA ASP LYS SER SER LEU LEU MET SER PHE LEU ASN TRP ARG VAL ASN MET ASP ILE ARG ALA SER ASP CYS
PRO LEU SER ASN HIS GLU ALA SER ILE LEU SER GLU PHE ASP GLY GLN VAL ILE ALA ASN ILE LEU ALA SER GLU LEU SER SER VAL LYS ARG ASP SER GLU ARG GLY LEU THR ASP LEU LEU ASP TYR LEU ASN SER PRO THR GLU LEU LEU LYS LYS LYS PRO TYR LEU GLY THR
THR CYS LYS PHE ASN THR TRP GLY ASP SER ASN ARG SER GLY LYS PHE THR TYR SER SER ARG SER GLY GLU SER ILE ALA LEU LEU CYS GLU THR GLU ARG GLN VAL LEU LYS SER TRP MET SER LYS ARG
ARG THR GLU VAL ILE THR LYS GLU GLN HIS GLN LEU PHE LEU SER LEU LEU LEU PRO GLN SER HIS GLU CYS LEU GLN LYS HIS LYS ASP GLY SER ALA LEU SER VAL ILE PRO ASP GLY SER ASN PRO ARG LEU LEU LYS PHE VAL PRO LEU ARG ASP THR THR TYR HIS GLU ASN LEU LEU LYS VAL PHE ASP GLU THR ASP THR GLN THR THR TYR HIS GLU ASN LEU LEU LYS VAL ASP CYS SER THR ASP ARG LYS LYS LEU
LYS GLN ILE LEU THR VAL LYS LYS GLN VAL VAL PHE ASP ALA GLU SER GLU PRO ARG LEU GLN TRP GLY HIS GLY CYS LEU SER ILE VAL TYR ASP GLU THR ASP THR GLN THR THR TYR HIS GLU ASN LEU LEU LYS VAL LYS GLN LEU LEU VAL LYS LYS LYS GLY LEU LYS LYS PHE LEU LEU LYS LYS ILE
LEU PRO GLN SER VAL PHE SER ASP SER LYS VAL LEU SER ARG ILE LYS PHE LYS THR GLU LEU LEU LEU ASN SER LEU THR LEU LEU LEU HIS CYS PHE LEU LYS HIS ALA PRO SER ASP ALA ILE MET GLU VAL GLU SER LYS SER SER LEU HIS LYS HIS LEU LYS LEU GLY GLY
VAL ARG GLN ARG ASN THR GLU VAL LEU LEU ARG GLU LYS MET ASN LYS VAL VAL ILE LYS ASP ASN GLY MET GLU GLU GLU ILE GLU PHE CYS ASN ASN LEU THR LYS THR VAL SER GLU ASN PRO LEU PRO LEU SER CYS TRP SER GLU VAL GLN ASN TYR ILE GLU ASP
ILE GLY PHE ASN ASN VAL LEU VAL ASN ILE ASP ARG ASN THR VAL LYS SER GLU LEU LEU LEU ASP THR ASN VAL VAL SER THR THR SER THR ILE LYS ASP VAL ARG THR LEU VAL SER TYR VAL SER THR GLU THR ILE PRO LYS PHE LEU LEU ALA PHE LEU LEU TYR
GLU GLU VAL LEU MET ASN GLN CYS LYS ALA VAL LYS GLU LEU ILE ASN SER THR GLY LEU SER ASP LEU GLU LEU GLU SER LEU LEU LEU CYS ALA PHE TYR PHE GLN SER GLU CYS SER LYS ARG ASP VAL LEU SER LEU VAL
HIS GLU ASP TRP GLN LYS ILE GLY LYS ASN ASN GLU LEU GLY ASP VAL SER LEU LYS VAL ASN ILE VAL LEU VAL PRO LEU LYS ASP MET SER LYS PRO HIS LYS HIS GLU ARG VAL VAL ILE ALA ARG ARG SER LEU ASN HIS ALA LEU SER LEU MET PHE LEU



• Molecule 2: RNA (5'-R(P*UP*CP*UP*CP*AP*AP*AP*GP*AP*AP*AP*UP*CP*GP*UP*UP*CP*C)-3')





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19012	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.180	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	298.8, 298.8, 298.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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	0.17	0/17317	0.47	8/23345 (0.0%)
2	C	0.37	0/239	0.99	1/368 (0.3%)
All	All	0.17	0/17556	0.49	9/23713 (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	4

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1668	PRO	CA-N-CD	-12.50	94.50	112.00
1	A	2751	PRO	CA-N-CD	-10.09	97.87	112.00
1	A	1592	PRO	N-CD-CG	-6.96	92.76	103.20
1	A	1592	PRO	CA-N-CD	-6.82	102.45	112.00
1	A	1668	PRO	N-CD-CG	-6.36	93.66	103.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1196	SER	Peptide,Mainchain
1	A	1198	TYR	Peptide
1	A	2473	GLN	Peptide

5.2 Too-close contacts

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	17029	0	17299	707	0
2	C	214	0	109	16	0
All	All	17243	0	17408	712	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 21.

