wwPDB EM Validation Summary Report

Feb 18, 2023 – 03:30 pm GMT

PDB ID	:	7Z88
EMDB ID	:	EMD-14546
Title	:	DNA-PK in the intermediate state
Authors	:	Liang, S.; Blundell, T.L.
Deposited on	:	2022-03-16
Resolution	:	3.33 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:

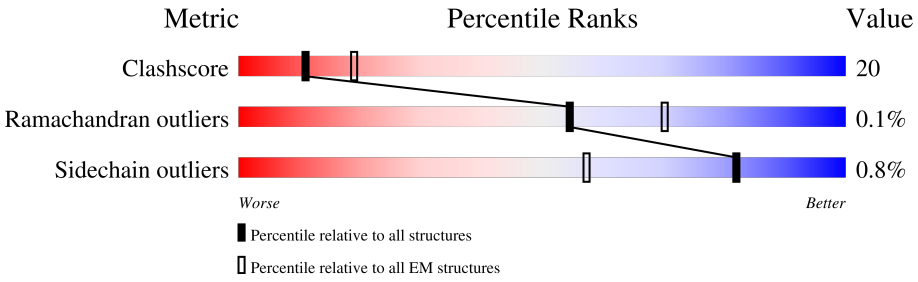
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 3.33 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	4128	15% 50% 36% 13%
2	B	609	10% 46% 33% • 20%
3	C	732	43% 53% 37% • 10%
4	D	26	12% 50% 50%
5	E	26	15% 46% 54%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 38754 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 DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3599	28443	18257	4823	5179	184	0	0

- Molecule 2 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	490	3937	2525	667	728	17	0	0

- Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	661	5274	3372	882	994	26	0	0

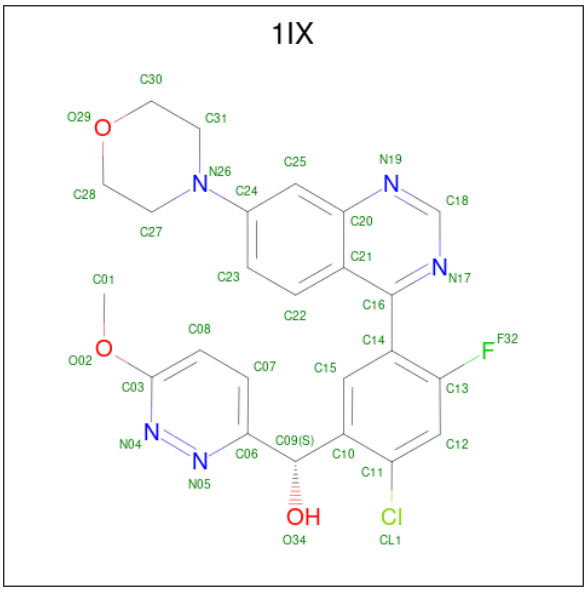
- Molecule 4 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	D	26	526	250	92	158	26	0	0

- Molecule 5 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	E	26	540	254	106	154	26	0	0

- Molecule 6 is ({S})-[2-chloranyl-4-fluoranyl-5-(7-morpholin-4-ylquinazolin-4-yl)phenyl]-(6-methoxypyridazin-3-yl)methanol (three-letter code: 1IX) (formula: $C_{24}H_{21}ClFN_5O_3$) (labeled as "Ligand of Interest" by depositor).



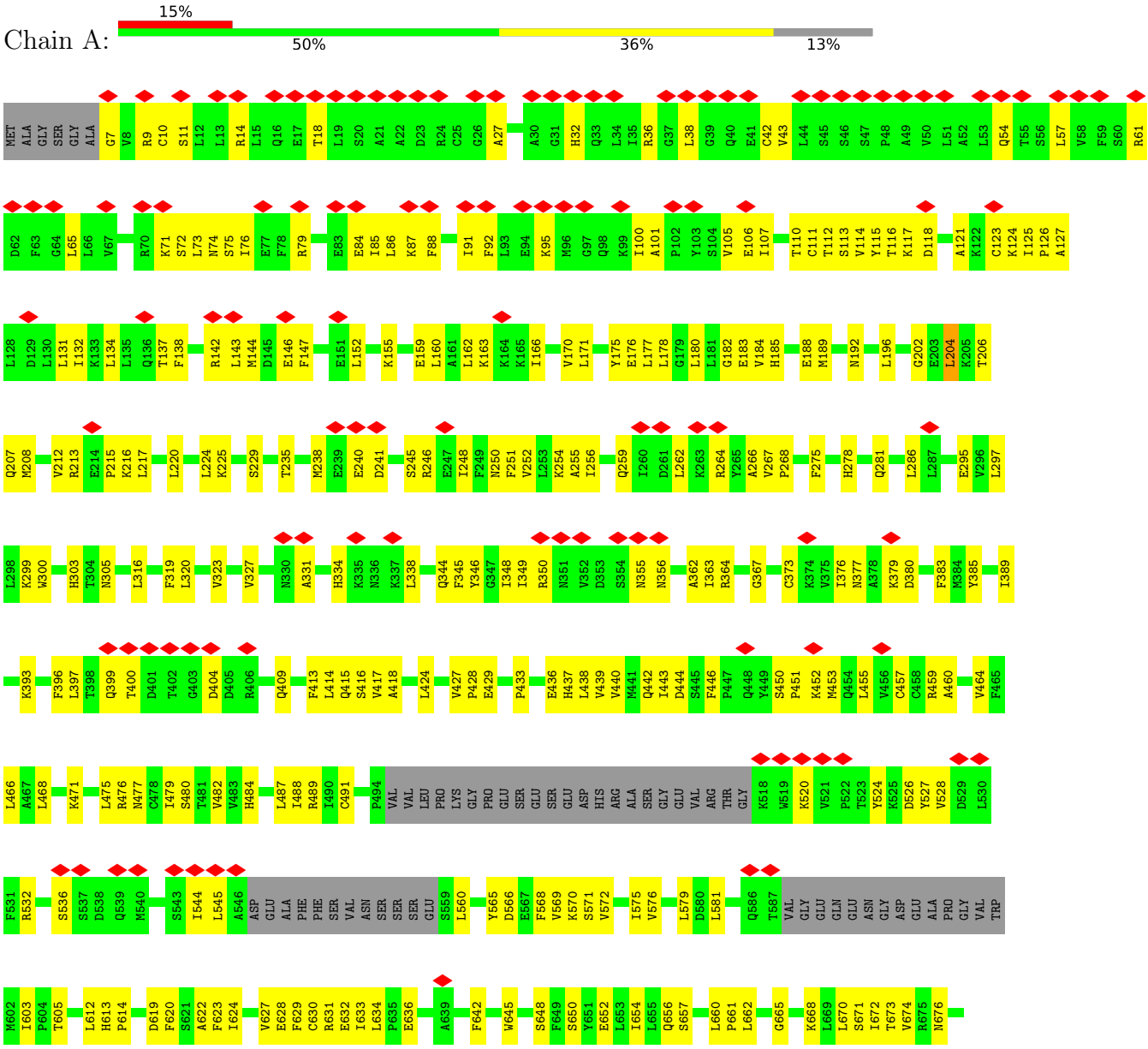
Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	Cl	F	N	O	0
			34	24	1	1	5	3	

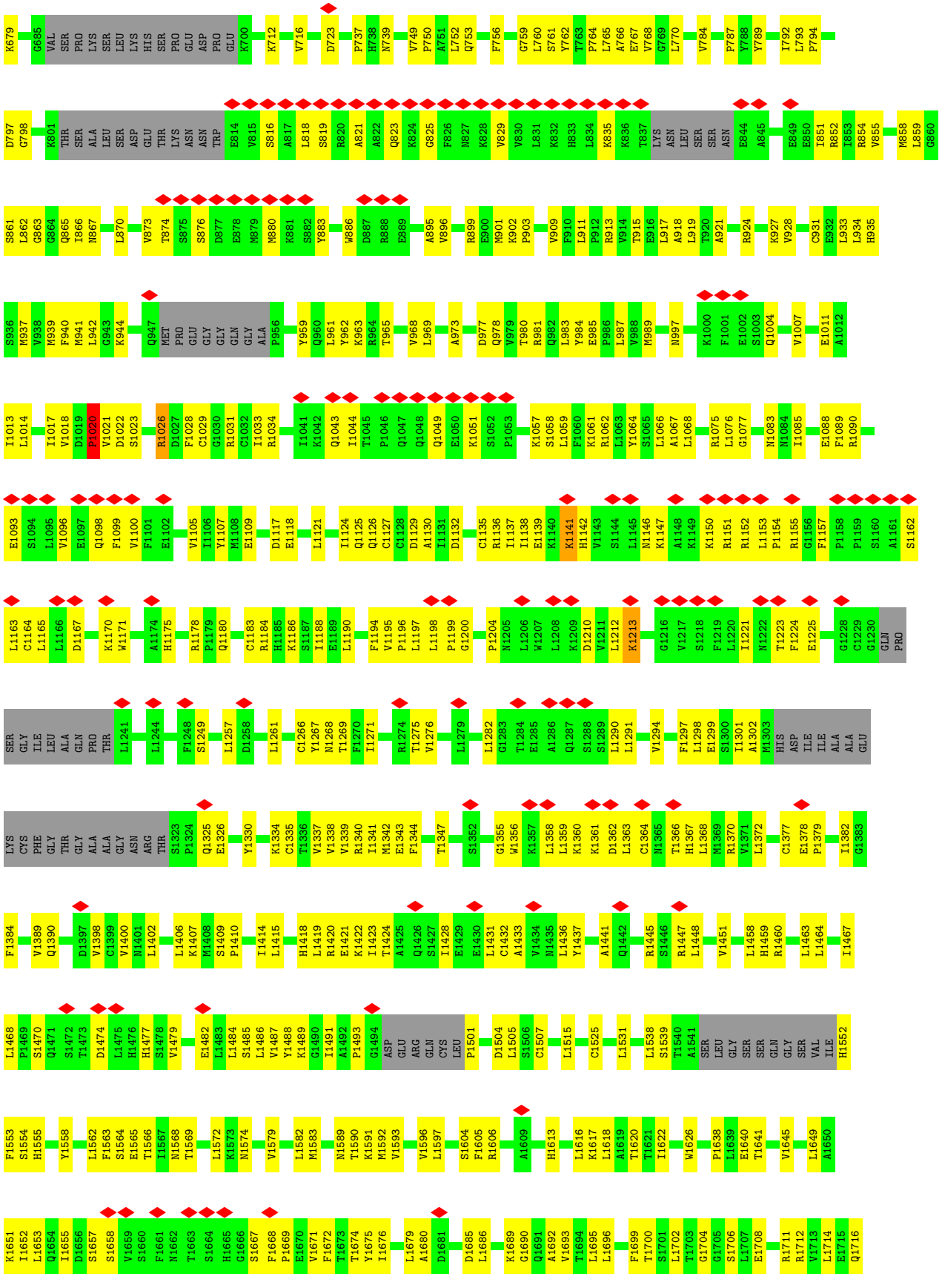
3 Residue-property plots (i)

