# wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 06:25 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 5OEJ |
| EMDB ID | : | EMD-3790 |
| Title | : | Structure of Tra1 subunit within the chromatin modifying complex SAGA |
| Authors | : | Sharov, G.; Voltz, K.; Durand, A.; Kolesnikova, O.; Papai, G.; Myasnikov, A.G.; Dejaegere, A.; Ben-Shem, A.; Schultz, P. |
| Deposited on | : | 2017-07-07 |
| Resolution | : | 5.70 Å(reported) |
| Based on initial model | : | 4JSN |

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:

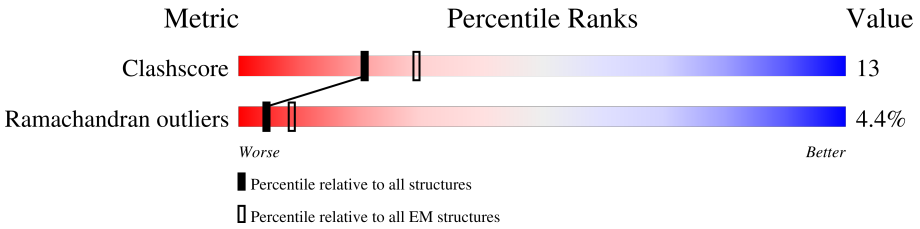
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | 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 5.70 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 |

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 | B | 3825 | 19% 60% 14% 26% |

# 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 14023 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 Tra1 subunit within the chromatin modifying complex SAGA.

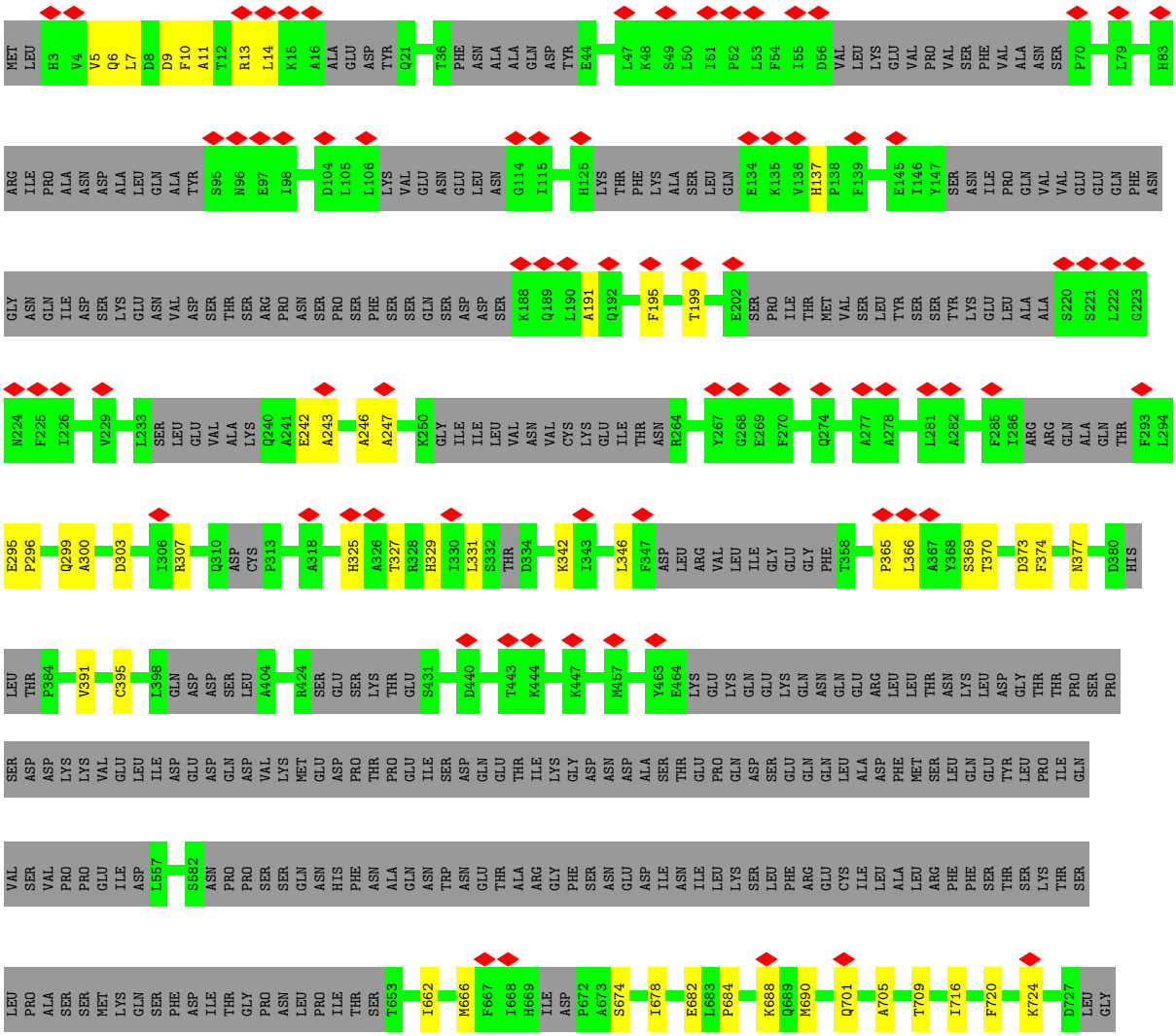
| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 1 | B | 2825 | 14023 | 8373 | 2825 | 2825 | 0 | 0 |