The worst 5 of 712 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:A:1196:SER:O	1:A:1198:TYR:N	1.73	1.20
1:A:1765:ASP:O	1:A:1768:GLN:HB3	1.71	0.90
1:A:1536:LEU:HB2	1:A:2569:VAL:HB	1.56	0.86
1:A:2282:LEU:HA	1:A:2473:GLN:HA	1.57	0.83
1:A:2549:LYS:NZ	1:A:2563:ASP:OD2	2.11	0.83

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	2112/3982 (53%)	1935 (92%)	160 (8%)	17 (1%)	16 47

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	972	ILE
1	A	1197	THR
1	A	2405	ALA
1	A	2467	SER
1	A	3109	MET

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	1953/3629 (54%)	1949 (100%)	4 (0%)	87 87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1305	MET
1	A	1519	ASN
1	A	2623	ASN
1	A	2902	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2512	HIS
1	A	2822	ASN
1	A	3083	ASN
1	A	2996	HIS
1	A	2196	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	9/18 (50%)	4 (44%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	3	U
2	C	6	A
2	C	7	A
2	C	8	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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.

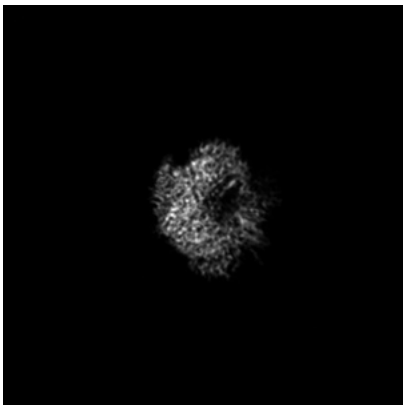
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-67169. 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

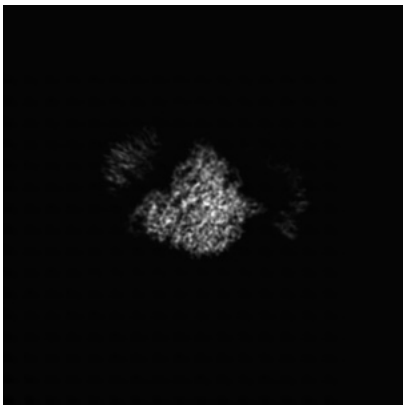
6.1.1 Primary map



X

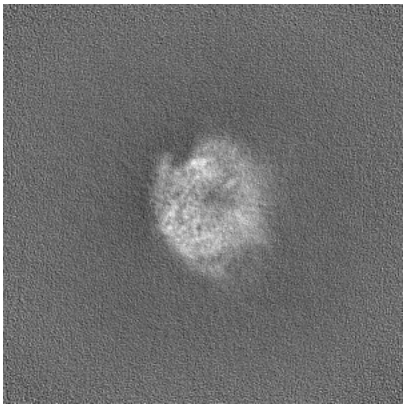


Y

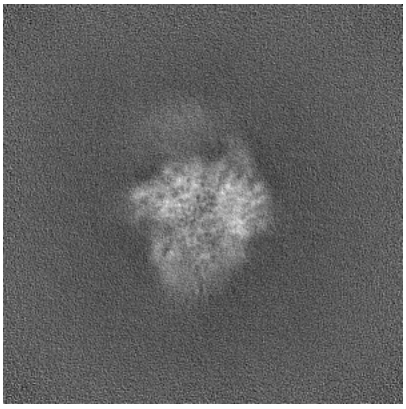


Z

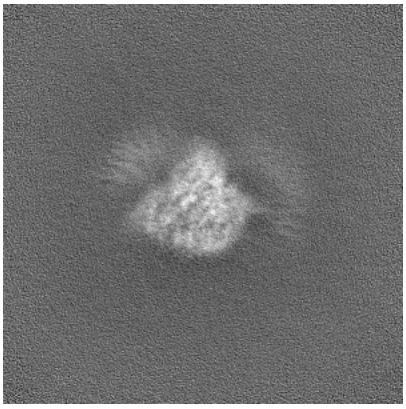
6.1.2 Raw map



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: 180

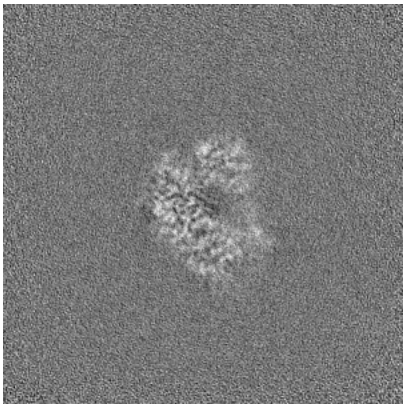


Y Index: 180

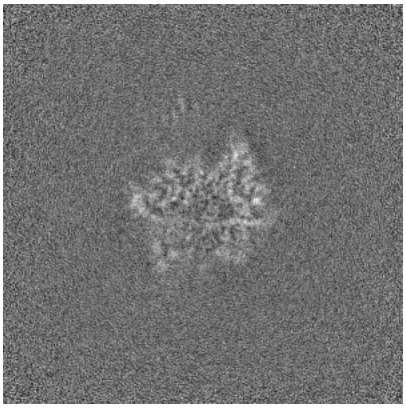


Z Index: 180

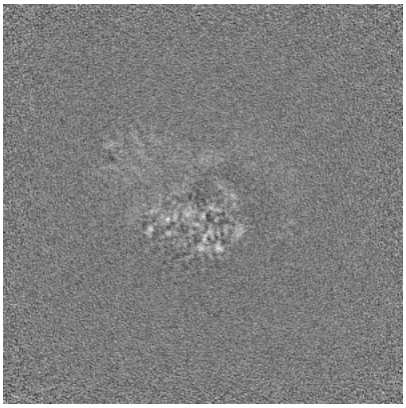
6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