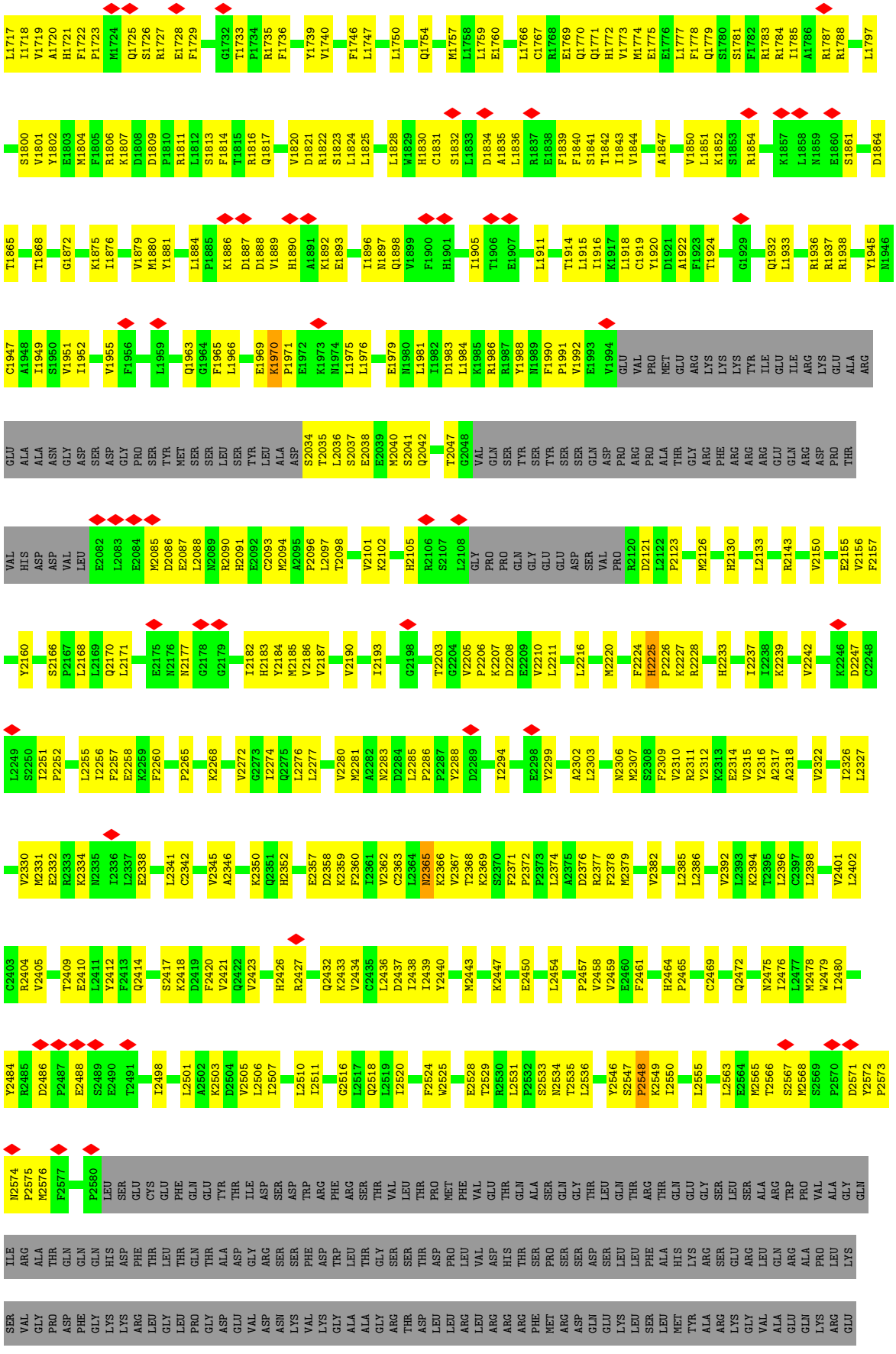
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain A:






L1717 I1718 V1719 A1720 H1721 F1722 P1723 M1724 Q1725 S1726 R1727 E1728 F1729 G1732 T1733 P1734 R1735 F1736 Y1739 V1740 F1746 L1747 L1750 Q1754 M1757 L1758 L1759 E1760 L1766 C1767 R1768 E1769 Q1770 Q1771 H1772 V1773 M1774 E1775 E1776 L1777 F1778 Q1779 S1780 S1781 F1782 R1783 R1784 I1785 A1786 R1787 R1788 L1797
S1800 V1801 Y1802 E1803 M1804 F1805 R1806 K1807 D1808 D1809 P1810 R1811 L1812 S1813 F1814 T1815 R1816 Q1817 V1820 D1821 R1822 S1823 L1824 L1825 L1828 W1829 H1830 C1831 S1832 L1833 D1834 A1835 L1836 R1837 E1838 F1839 F1840 S1841 T1842 I1843 V1844 A1847 V1850 L1851 K1852 S1853 R1854 K1857 L1858 N1859 E1860 S1861 D1864
T1865 T1868 G1872 K1875 I1876 V1879 M1880 Y1881 L1884 P1885 K1886 D1887 D1888 V1889 H1890 A1891 K1892 E1893 I1896 N1897 Q1898 V1899 F1900 H1901 I1905 T1906 E1907 L1911 T1914 L1915 I1916 K1917 L1918 C1919 Y1920 D1921 A1922 F1923 T1924 G1929 Q1932 L1933 R1936 R1937 R1938 Y1945 N1946
C1947 A1948 I1949 S1950 V1951 I1952 V1955 F1956 L1959 Q1963 G1964 F1965 L1966 E1969 K1970 P1971 E1972 K1973 N1974 L1975 L1976 E1979 N1980 L1981 I1982 D1983 L1984 K1985 R1986 R1987 Y1988 N1989 F1990 P1991 V1992 E1993 V1994 GLU VAL PRO MET GLU ARG LYS LYS TYR ILE GLU ILE ARG LYS GLU ALA ARG
GLU ALA ALA ASN GLY ASP SER ASP GLY PRO SER TYR MET SER SER LEU SER TYR LEU ALA ASP S2034 T2035 L2036 S2037 E2038 E2039 M2040 S2041 Q2042 T2047 G2048 VAL GLN SER TYR SER TYR SER SER GLN ASP PRO ARG PRO ALA THR GLY ARG PHE ARG ARG ARG GLU GLN ARG ASP PRO THR
VAL HIS ASP ASP VAL LEU E2082 L2083 E2084 M2085 D2086 E2087 L2088 N2089 R2090 H2091 E2092 C2093 M2094 A2095 P2096 L2097 T2098 V2101 K2102 H2105 R2106 S2107 L2108 GLY PRO PRO GLN GLY GLU GLU ASP SER VAL PRO R2120 D2121 L2122 P2123 M2126 H2130 L2133 R2143 V2150 E2155 V2156 F2157
Y2160 S2166 P2167 L2168 L2169 Q2170 L2171 E2175 N2176 N2177 G2178 G2179 I2182 H2183 Y2184 M2185 V2186 V2187 V2190 I2193 G2198 T2203 G2204 V2205 P2206 K2207 D2208 E2209 V2210 L2211 L2216 M2220 F2224 H2225 P2226 K2227 R2228 H2233 I2237 I2238 K2239 V2242 K2246 D2247 C2248
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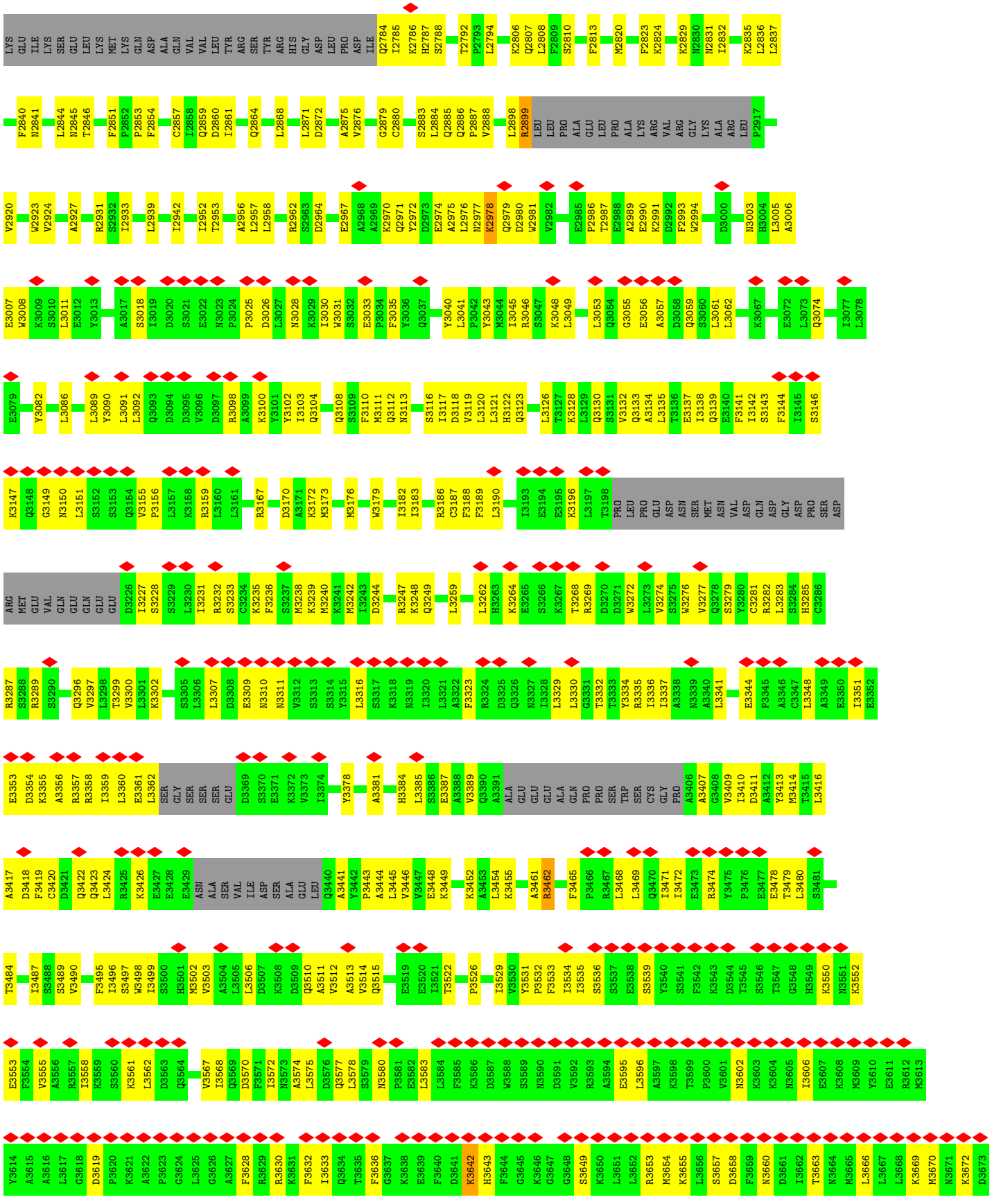
V2330 M2331 E2332 R2333 K2334 N2335 I2336 L2337 E2338 L2341 C2342 V2345 A2346 K2350 Q2351 H2352 E2357 D2358 K2359 F2360 I2361 V2362 C2363 L2364 N2365 K2366 V2367 T2368 K2369 S2370 F2371 P2372 P2373 L2374 A2375 D2376 R2377 F2378 M2379 V2382 L2385 L2386 V2392 L2393 K2394 T2395 L2396 C2397 L2398 V2401 L2402
C2403 R2404 V2405 T2409 E2410 L2411 Y2412 F2413 Q2414 S2417 K2418 D2419 F2420 V2421 Q2422 V2423 H2426 R2427 Q2432 K2433 V2434 C2435 L2436 D2437 I2438 I2439 Y2440 M2443 K2447 E2450 L2454 P2457 V2458 V2459 E2460 F2461 H2464 P2465 C2469 Q2472 N2475 I2476 L2477 M2478 W2479 I2480
Y2484 R2485 D2486 P2487 E2488 S2489 E2490 T2491 I2498 L2501 A2502 K2503 D2504 V2505 L2506 I2507 L2510 I2511 G2516 L2517 Q2518 L2519 I2520 F2524 W2525 E2528 T2529 R2530 L2531 P2532 S2533 N2534 T2535 L2536 Y2546 S2547 P2548 K2549 I2550 L2555 L2563 E2564 M2565 T2566 S2567 M2568 S2569 P2570 D2571 Y2572 P2573
N2574 P2575 M2576 F2577 F2580 LEU SER GLU CYS GLU PHE GLN GLU TYR THR ILE ASP SER ASP TRP ARG PHE ARG SER THR VAL LEU THR PRO MET PHE VAL GLU THR GLN ALA SER GLN GLY THR LEU GLN THR ARG THR GLN GLU GLY SER LEU SER ALA ARG TRP PRO VAL ALA GLY GLN
ILE ARG ALA THR GLN GLN GLN HIS ASP PHE THR LEU THR GLN THR ALA ASP GLY ARG SER SER PHE ASP TRP LEU THR GLY SER SER THR ASP PRO LEU VAL ASP HIS THR SER PRO SER SER ASP SER LEU LEU PHE ALA HIS LYS ARG SER GLU ARG LEU GLN ARG ALA PRO LEU LYS
SER VAL GLY PRO ASP PHE GLY LYS LYS ARG LEU GLY LEU PRO GLY ASP GLU VAL ASP ASN LYS VAL LYS GLY ALA ALA GLY ASP LEU ARG ASP GLN GLU LYS LEU SER LEU MET TYR ALA ARG LYS GLY VAL ALA GLU GLN LYS ARG GLU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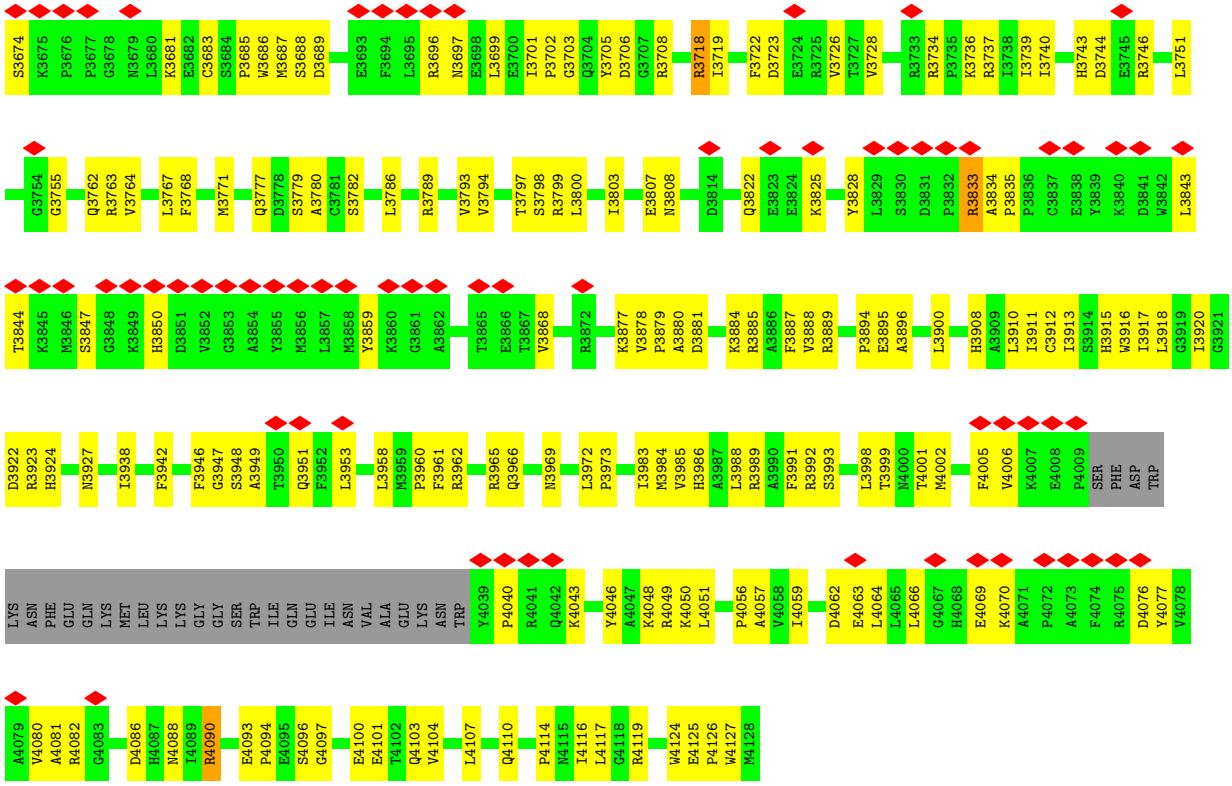
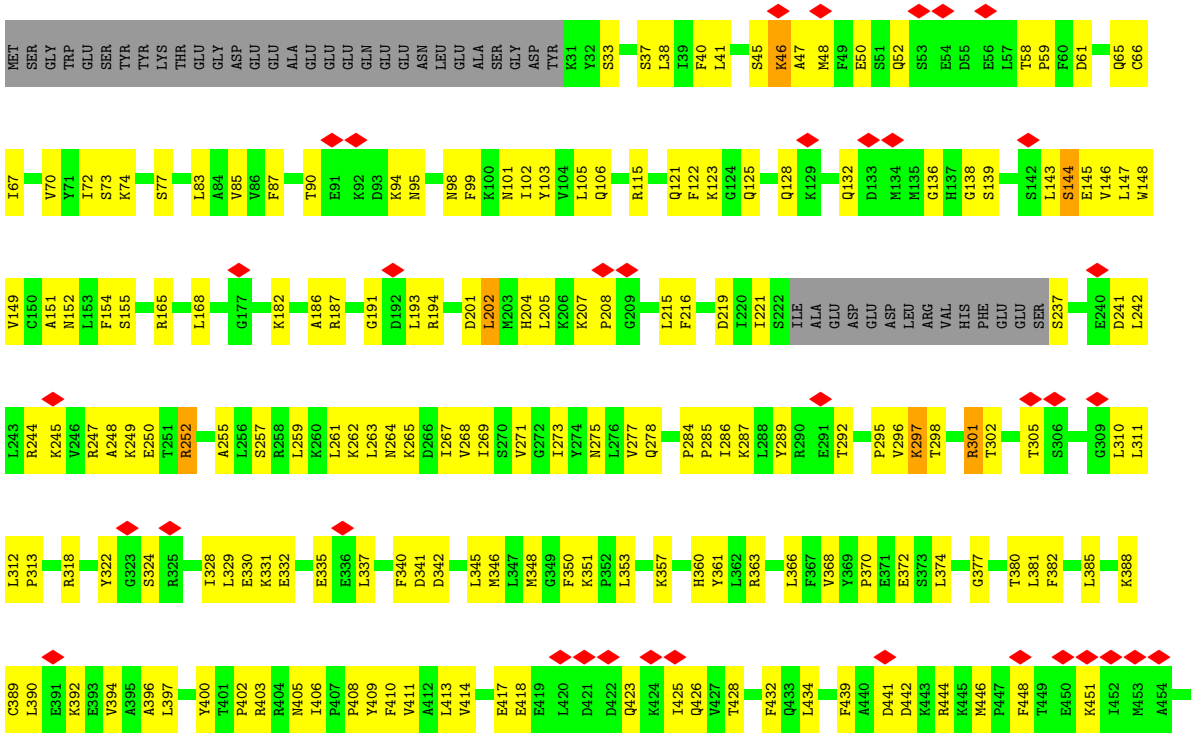
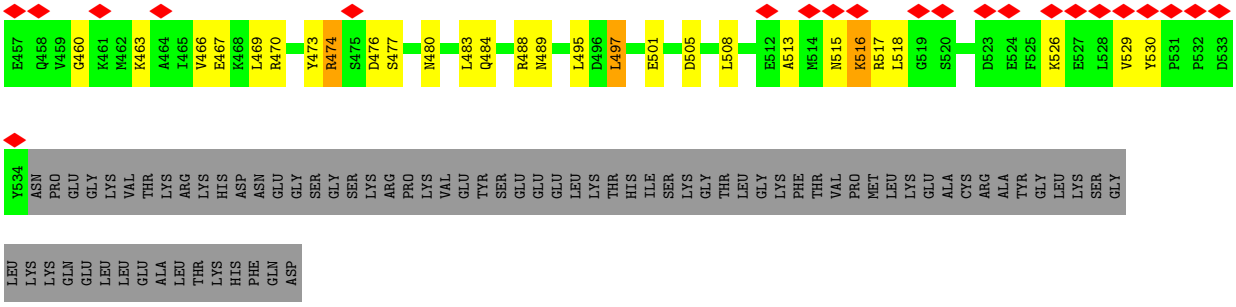
F2840 N2841 L2844 N2845 T2846 F2851 P2852 P2853 F2854 C2857 I2858 Q2859 D2860 I2861 Q2864 L2868 L2871 D2872 A2875 V2876 G2879 C2880 S2883 L2884 Q2885 Q2886 P2887 V2888 L2898 R2899 LEU LEU PRO ALA GLU LEU PRO ALA LYS ARG VAL ARG GLY LYS ALA ARG LEU P2917
V2920 W2923 V2924 A2927 R2931 S2932 I2933 L2939 I2942 I2952 T2953 A2956 L2957 L2958 R2962 S2963 D2964 E2967 A2968 A2969 K2970 Q2971 Y2972 D2973 E2974 A2975 L2976 N2977 K2978 Q2979 D2980 W2981 V2982 E2985 P2986 T2987 E2988 A2989 E2990 K2991 D2992 F2993 W2994 D3000 N3003 H3004 L3005 A3006
E3007 W3008 K3009 S3010 L3011 E3012 Y3013 A3017 S3018 I3019 D3020 S3021 E3022 N3023 P3024 P3025 D3026 L3027 N3028 K3029 I3030 W3031 S3032 E3033 P3034 F3035 Y3036 Q3037 Y3040 L3041 P3042 Y3043 M3044 I3045 R3046 S3047 K3048 L3049 L3053 Q3054 G3055 E3056 A3057 D3058 Q3059 S3060 L3061 L3062 K3067 E3072 L3073 Q3074 I3077 L3078
E3079 Y3082 L3086 L3089 Y3090 L3091 L3092 Q3093 D3094 D3095 V3096 D3097 R3098 A3099 K3100 Y3101 Y3102 I3103 Q3104 Q3108 S3109 F3110 M3111 Q3112 N3113 S3116 I3117 D3118 V3119 L3120 L3121 H3122 Q3123 L3126 T3127 K3128 L3129 Q3130 S3131 V3132 Q3133 A3134 L3135 T3136 E3137 I3138 Q3139 E3140 F3141 I3142 S3143 F3144 I3145 S3146
K3147 Q3148 G3149 N3150 L3151 S3152 S3153 Q3154 V3155 P3156 L3157 K3158 R3159 L3160 L3161 R3167 D3170 A3171 K3172 M3173 M3176 W3179 I3182 I3183 R3186 C3187 F3188 F3189 L3190 I3193 E3194 E3195 K3196 L3197 T3198 PRO LEU PRO GLU ASP ASN SER MET ASN VAL ASP GLN ASP GLY ASP PRO SER ASP
ARG MET GLU VAL GLN GLU GLN GLU GLU D3226 I3227 S3228 S3229 L3230 I3231 R3232 S3233 C3234 K3235 F3236 S3237 M3238 K3239 M3240 K3241 M3242 T3243 D3244 R3247 K3248 Q3249 L3259 L3262 H3263 K3264 E3265 S3266 K3267 T3268 R3269 D3270 D3271 W3272 L3273 V3274 S3275 W3276 V3277 Q3278 S3279 Y3280 C3281 R3282 L3283 S3284 H3285 C3286
R3287 S3288 R3289 S3290 Q3296 V3297 L3298 T3299 V3300 L3301 K3302 S3305 L3306 L3307 D3308 E3309 N3310 N3311 V3312 S3313 S3314 Y3315 L3316 S3317 K3318 N3319 I3320 L3321 A3322 F3323 R3324 D3325 Q3326 N3327 I3328 L3329 L3330 G3331 T3332 T3333 Y3334 R3335 I3336 I3337 A3338 N3339 A3340 L3341 E3344 P3345 A3346 C3347 L3348 A3349 E3350 I3351 E3352
E3353 D3354 K3355 A3356 R3357 R3358 I3359 L3360 E3361 L3362 SER GLY SER SER SER GLU D3369 S3370 E3371 K3372 V3373 I3374 Y3378 A3381 H3384 L3385 S3386 E3387 A3388 V3389 Q3390 A3391 ALA GLU GLU GLU ALA GLN PRO PRO SER TRP SER CYS GLY PRO A3406 A3407 G3408 V3409 I3410 D3411 A3412 Y3413 M3414 T3415 L3416
A3417 D3418 F3419 C3420 D3421 Q3422 Q3423 L3424 R3425 K3426 E3427 E3428 E3429 ASN ALA SER VAL ILE ASP SER ALA GLU LEU Q3440 A3441 Y3442 P3443 A3444 L3445 V3446 V3447 E3448 K3449 K3452 A3453 L3454 K3455 A3461 R3462 F3465 P3466 R3467 L3468 L3469 Q3470 I3471 I3472 E3473 R3474 Y3475 P3476 E3477 E3478 T3479 L3480 S3481
T3484 I3487 S3488 S3489 V3490 F3495 I3496 S3497 W3498 I3499 S3500 H3501 M3502 V3503 A3504 L3505 L3506 D3507 K3508 D3509 Q3510 A3511 V3512 A3513 V3514 Q3515 E3519 E3520 I3521 T3522 P3526 I3529 V3530 Y3531 P3532 F3533 I3534 I3535 S3536 S3537 E3538 S3539 Y3540 S3541 F3542 K3543 D3544 T3545 S3546 T3547 G3548 H3549 K3550 N3551 K3552
E3553 F3554 V3555 A3556 R3557 I3558 K3559 S3560 K3561 L3562 D3563 Q3564 V3567 I3568 Q3569 D3570 F3571 I3572 N3573 A3574 L3575 D3576 Q3577 L3578 S3579 N3580 P3581 E3582 L3583 L3584 F3585 K3586 D3587 W3588 S3589 N3590 D3591 V3592 R3593 A3594 E3595 L3596 A3597 K3598 T3599 P3600 V3601 N3602 K3603 K3604 N3605 I3606 E3607 K3608 M3609 Y3610 E3611 R3612 M3613
Y3614 A3615 A3616 L3617 G3618 D3619 P3620 K3621 A3622 P3623 G3624 L3625 G3626 A3627 F3628 R3629 R3630 K3631 F3632 I3633 Q3634 T3635 F3636 G3637 K3638 E3639 F3640 D3641 K3642 H3643 F3644 G3645 K3646 G3647 G3648 S3649 K3650 L3651 L3652 R3653 M3654 K3655 L3656 S3657 D3658 F3659 N3660 D3661 I3662 T3663 N3664 M3665 L3666 L3667 L3668 K3669 M3670 N3671 K3672 D3673