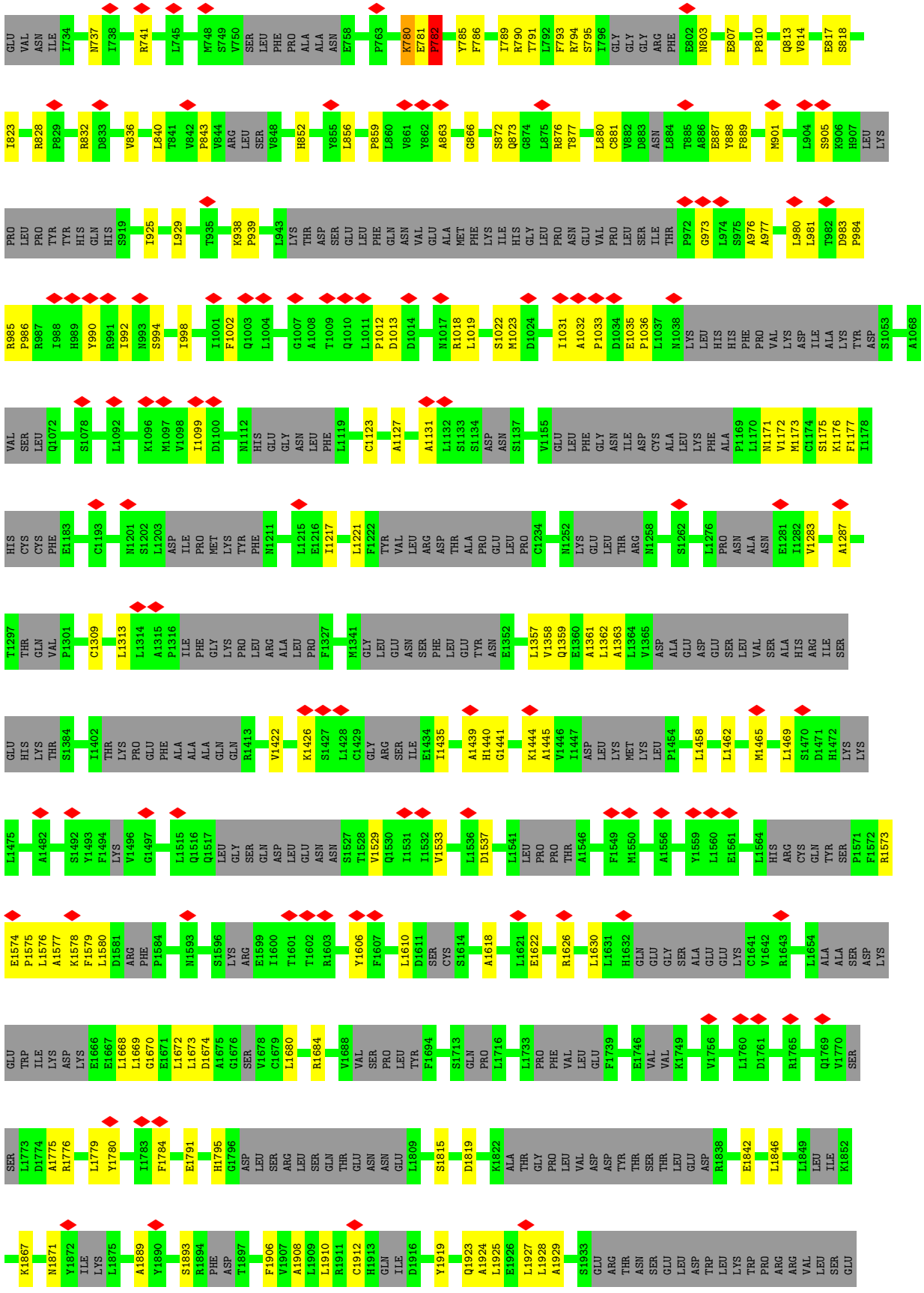
# 3 Residue-property plots (i)

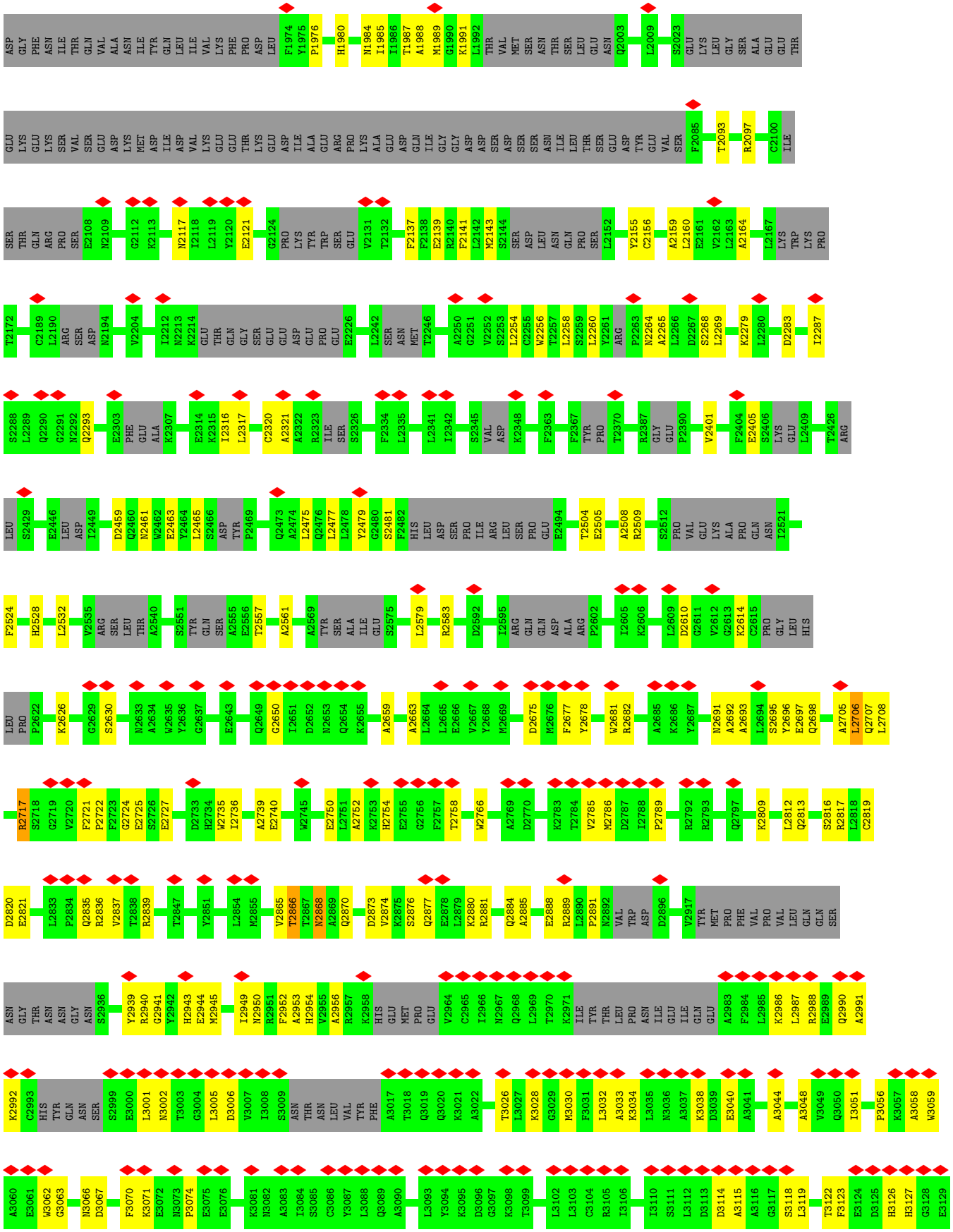
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