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: 182

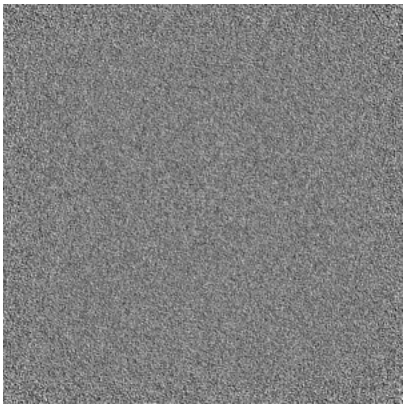


Y Index: 165

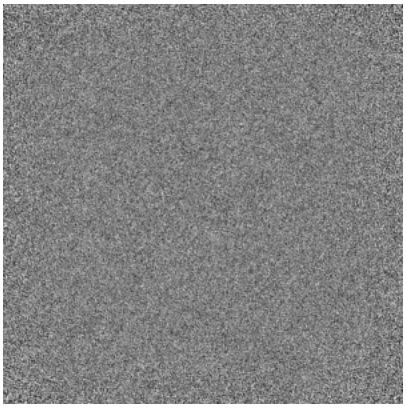


Z Index: 164

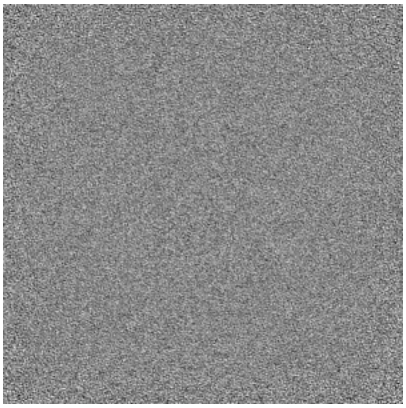
6.3.2 Raw map



X Index: 0



Y Index: 0

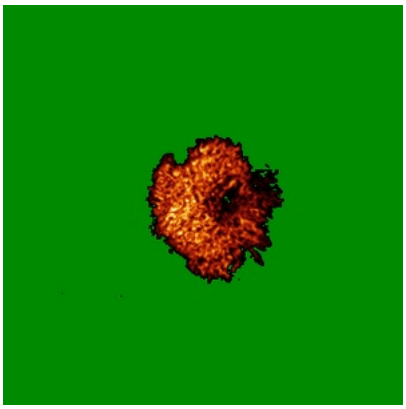


Z Index: 0

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

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

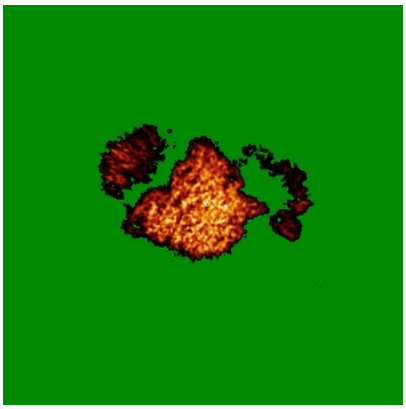