• Molecule 2: X-ray repair cross-complementing protein 6

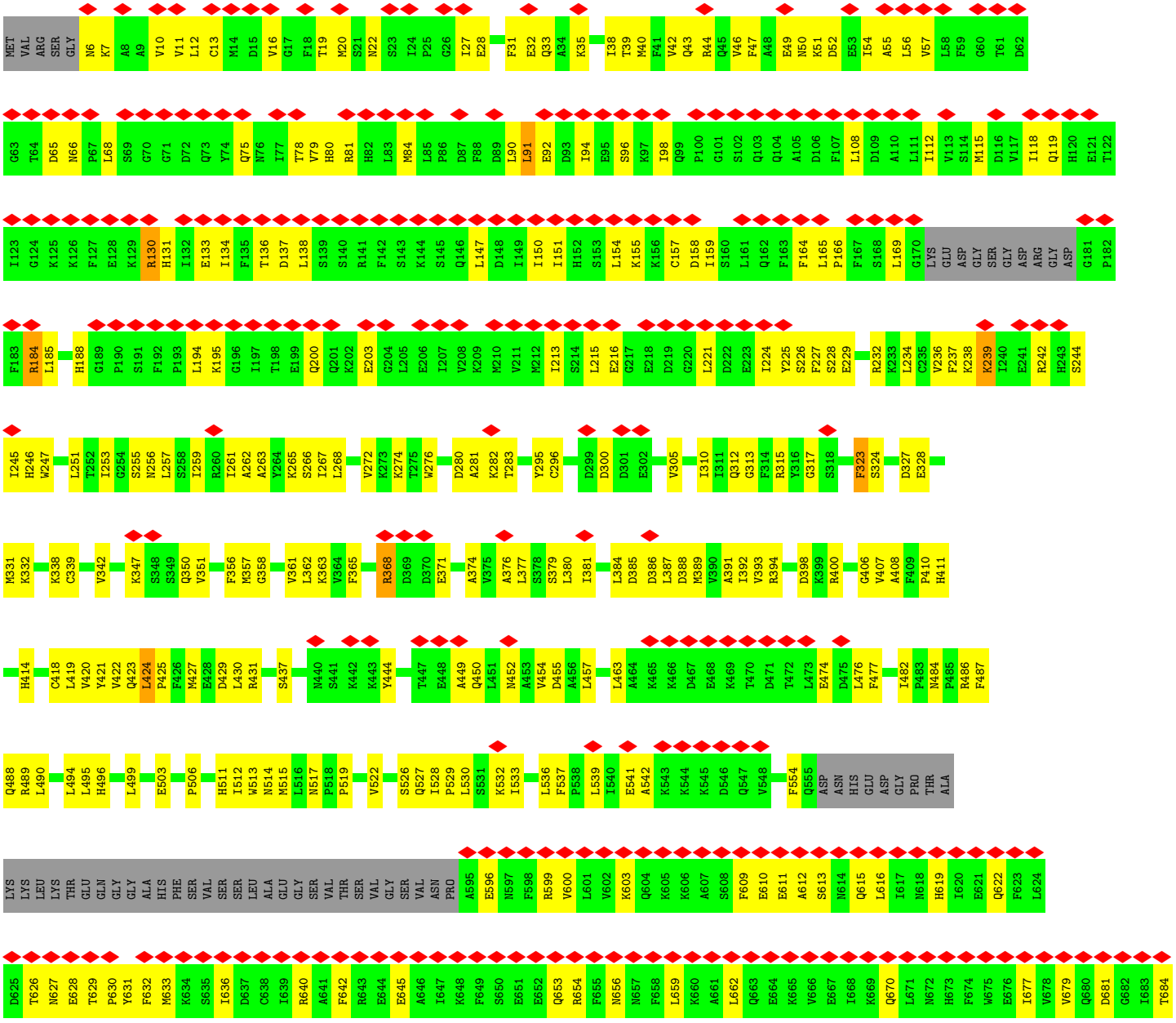
Chain B:

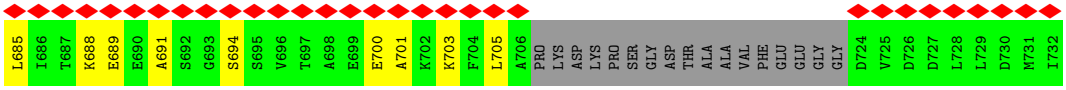




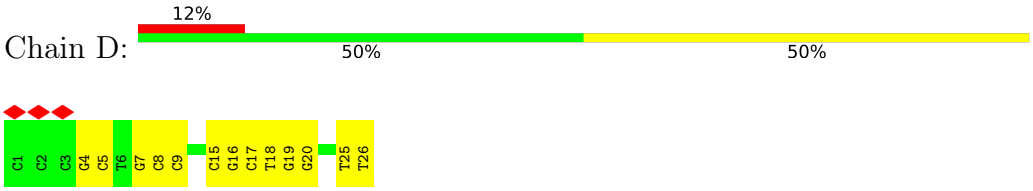
• Molecule 3: X-ray repair cross-complementing protein 5

Chain C:

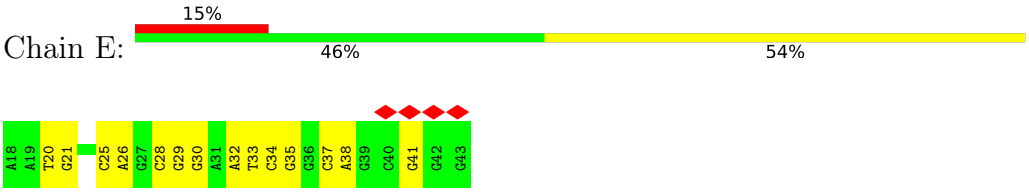




• Molecule 4: DNA (26-MER)



• Molecule 5: DNA (26-MER)



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	190498	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	47.22	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.648	Depositor
Minimum map value	-2.277	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	456.4, 456.4, 456.4	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.304, 1.304, 1.304	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1IX

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	0.30	0/29016	0.53	1/39251 (0.0%)
2	B	0.32	0/4014	0.60	3/5408 (0.1%)
3	C	0.27	0/5374	0.50	2/7246 (0.0%)
4	D	0.56	0/587	0.91	0/902
5	E	0.56	0/607	0.86	0/936
All	All	0.31	0/39598	0.55	6/53743 (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
2	B	0	2
All	All	0	6

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	424	LEU	CA-CB-CG	5.78	128.60	115.30
2	B	385	LEU	CA-CB-CG	5.65	128.29	115.30
1	A	204	LEU	CA-CB-CG	5.60	128.17	115.30
2	B	497	LEU	CA-CB-CG	5.34	127.57	115.30
2	B	202	LEU	CA-CB-CG	5.18	127.22	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1020	PRO	Peptide
1	A	1175	HIS	Peptide
1	A	3025	PRO	Peptide
1	A	3462	ARG	Peptide
2	B	252	ARG	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	28443	0	28622	1176	0
2	B	3937	0	4013	194	0
3	C	5274	0	5275	252	0
4	D	526	0	293	12	0
5	E	540	0	291	14	0
6	A	34	0	0	0	0
All	All	38754	0	38494	1577	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 20.

The worst 5 of 1577 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)
2:B:322:TYR:CE2	3:C:274:LYS:HG3	1.64	1.32
3:C:323:PHE:CE1	3:C:328:GLU:HB3	1.82	1.13
2:B:322:TYR:HE2	3:C:274:LYS:CG	1.68	1.05
1:A:2225:HIS:ND1	1:A:2226:PRO:HD2	1.72	1.04
1:A:3190:LEU:HB3	1:A:3235:LYS:HZ2	1.27	0.98

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	3555/4128 (86%)	3157 (89%)	395 (11%)	3 (0%)	51 82
2	B	486/609 (80%)	418 (86%)	67 (14%)	1 (0%)	47 78
3	C	653/732 (89%)	585 (90%)	68 (10%)	0	100 100
All	All	4694/5469 (86%)	4160 (89%)	530 (11%)	4 (0%)	54 82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2548	PRO
1	A	1021	VAL
2	B	144	SER
1	A	1020	PRO

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	3121/3671 (85%)	3099 (99%)	22 (1%)	84 91
2	B	439/548 (80%)	435 (99%)	4 (1%)	78 88
3	C	585/649 (90%)	578 (99%)	7 (1%)	71 84
All	All	4145/4868 (85%)	4112 (99%)	33 (1%)	82 90

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	239	LYS
3	C	323	PHE
3	C	670	GLN
1	A	2899	ARG
1	A	2365	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	480	ASN
3	C	488	GLN
3	C	511	HIS
3	C	452	ASN
1	A	2807	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)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	1IX	A	4201	-	37,38,38	2.25	10 (27%)	50,54,54	2.00	18 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1IX	A	4201	-	-	0/18/26/26	0/5/5/5

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	4201	1IX	C14-C16	6.37	1.56	1.49
6	A	4201	1IX	C12-C13	5.77	1.47	1.37
6	A	4201	1IX	C11-CL1	4.25	1.83	1.73
6	A	4201	1IX	C21-C20	-3.50	1.36	1.42
6	A	4201	1IX	C24-N26	3.36	1.48	1.38

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	4201	1IX	C21-C16-N17	-5.35	119.52	123.04
6	A	4201	1IX	C18-N19-C20	4.50	121.60	115.40
6	A	4201	1IX	C21-C20-N19	-4.21	118.34	122.83
6	A	4201	1IX	N19-C18-N17	-4.21	122.10	128.68
6	A	4201	1IX	C15-C10-C11	3.23	120.30	117.12

There are no chirality outliers.

There are no torsion outliers.

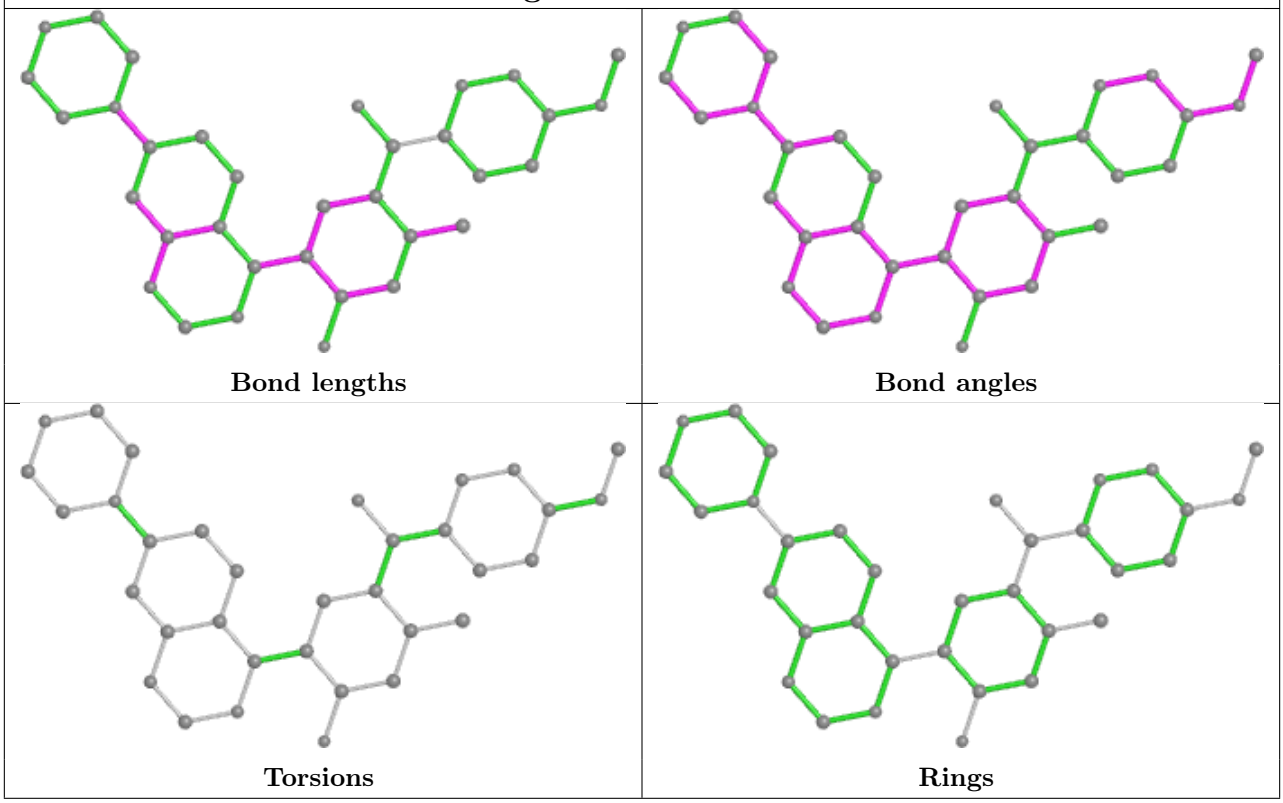
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 1IX A 4201



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.