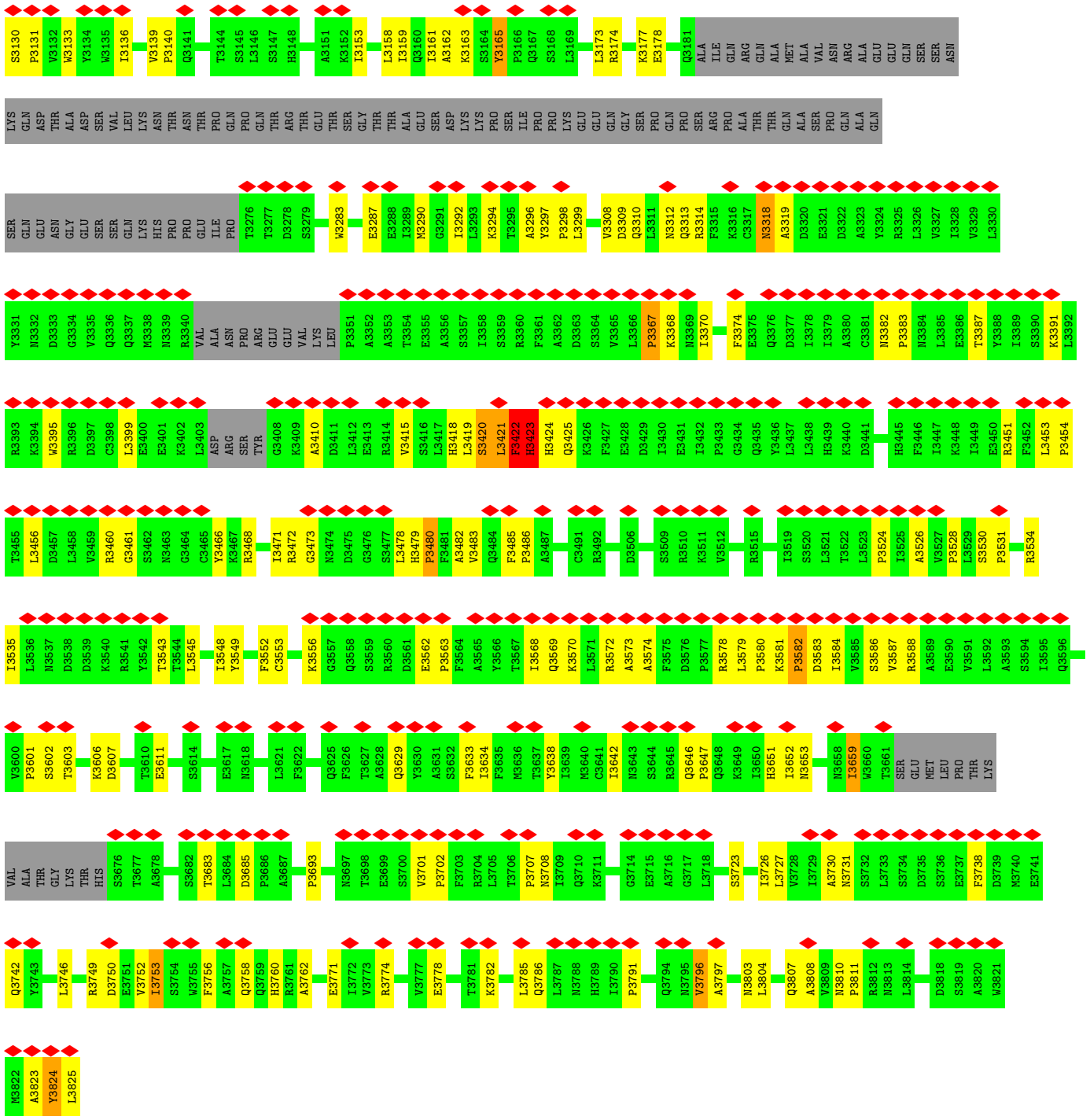
- Molecule 1: Tra1 subunit within the chromatin modifying complex SAGA

Chain B:




GLU VAL ASN ILE I734 N737 I738 R741 L745 M748 S749 V750 SER LEU PHE PRO ALA ALA ASN E758 P763 K780 E781 P782 Y785 F786 I789 R790 T791 L792 F793 R794 S795 I796 GLY GLY GLY ARG PHE E802 N803 E807 P810 Q813 V814 E817 S818
I823 R828 P829 R832 D833 V836 L840 T841 V842 P843 V844 ARG LEU SER V848 H852 Y855 L856 P859 L860 V861 Y862 A863 G866 S872 Q873 G874 L875 R876 T877 L880 C881 V882 D883 ASN L884 T885 A886 E887 Y888 F889 M901 L904 S905 K906 H907 LEU LYS
PRO LEU PRO TYR TYR HIS GLN HIS S919 I925 L929 T935 K938 P939 L943 LYS THR ASP SER GLU LEU PHE GLN ASN VAL GLU ALA MET PHE LYS ILE HIS GLY LEU PRO ASN GLU VAL PRO LEU SER ILE THR P972 G973 L974 S975 A976 A977 L980 L981 T982 D983 P984
R985 P986 R987 I988 H989 Y990 R991 I992 N993 S994 I998 I1001 F1002 Q1003 L1004 G1007 A1008 T1009 Q1010 L1011 P1012 D1013 D1014 N1017 R1018 L1019 S1022 M1023 D1024 I1031 A1032 P1033 D1034 E1035 P1036 L1037 N1038 LYS LEU HIS HIS PHE PRO VAL LYS ASP ILE ALA LYS TYR ASP S1053 A1068
VAL SER LEU Q1072 S1078 L1092 K1096 M1097 V1098 I1099 D1100 N1112 HIS GLU GLY ASN LEU PHE L1119 C1123 A1127 A1131 L1132 S1133 S1134 ASP ASN S1137 V1155 GLU LEU PHE GLY ASN ILE ASP CYS ALA LEU LYS PHE ALA P1169 L1170 N1171 V1172 M1173 C1174 S1175 K1176 F1177 I1178
HIS CYS CYS PHE E1183 C1193 N1201 S1202 L1203 ASP ILE PRO MET LYS TYR PHE N1211 L1215 E1216 I1217 L1221 F1222 TYR VAL LEU ARG ASP THR ALA PRO GLU LEU PRO C1234 N1252 LYS GLU LEU THR ARG N1258 S1262 L1276 PRO ASN ALA ASN E1281 I1282 V1283 A1287
T1297 THR GLN VAL P1301 C1309 L1313 L1314 A1315 P1316 ILE PHE GLY LYS PRO LEU ARG ALA LEU PRO F1327 M1341 GLY LEU GLU ASN SER PHE LEU GLU TYR ASN E1352 L1357 V1358 Q1359 E1360 A1361 L1362 A1363 L1364 V1365 ASP ALA GLU ASP GLU SER LEU VAL SER ALA HIS ARG ILE SER
GLU HIS LYS THR S1384 I1402 THR LYS PRO GLU PHE ALA ALA ALA GLN GLN R1413 V1422 K1426 S1427 L1428 C1429 GLY ARG SER ILE E1434 I1435 A1439 H1440 G1441 K1444 A1445 V1446 I1447 ASP LEU LYS MET LYS LEU P1454 L1458 L1462 M1465 L1469 S1470 D1471 H1472 LYS LYS
L1475 A1482 S1492 Y1493 F1494 LYS V1496 G1497 L1515 Q1516 Q1517 LEU GLY GLY SER GLN ASP LEU GLU ASN ASN S1527 T1528 V1529 Q1530 I1531 I1532 V1533 L1536 D1537 L1541 LEU PRO PRO THR A1546 F1549 M1550 A1556 Y1559 L1560 E1561 L1564 HIS ARG CYS GLN TYR SER P1571 F1572 R1573
E1574 P1575 L1576 A1577 K1578 F1579 L1580 D1581 ARG PHE P1584 N1593 S1596 LYS ARG E1599 I1600 T1601 T1602 R1603 Y1606 F1607 L1610 D1611 SER CYS S1614 A1618 L1621 E1622 R1626 L1630 L1631 H1632 GLN GLU GLY SER ALA GLU GLU LYS C1641 V1642 R1643 L1654 ALA ALA SER ASP LYS
GLU TRP ILE LYS ASP LYS E1666 E1667 L1668 L1669 G1670 E1671 L1672 L1673 D1674 A1675 G1676 SER V1678 C1679 L1680 R1684 V1688 VAL SER PRO LEU TYR F1694 S1713 GLN PRO L1716 L1733 PRO PHE VAL LEU GLU F1739 E1746 VAL VAL K1749 V1756 L1760 D1761 R1765 Q1769 V1770 SER
SER L1773 D1774 A1775 R1776 L1779 Y1780 I1783 F1784 E1791 H1795 G1796 ASP LEU SER ARG LEU SER GLN THR GLU ASN ASN GLU L1809 S1815 D1819 K1822 ALA THR GLY PRO LEU VAL ASP ASP TYR THR SER THR LEU GLU ASP R1838 E1842 L1846 L1849 LEU ILE K1852
K1867 N1871 Y1872 ILE LYS L1875 A1889 Y1890 S1893 R1894 PHE ASP T1897 F1906 V1907 A1908 L1909 L1910 R1911 C1912 H1913 GLN ILE D1916 Y1919 Q1923 A1924 L1925 E1926 L1927 L1928 A1929 S1933 GLU ARG THR ASN SER GLU LEU ASP TRP LEU LYS TRP PRO ARG ARG VAL LEU SER GLU