6.4.1 Primary map



X

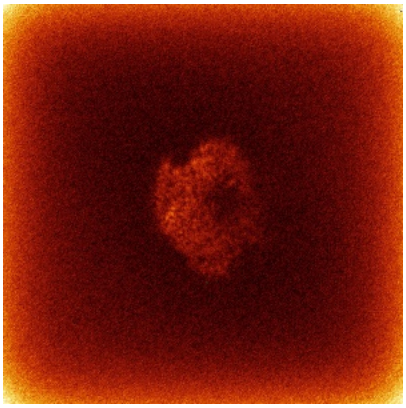


Y

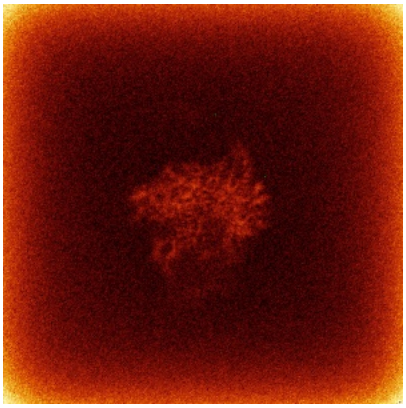


Z

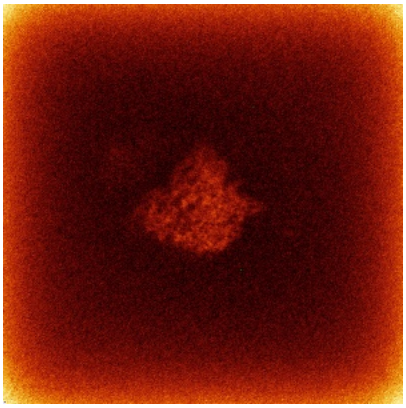
6.4.2 Raw map



X



Y

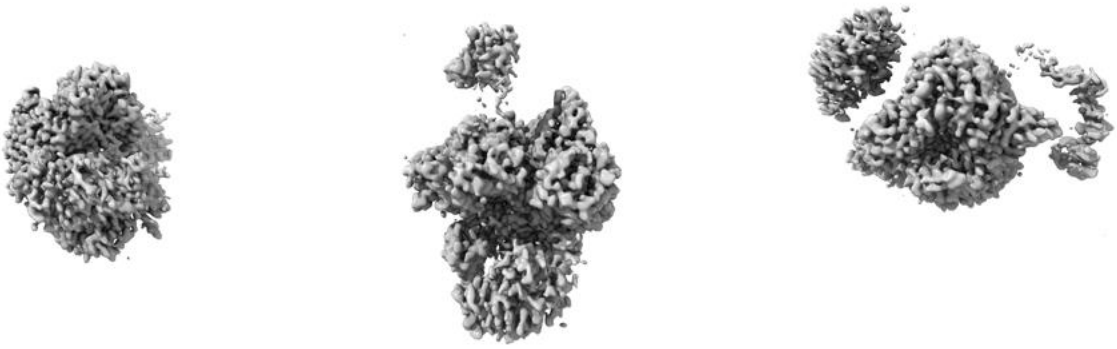


Z

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

6.5 Orthogonal surface views (i)

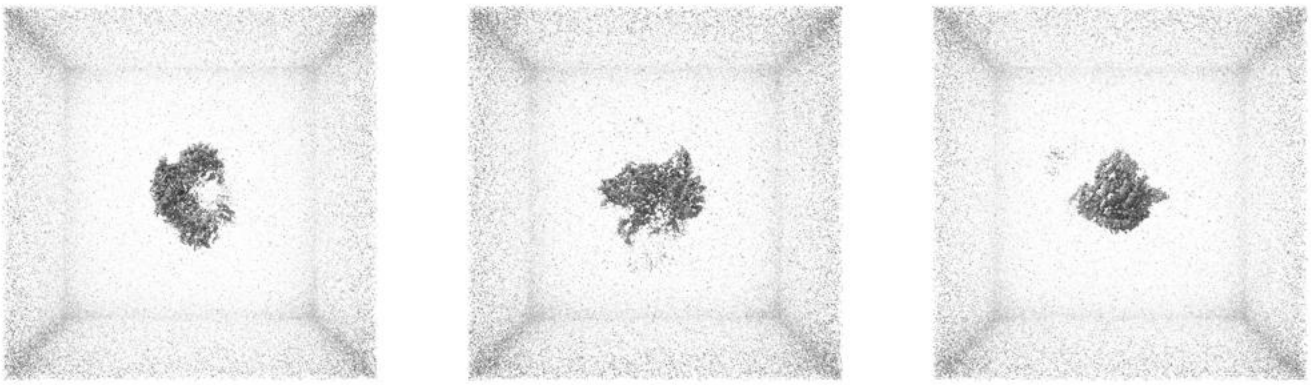
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

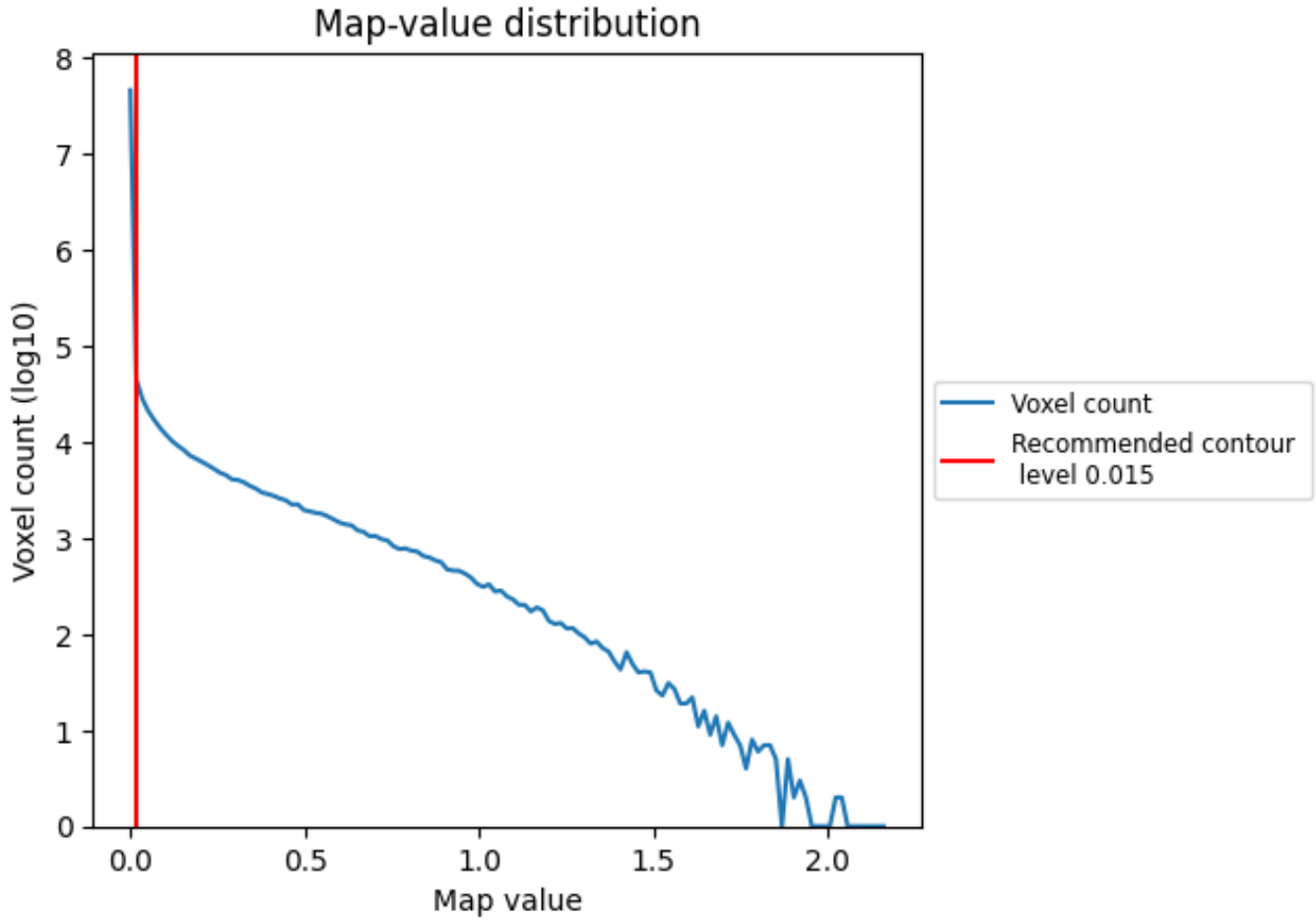
6.6 Mask visualisation (i)