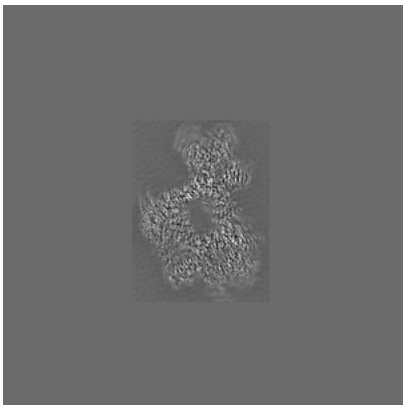
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14546. 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

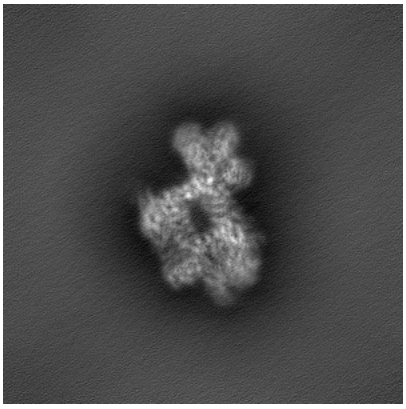


X

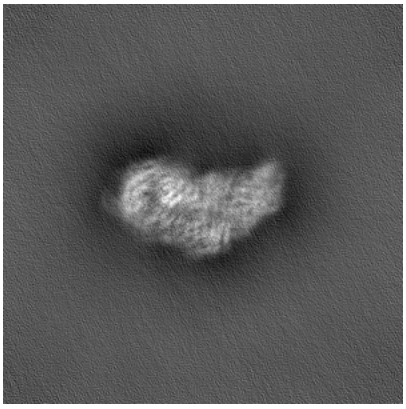
Y

Z

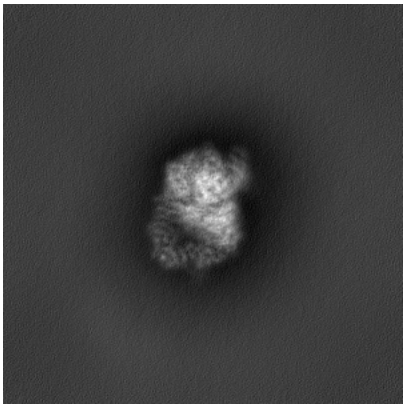
6.1.2 Raw map



X



Y

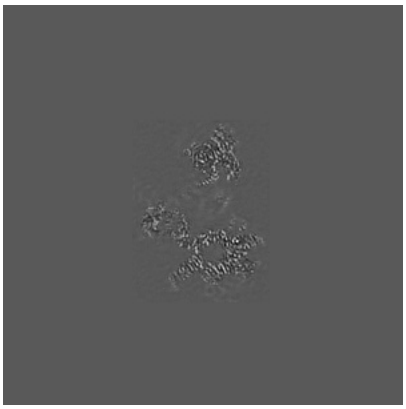


Z

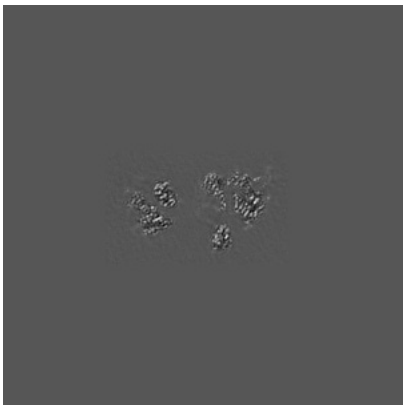
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



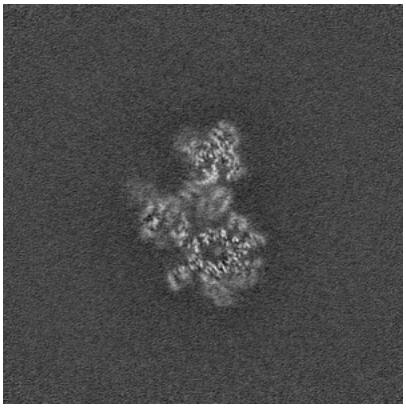
X Index: 175



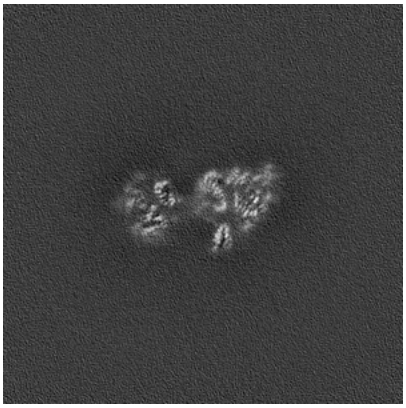
Y Index: 175

Z Index: 175

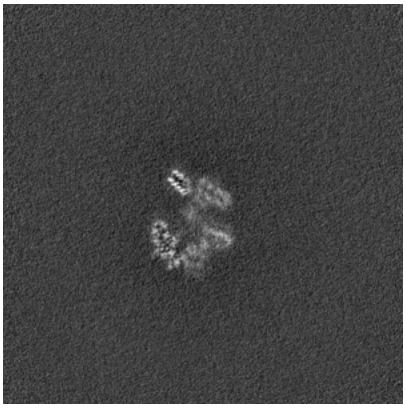
6.2.2 Raw map



X Index: 175



Y Index: 175



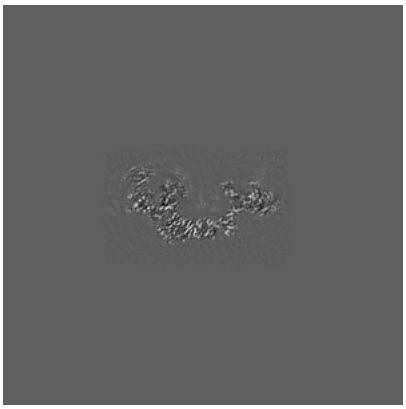
Z Index: 175

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

6.3 Largest variance slices (i)

6.3.1 Primary map

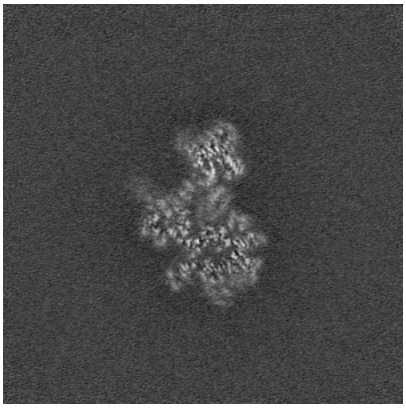
X Index: 182



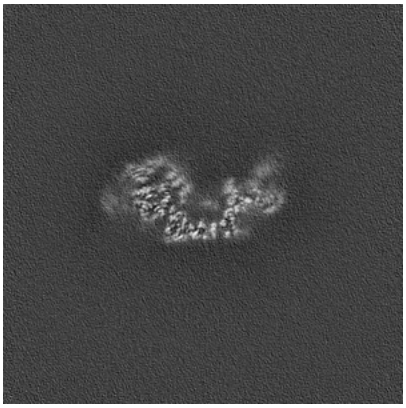
Y Index: 194

Z Index: 143

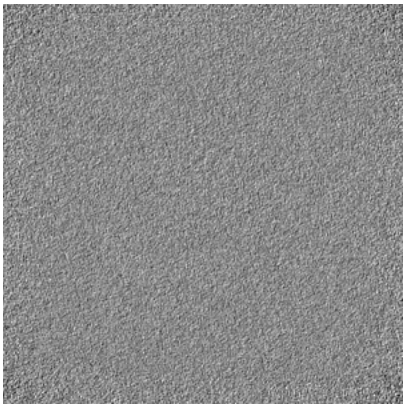
6.3.2 Raw map



X Index: 177



Y Index: 197



Z Index: 0

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 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

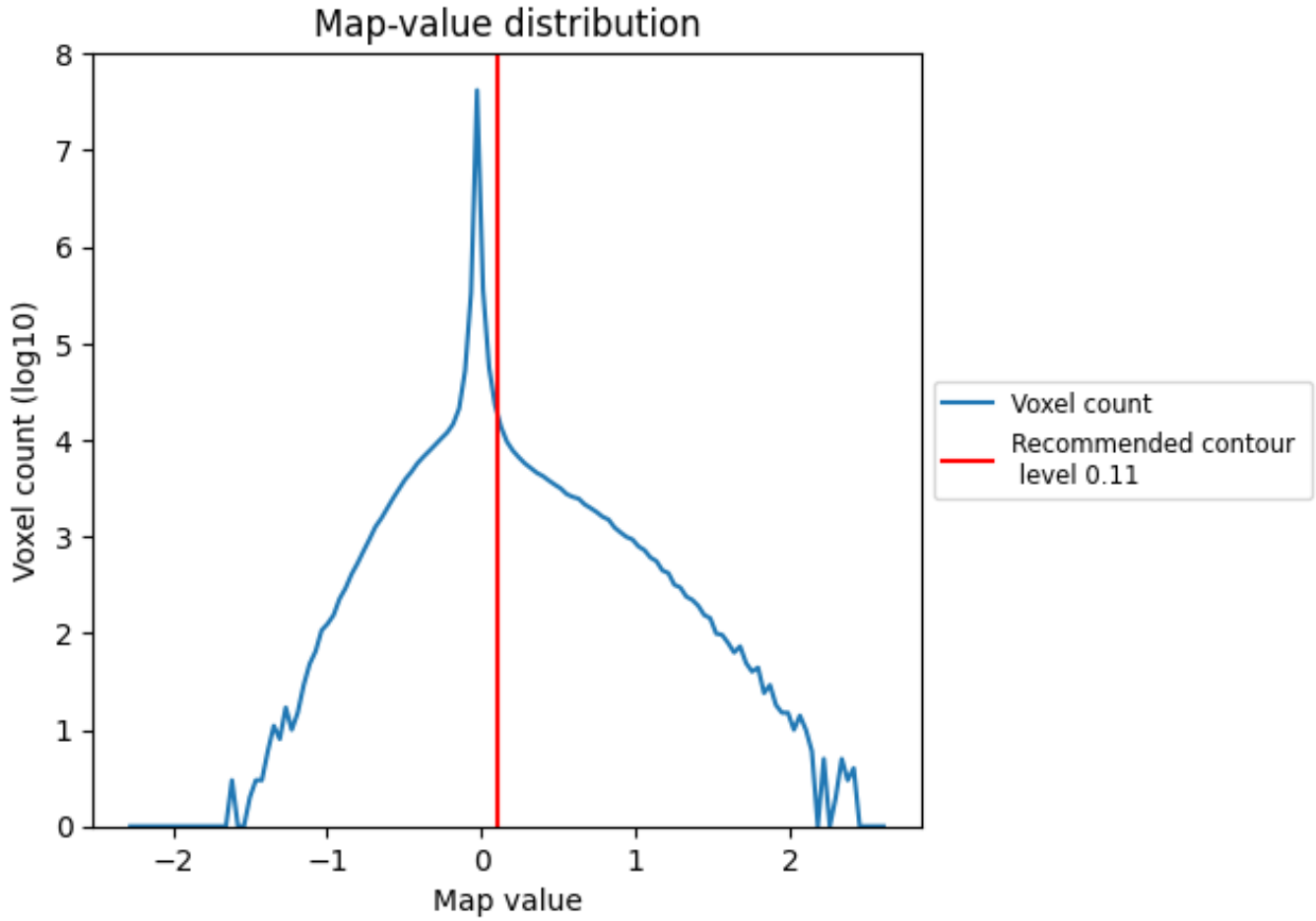
6.5 Mask visualisation (i)