ASP GLY PHE ASN ILE THR GLN VAL ALA ASN ILE TYR GLN LEU ILE VAL LYS PHE PRO ASP LEU F1974 Y1975 P1976 H1980 N1984 I1985 I1986 T1987 A1988 M1989 G1990 K1991 L1992 THR VAL MET SER ASN THR SER LEU GLU ASN Q2003 L2009 S2023 GLU LYS LEU GLY SER ALA GLU GLU THR
GLU LYS GLU LYS SER VAL SER GLU ASP LYS MET ASP ILE ASP VAL LYS GLU GLU THR LYS GLU ASP ILE ALA GLU ARG PRO LYS ALA GLU ASP GLN ILE GLY GLY ASP ASP SER ASP SER SER ASN ILE LEU THR SER GLU ASP TYR GLU VAL SER F2085 T2093 R2097 C2100 ILE
SER THR GLN ARG PRO SER E2108 N2109 G2112 K2113 N2117 I2118 L2119 Y2120 E2121 G2124 PRO LYS TYR TRP SER GLU V2131 T2132 F2137 F2138 E2139 R2140 F2141 L2142 M2143 S2144 SER ASP LEU ASN GLN PRO SER L2152 Y2155 C2156 A2159 L2160 E2161 V2162 L2163 A2164 L2167 LYS TRP LYS PRO
T2172 C2189 L2190 ARG SER ASP N2194 V2204 I2212 N2213 K2214 GLU THR GLN GLY SER GLU GLU ASP GLU PRO GLU E2226 L2242 SER ASN MET T2246 A2250 G2251 V2252 S2253 L2254 C2255 W2256 T2257 L2258 S2259 L2260 Y2261 ARG P2263 N2264 A2265 L2266 D2267 S2268 L2269 K2279 L2280 D2283 I2287
S2288 L2289 Q2290 G2291 N2292 Q2293 E2303 PHE GLU ALA K2307 E2314 K2315 I2316 L2317 C2320 A2321 A2322 R2323 ILE SER S2326 F2334 L2335 L2341 I2342 S2345 VAL ASP K2348 F2363 F2367 TYR PRO T2370 R2387 GLY GLU P2390 V2401 F2404 E2405 S2406 LYS GLU L2409 T2426 ARG
LEU S2429 E2446 LEU ASP I2449 D2459 Q2460 N2461 W2462 E2463 Y2464 L2465 S2466 ASP TYR P2469 Q2473 A2474 L2475 Q2476 L2477 L2478 Y2479 G2480 S2481 F2482 HIS LEU ASP SER PRO ILE ARG LEU SER PRO GLU E2494 T2504 E2505 A2508 R2509 S2512 PRO VAL GLU LYS ALA PRO GLN ASN I2521
F2524 H2528 L2532 V2535 ARG SER LEU THR A2540 S2551 TYR GLN SER A2555 E2556 T2557 A2561 A2569 TYR SER ALA ILE GLU S2575 L2579 R2583 D2592 I2595 ARG GLN GLN ASP ALA ARG P2602 I2605 K2606 L2609 D2610 G2611 V2612 G2613 K2614 G2615 PRO GLY LEU HIS
LEU PRO P2622 K2626 G2629 S2630 N2633 A2634 W2635 Y2636 G2637 E2643 Q2649 G2650 T2651 D2652 N2653 Q2654 K2655 A2659 A2663 L2664 L2665 E2666 V2667 Y2668 M2669 D2675 W2676 F2677 Y2678 W2681 R2682 A2685 K2686 Y2687 N2691 A2692 A2693 L2694 S2695 Y2696 E2697 Q2698 A2705 L2706 Q2707 L2708
R2717 S2718 G2719 V2720 F2721 P2722 F2723 G2724 E2725 S2726 E2727 D2733 H2734 W2735 I2736 A2739 E2740 W2745 E2750 L2751 A2752 K2753 H2754 E2755 G2756 F2757 T2758 W2766 A2769 D2770 K2783 T2784 V2785 M2786 D2787 I2788 P2789 R2792 R2793 Q2797 K2809 L2812 Q2813 S2816 R2817 L2818 C2819
D2820 E2821 L2833 P2834 Q2835 R2836 V2837 T2838 R2839 T2847 Y2851 L2854 M2855 V2865 T2866 T2867 N2868 A2869 Q2870 D2873 V2874 K2875 S2876 Q2877 E2878 L2879 K2880 R2881 Q2884 A2885 E2888 R2889 L2890 P2891 N2892 VAL TRP ASP D2896 V2917 TYR MET PRO PHE VAL PRO VAL LEU GLN GLN SER
ASN GLY THR ASN ASN GLY ASN S2936 Y2939 R2940 G2941 Y2942 H2943 E2944 M2945 I2949 N2950 R2951 F2952 A2953 H2954 V2955 A2956 R2957 K2958 HIS GLU MET PRO GLU V2964 C2965 I2966 N2967 Q2968 L2969 T2970 K2971 ILE TYR THR LEU PRO ASN ILE GLU ILE GLN GLU A2983 F2984 L2985 K2986 L2987 R2988 E2989 Q2990 A2991
K2992 C2993 HIS TYR GLN ASN SER S2999 E3000 L3001 N3002 T3003 G3004 L3005 D3006 V3007 I3008 S3009 ASN THR ASN LEU VAL TYR PHE A3017 T3018 Q3019 Q3020 K3021 A3022 T3026 L3027 K3028 G3029 M3030 F3031 L3032 A3033 K3034 L3035 N3036 A3037 K3038 D3039 E3040 A3041 A3044 A3048 V3049 Q3050 I3051 P3056 K3057 A3058 W3059
A3060 E3061 W3062 G3063 N3066 D3067 F3070 K3071 E3072 N3073 P3074 E3075 E3076 K3081 N3082 A3083 I3084 S3085 C3086 Y3087 L3088 Q3089 A3090 L3093 Y3094 K3095 D3096 G3097 K3098 T3099 L3102 L3103 C3104 R3105 I3106 I3110 S3111 L3112 D3113 D3114 A3115 A3116 G3117 S3118 L3119 T3122 F3123 E3124 D3125 H3126 H3127 G3128 E3129