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

7 Map analysis

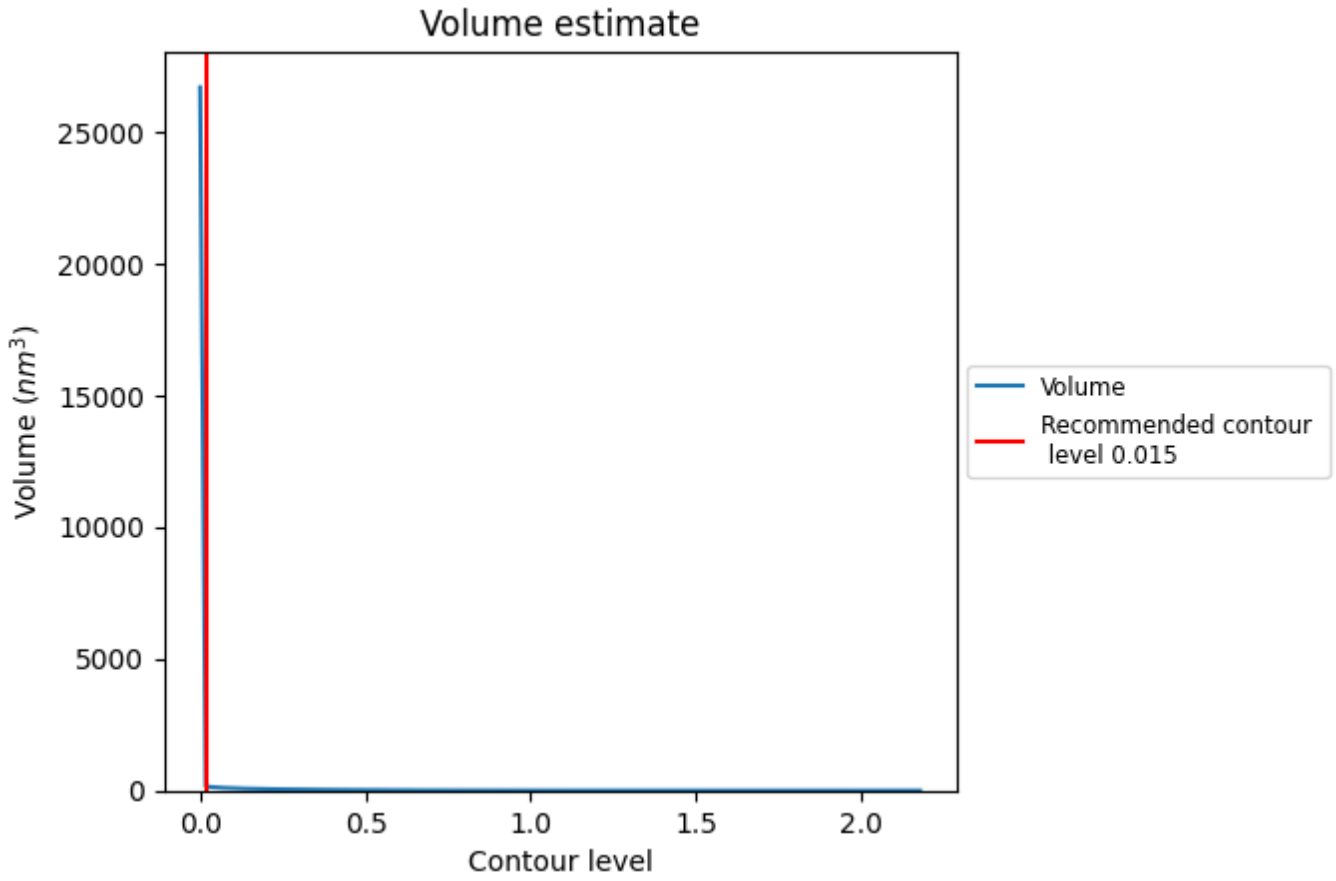
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