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

7 Map analysis

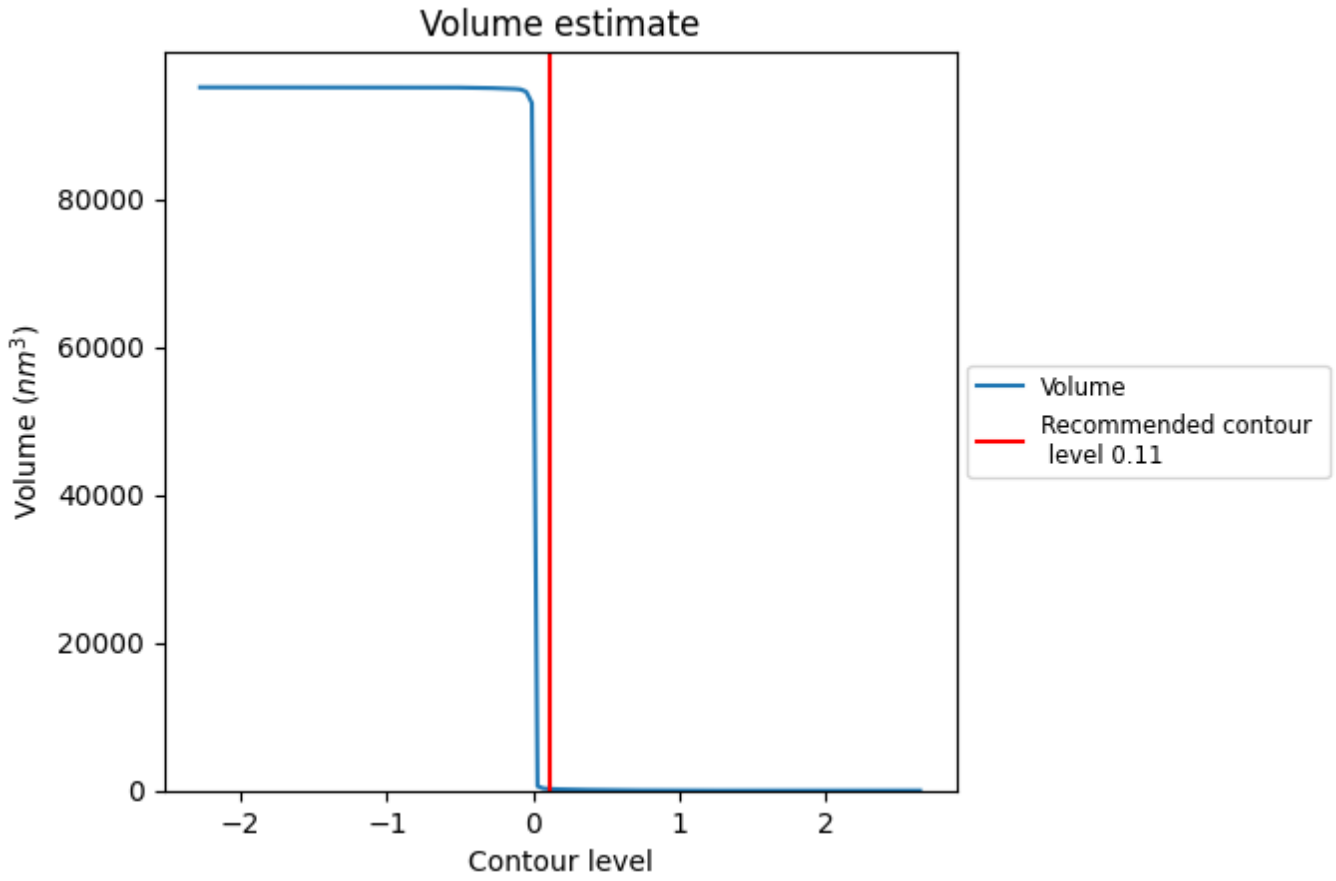
This section contains the results of statistical analysis of the map.

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.

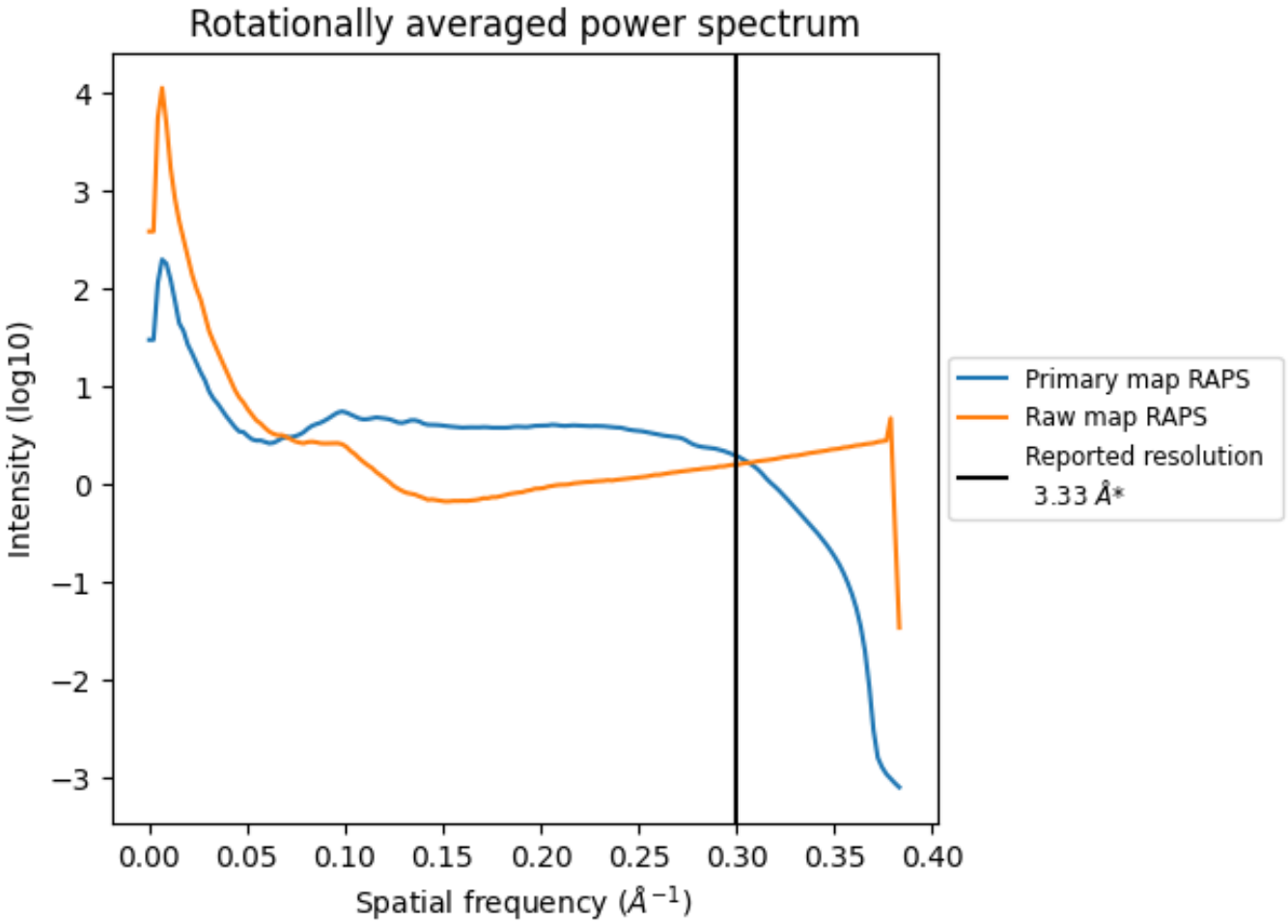
7.2 Volume estimate (i)



The volume at the recommended contour level is 229 nm^3; this corresponds to an approximate mass of 207 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)