S3130 P3131 V3132 W3133 Y3134 W3135 I3136 V3139 P3140 Q3141 T3144 S3145 L3146 S3147 H3148 A3151 K3152 I3153 L3158 I3159 Q3160 I3161 A3162 K3163 S3164 Y3165 P3166 Q3167 S3168 L3169 L3173 R3174 K3177 E3178 Q3181
ALA ILE GLN ARG GLN ALA MET ALA VAL ASN ARG ALA GLU GLU GLN SER SER ASN
LYS GLN ASP THR ALA ASP SER VAL LEU LYS ASN THR ASN THR PRO GLN PRO GLN THR ARG THR GLU THR SER GLY THR THR ALA GLU SER ASP LYS LYS PRO SER ILE PRO PRO LYS GLU GLU GLN GLY SER PRO GLN PRO SER ARG PRO ALA THR THR GLN ALA SER PRO GLN ALA GLN
SER GLN GLU ASN GLY GLU SER SER GLN LYS HIS PRO PRO GLU ILE PRO T3276 T3277 D3278 S3279 W3283 E3287 E3288 I3289 M3290 G3291 I3292 L3293 K3294 T3295 A3296 Y3297 P3298 L3299 V3308 D3309 Q3310 L3311 N3312 Q3313 R3314 F3315 K3316 C3317 N3318 A3319 D3320 E3321 D3322 A3323 Y3324 R3325 L3326 V3327 I3328 V3329 L3330
Y3331 N3332 D3333 G3334 V3335 Q3336 Q3337 M3338 N3339 R3340 VAL ALA ASN PRO ARG GLU GLU VAL LYS LEU P3351 A3352 A3353 T3354 E3355 A3356 S3357 I3358 S3359 R3360 F3361 A3362 D3363 S3364 V3365 L3366 P3367 K3368 N3369 I3370 F3374 E3375 Q3376 D3377 I3378 I3379 A3380 C3381 N3382 P3383 N3384 L3385 E3386 T3387 Y3388 S3390 K3391 L3392
R3393 K3394 W3395 R3396 D3397 C3398 L3399 E3400 E3401 K3402 L3403 ASP ARG SER TYR G3408 K3409 A3410 D3411 L3412 E3413 R3414 V3415 S3416 L3417 H3418 L3419 S3420 L3421 F3422 H3423 H3424 Q3425 K3426 F3427 E3428 D3429 I3430 E3431 I3432 P3433 G3434 Q3435 Y3436 L3437 L3438 H3439 K3440 D3441 H3445 F3446 I3447 K3448 I3449 E3450 R3451 F3452 L3453 P3454
T3455 L3456 D3457 L3458 V3459 R3460 G3461 S3462 N3463 G3464 C3465 Y3466 K3467 R3468 I3471 R3472 G3473 N3474 D3475 G3476 S3477 L3478 H3479 P3480 F3481 A3482 V3483 Q3484 F3485 P3486 A3487 C3491 R3492 D3506 S3509 R3510 K3511 V3512 R3515 I3519 S3520 L3521 T3522 L3523 P3524 I3525 A3526 V3527 P3528 L3529 S3530 P3531 R3534
I3535 L3536 N3537 D3538 D3539 K3540 R3541 Y3542 T3543 T3544 L3545 I3548 Y3549 F3552 C3553 K3556 G3557 Q3558 S3559 R3560 D3561 E3562 P3563 F3564 A3565 Y3566 T3567 I3568 Q3569 K3570 L3571 R3572 A3573 A3574 F3575 D3576 P3577 R3578 L3579 P3580 K3581 P3582 D3583 I3584 V3585 S3586 V3587 R3588 A3589 E3590 V3591 L3592 A3593 S3594 I3595 Q3596
V3600 P3601 S3602 T3603 K3606 D3607 T3610 E3611 S3614 E3617 N3618 L3621 F3622 Q3625 F3626 T3627 A3628 Q3629 Y3630 A3631 S3632 F3633 I3634 F3635 M3636 T3637 Y3638 I3639 M3640 C3641 I3642 N3643 S3644 R3645 Q3646 P3647 Q3648 K3649 I3650 H3651 I3652 N3653 N3658 I3659 W3660 T3661
SER GLU MET LEU PRO THR LYS
VAL ALA THR GLY LYS THR HIS S3676 T3677 A3678 S3682 T3683 L3684 D3685 P3686 A3687 P3693 N3697 T3698 E3699 S3700 V3701 P3702 F3703 R3704 L3705 T3706 P3707 N3708 I3709 Q3710 K3711 G3714 E3715 A3716 G3717 L3718 S3723 I3726 L3727 V3728 I3729 A3730 N3731 S3732 L3733 S3734 D3735 S3736 E3737 F3738 D3739 M3740 E3741
Q3742 Y3743 L3746 R3749 D3750 E3751 V3752 I3753 S3754 W3755 F3756 A3757 Q3758 Q3759 H3760 R3761 A3762 E3771 I3772 V3773 R3774 V3777 E3778 T3781 K3782 L3785 Q3786 L3787 N3788 H3789 I3790 P3791 Q3794 N3795 Y3796 A3797 N3803 L3804 Q3807 A3808 V3809 N3810 P3811 R3812 N3813 L3814 D3818 S3819 A3820 W3821
M3822 A3823 Y3824 L3825

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 105916 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION; Full CTF correction in Relion | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 60 | Depositor |
| Minimum defocus (nm) | 1400 | Depositor |
| Maximum defocus (nm) | 3400 | Depositor |
| Magnification | 127272 | Depositor |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |
| Maximum map value | 0.192 | Depositor |
| Minimum map value | -0.114 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.006 | Depositor |
| Recommended contour level | 0.0429 | Depositor |
| Map size (Å) | 352.0, 352.0, 352.0 | wwPDB |
| Map dimensions | 320, 320, 320 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.1, 1.1, 1.1 | 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 | B | 0.23 | 0/13920 | 0.40 | 3/19262 (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 | B | 0 | 2 |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 782 | PRO | N-CA-CB | 5.66 | 110.09 | 103.30 |
| 1 | B | 2717 | ARG | O-C-N | 5.64 | 131.73 | 122.70 |
| 1 | B | 3422 | PHE | C-N-CA | 5.40 | 135.21 | 121.70 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | B | 3421 | LEU | Peptide |
| 1 | B | 3423 | HIS | 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 | B | 14023 | 0 | 6129 | 270 | 0 |
| All | All | 14023 | 0 | 6129 | 270 | 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 13.

The worst 5 of 270 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:B:3651:HIS:O | 1:B:3659:ILE:HA | 1.02 | 1.20 |
| 1:B:3651:HIS:O | 1:B:3659:ILE:CA | 1.95 | 1.12 |
| 1:B:3420:SER:O | 1:B:3423:HIS:CA | 2.00 | 1.09 |
| 1:B:3420:SER:O | 1:B:3423:HIS:HA | 1.50 | 1.09 |
| 1:B:3420:SER:O | 1:B:3423:HIS:N | 1.95 | 0.99 |

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 | B | 2619/3825 (68%) | 2264 (86%) | 240 (9%) | 115 (4%) | 2 22 |

5 of 115 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 137 | HIS |
| 1 | B | 781 | GLU |
| 1 | B | 782 | PRO |
| 1 | B | 939 | PRO |
| 1 | B | 983 | ASP |

#### 5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

#### 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-3790. 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: 160