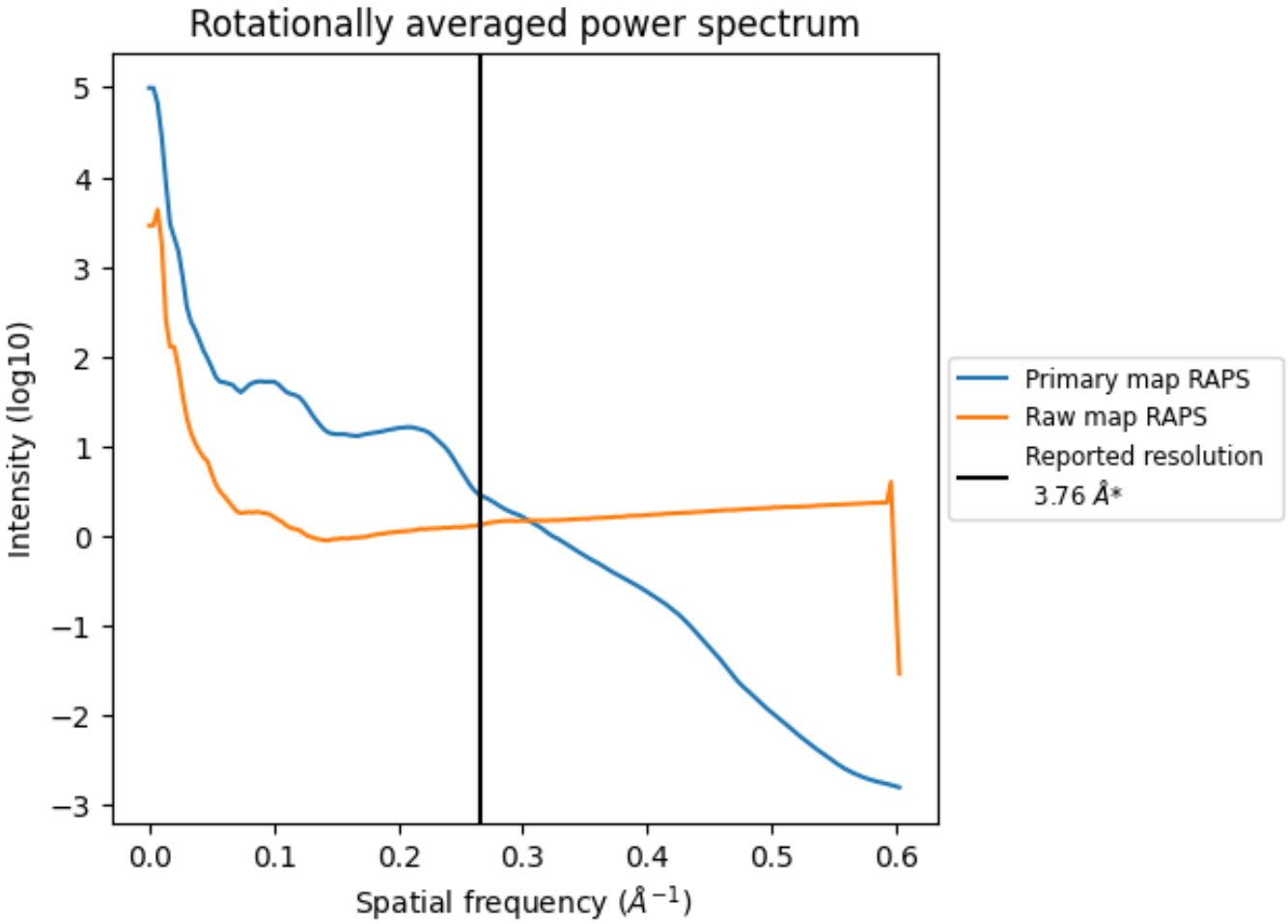
7.2 Volume estimate (i)



The volume at the recommended contour level is 603 nm^3; this corresponds to an approximate mass of 545 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)