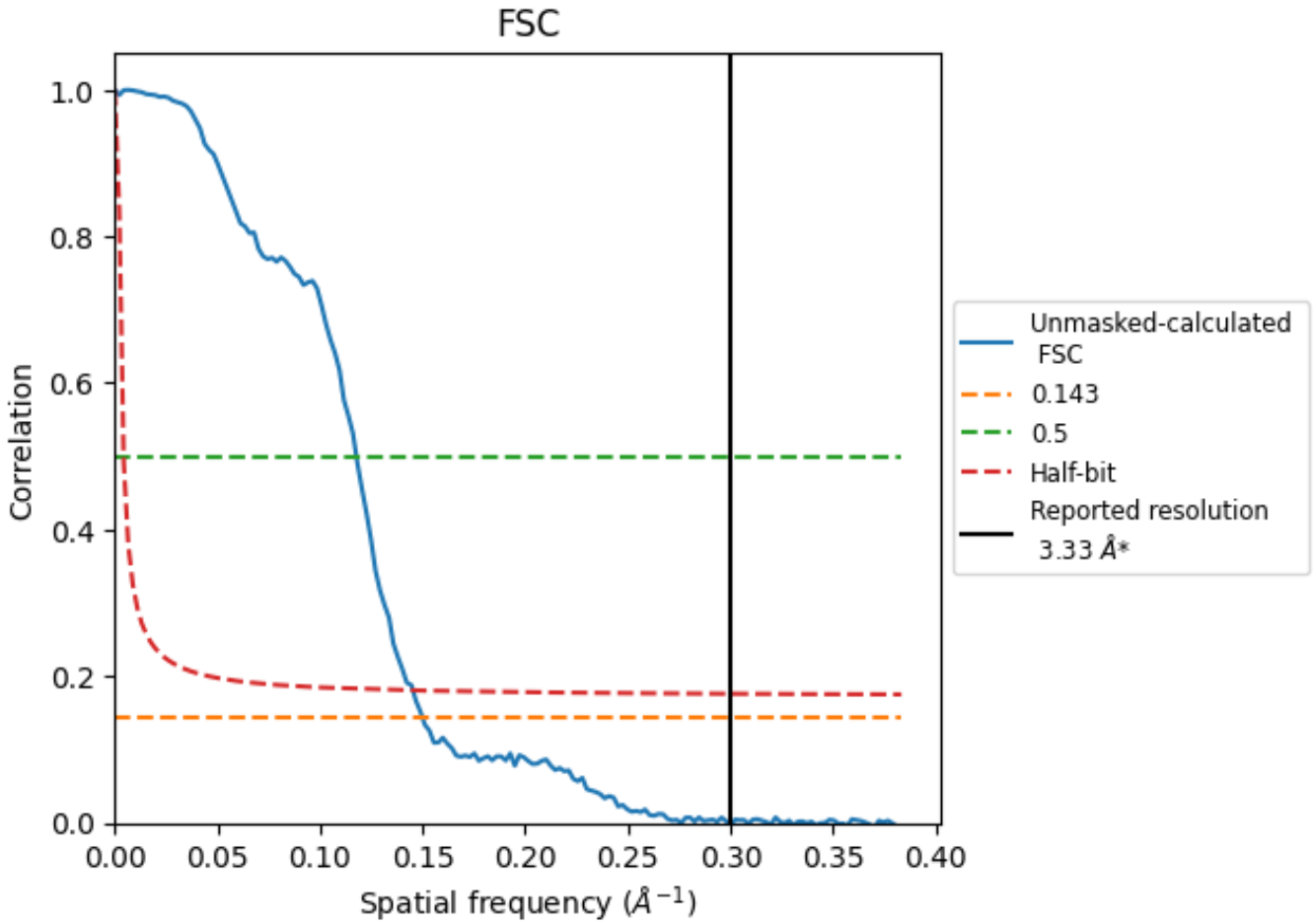


*Reported resolution corresponds to spatial frequency of 0.300 Å^{-1}

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 0.300 Å^{-1}

8.2 Resolution estimates (i)

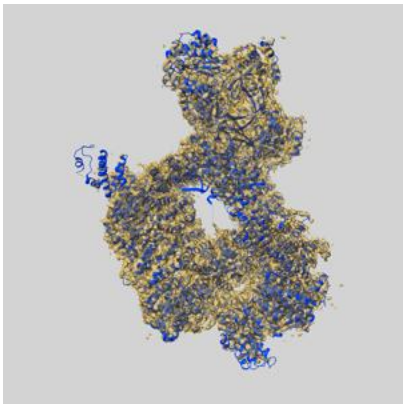
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.33	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.67	8.49	6.88

*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 6.67 differs from the reported value 3.33 by more than 10 %

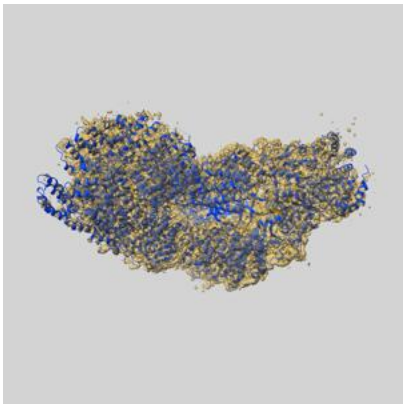
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14546 and PDB model 7Z88. Per-residue inclusion information can be found in section 3 on page 5.

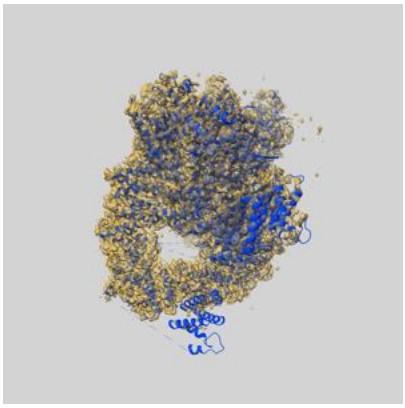
9.1 Map-model overlay



X



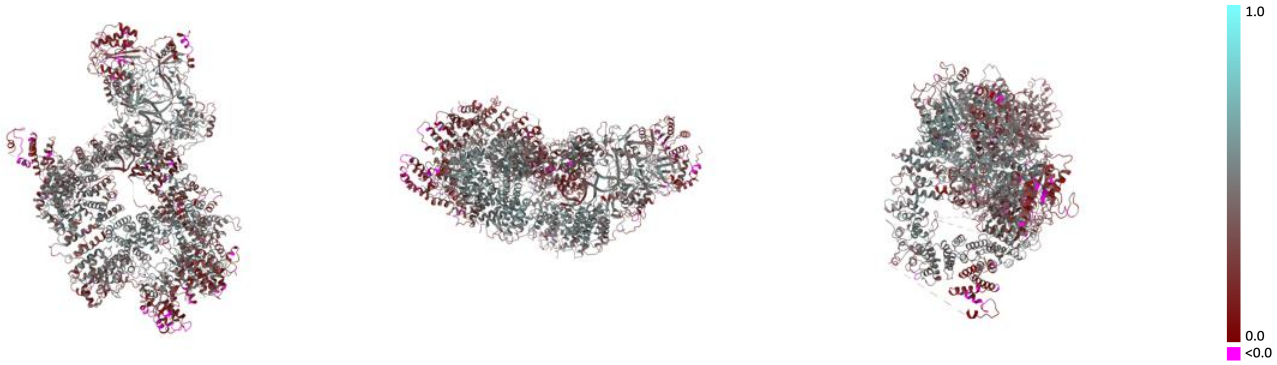
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.11 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.

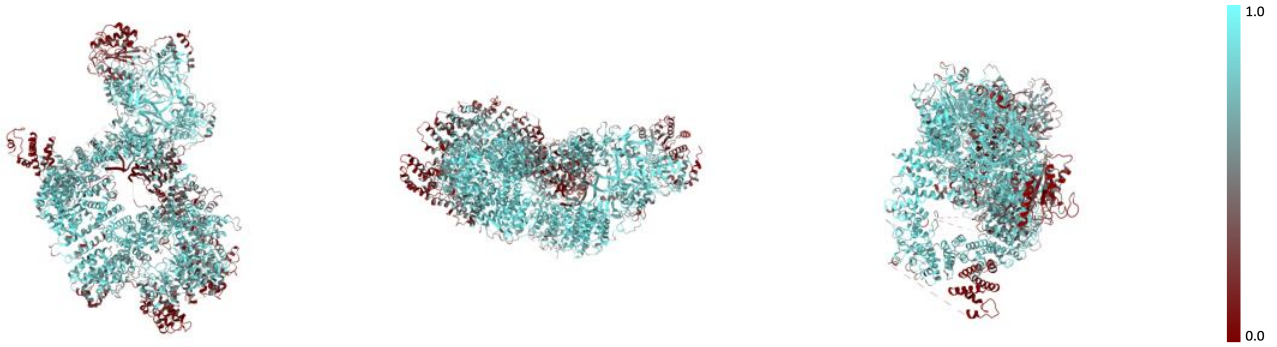
9.2 Q-score mapped to coordinate model (i)



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.

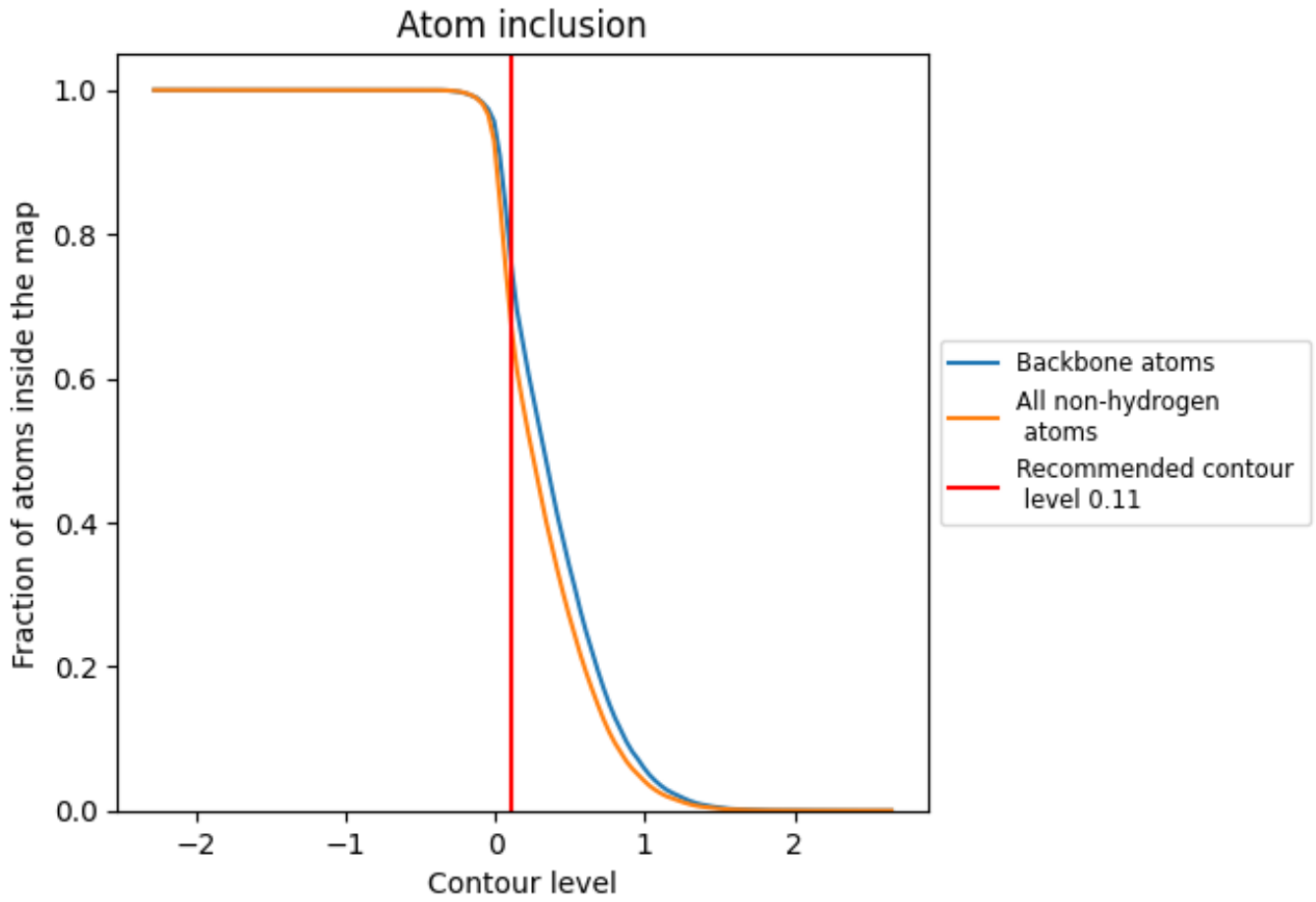
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.11).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 67% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6701	0.3890
A	0.6996	0.4010
B	0.7341	0.4110
C	0.4538	0.3040
D	0.7452	0.4420
E	0.6944	0.3990