Y Index: 160

Z Index: 160

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: 161

Y Index: 138

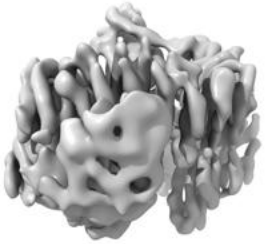
Z Index: 148

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 0.0429. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

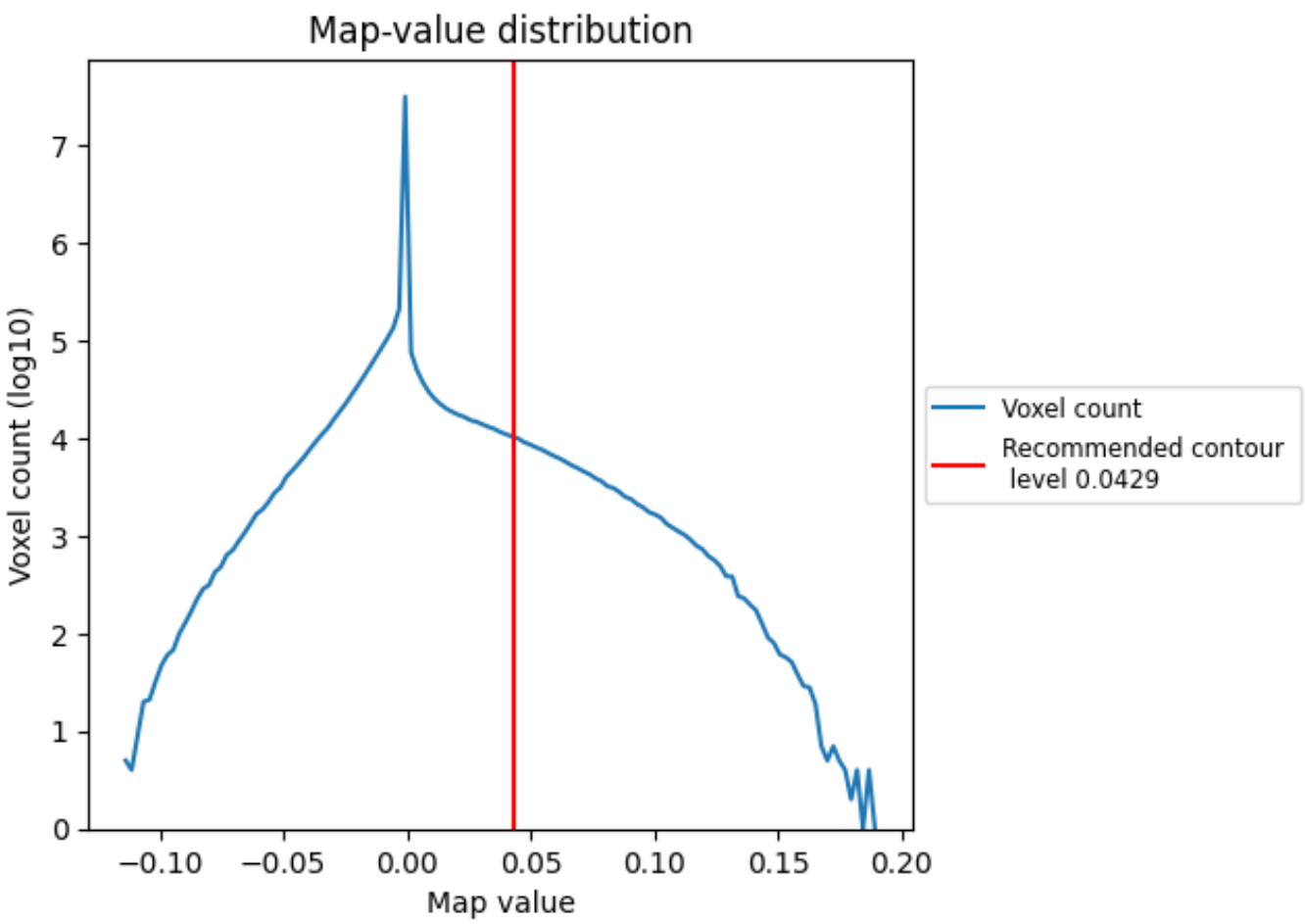
## 6.5 Mask visualisation (i)