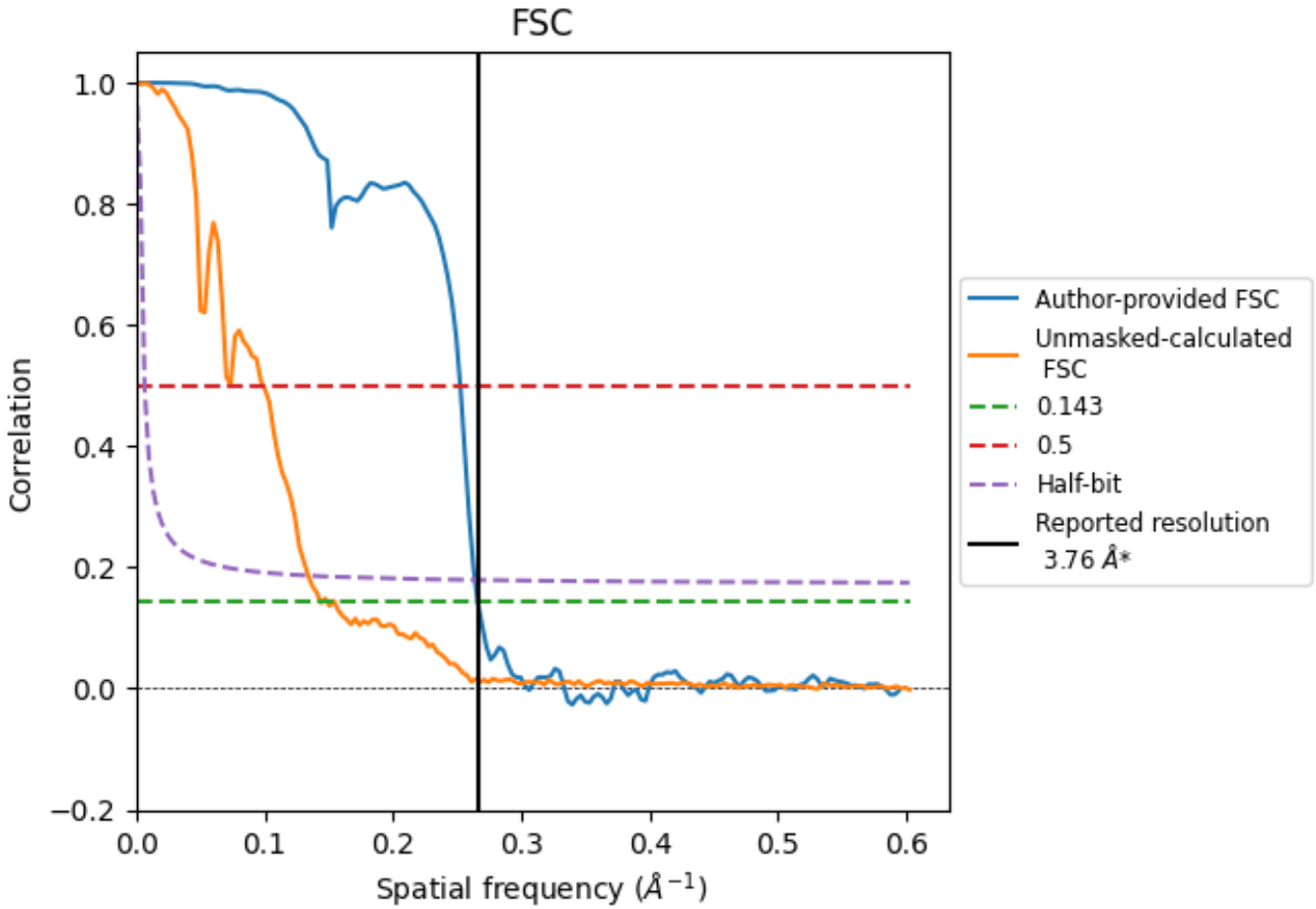


*Reported resolution corresponds to spatial frequency of 0.266 Å^{-1}

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 0.266 Å^{-1}

8.2 Resolution estimates (i)

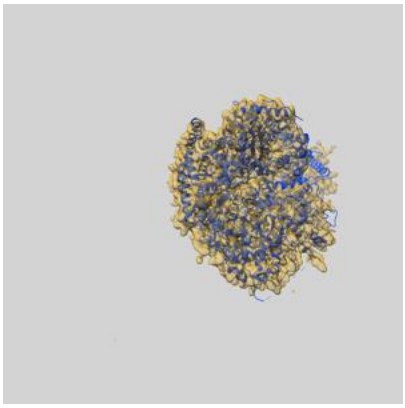
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.76	-	-
Author-provided FSC curve	3.76	3.96	3.79
Unmasked-calculated*	6.96	10.11	7.46

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.96 differs from the reported value 3.76 by more than 10 %

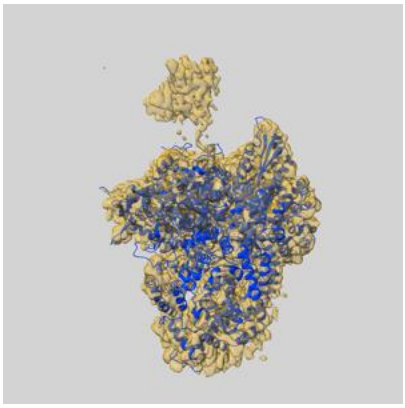
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-67169 and PDB model 9XSB. Per-residue inclusion information can be found in section 3 on page 5.

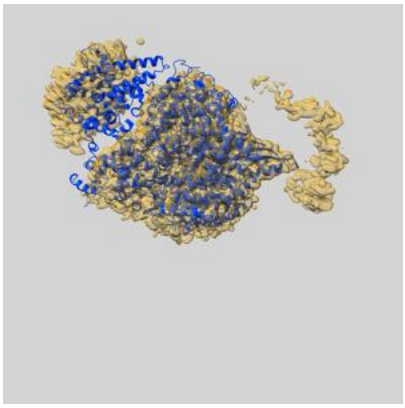
9.1 Map-model overlay



X



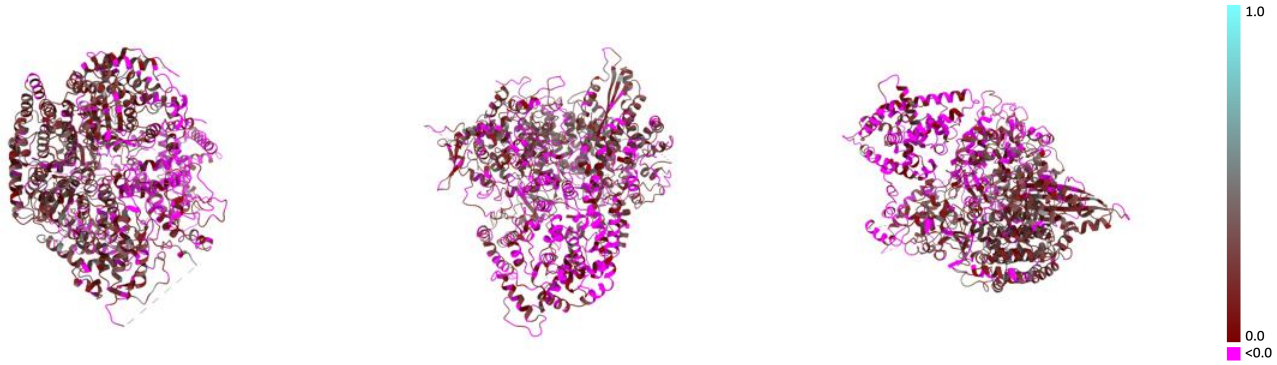
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

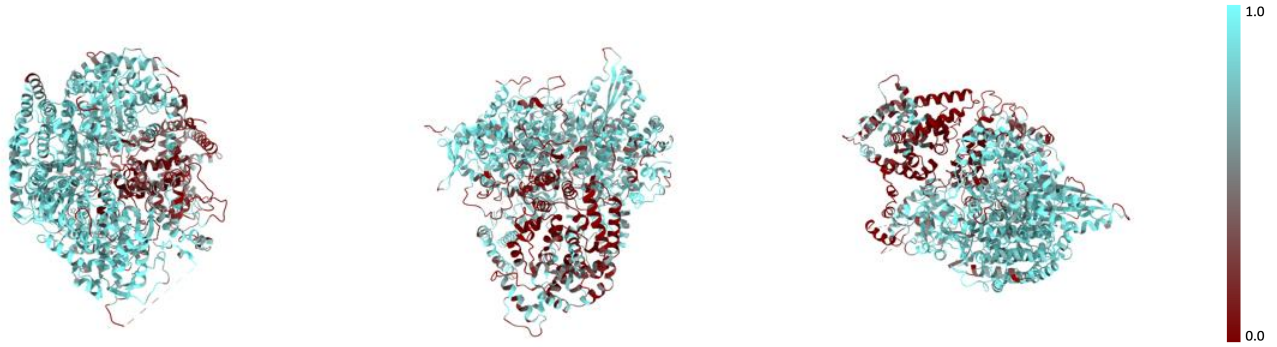
9.2 Q-score mapped to coordinate model (i)



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.

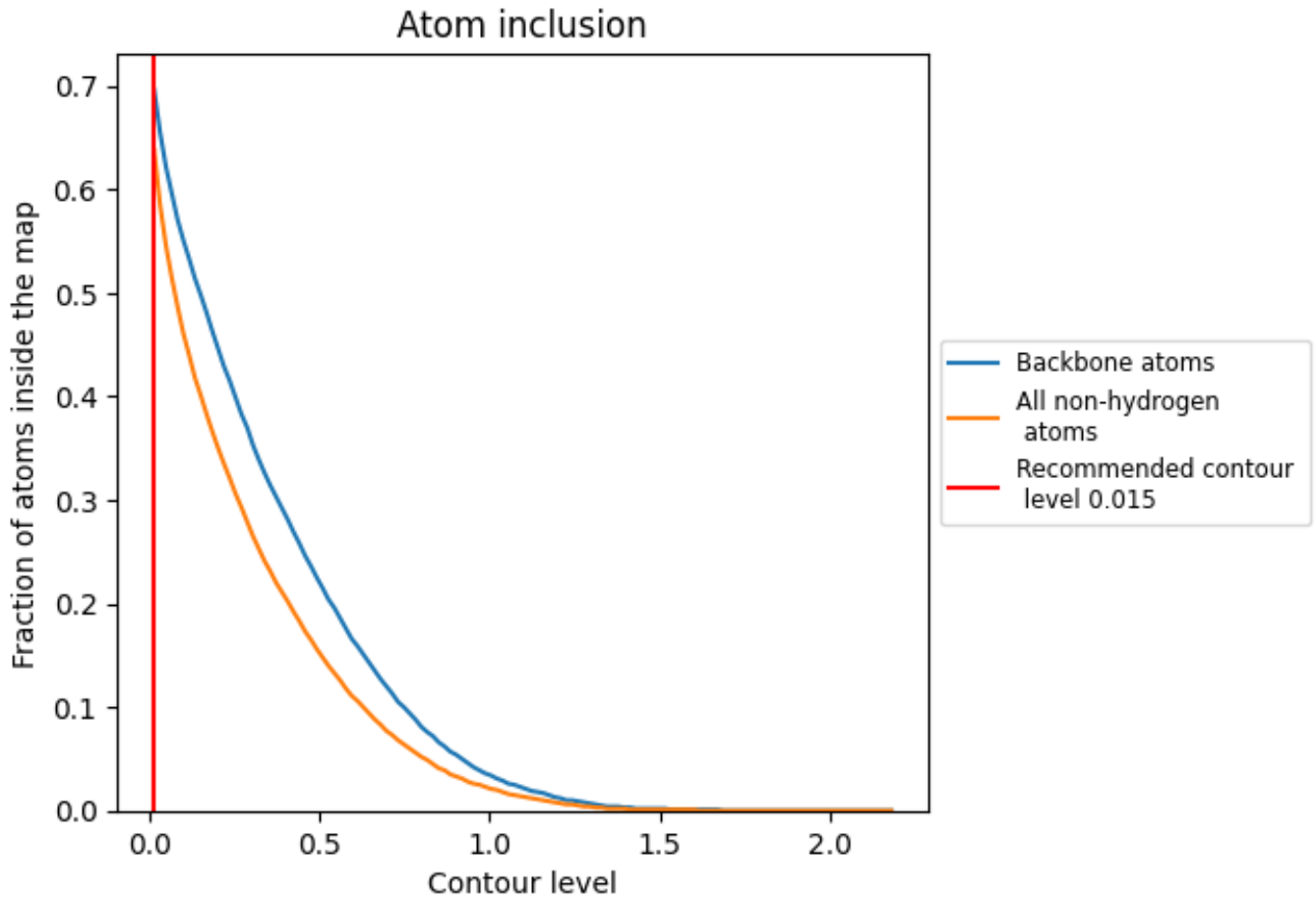
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 64% 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 (0.015) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.6380	0.1280
A	0.6380	0.1290
C	0.6350	0.0020