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

# 7 Map analysis (i)

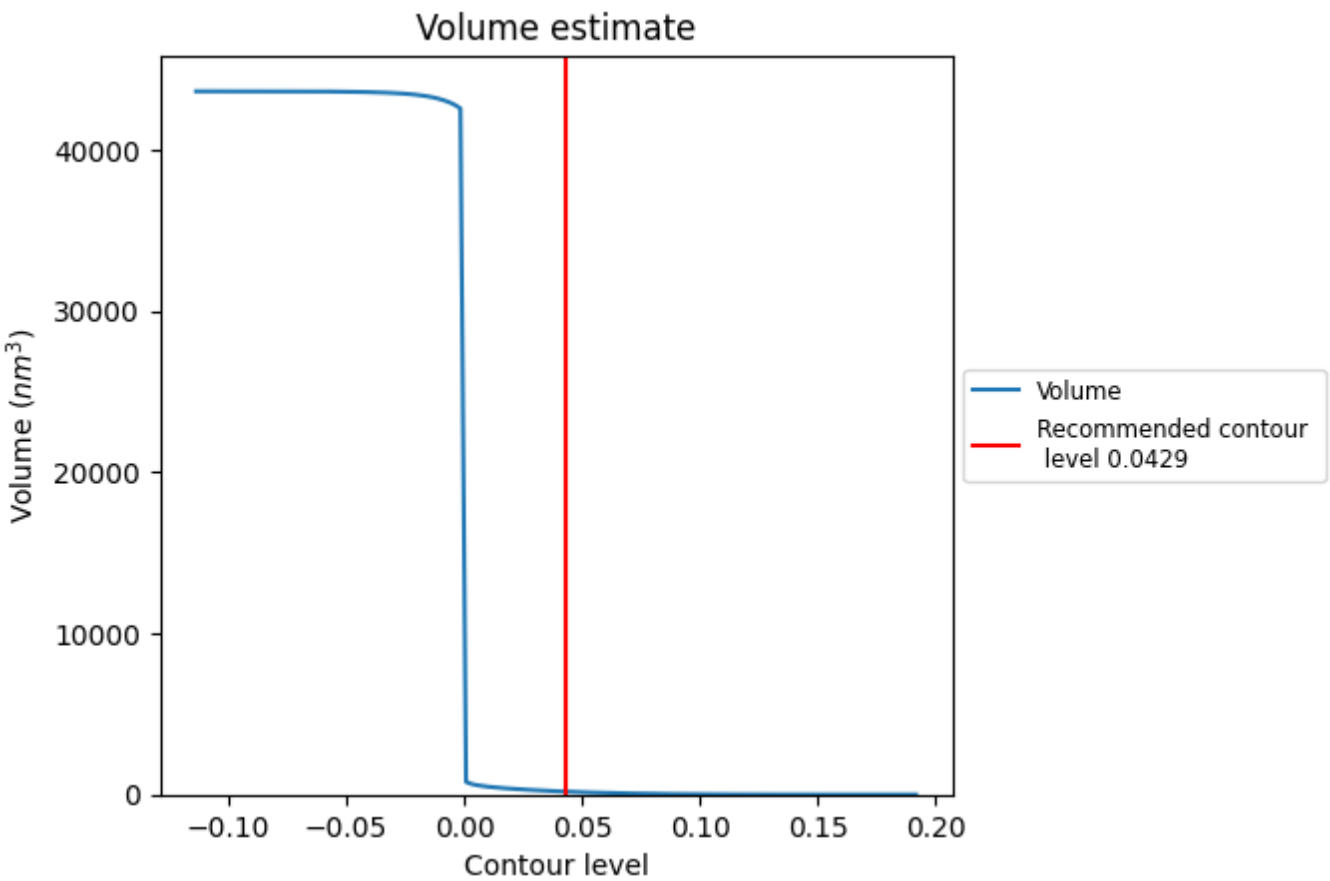
This section contains the results of statistical analysis of the map.

## 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.

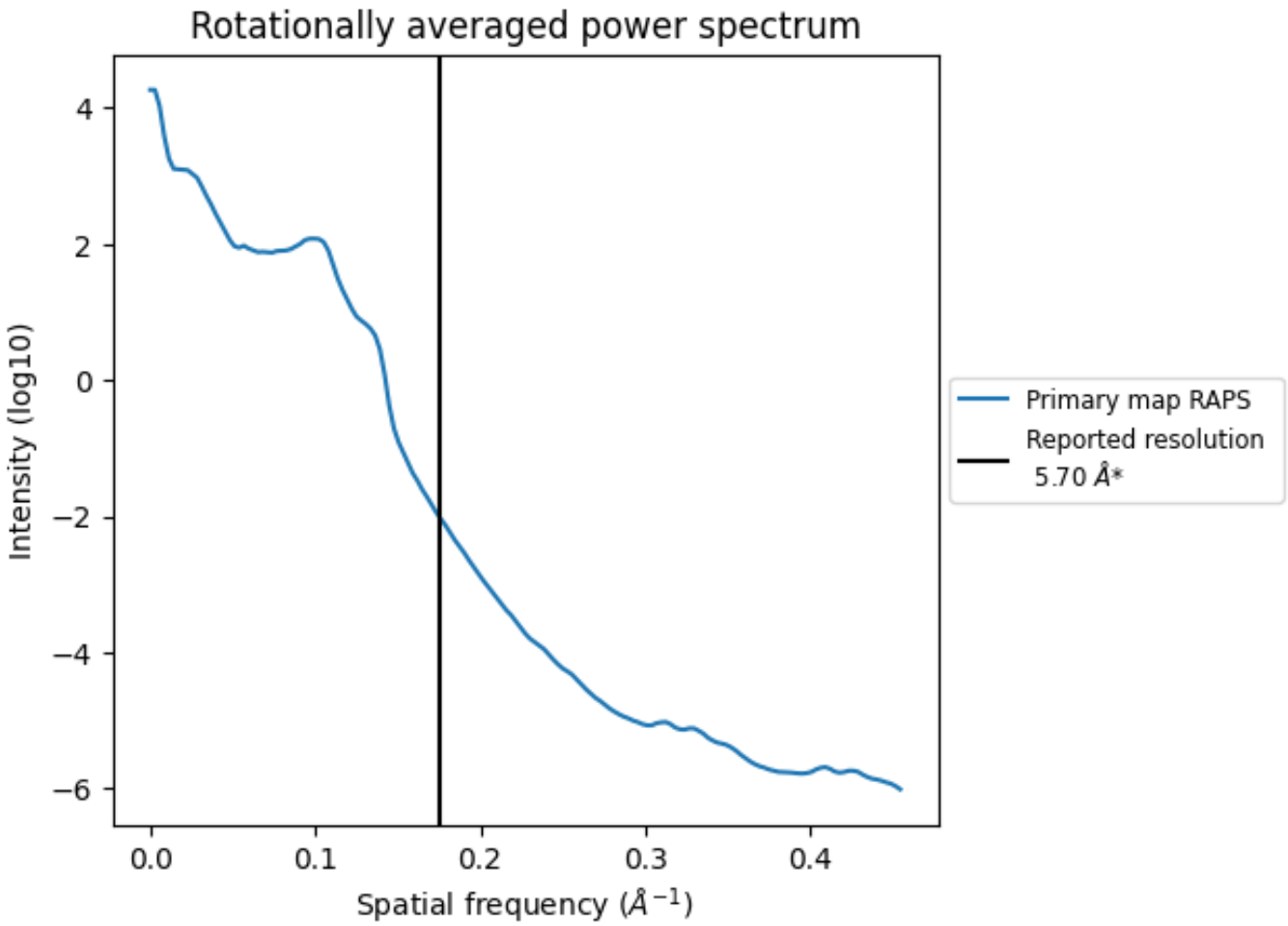
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 184 $nm^3$; this corresponds to an approximate mass of 166 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)

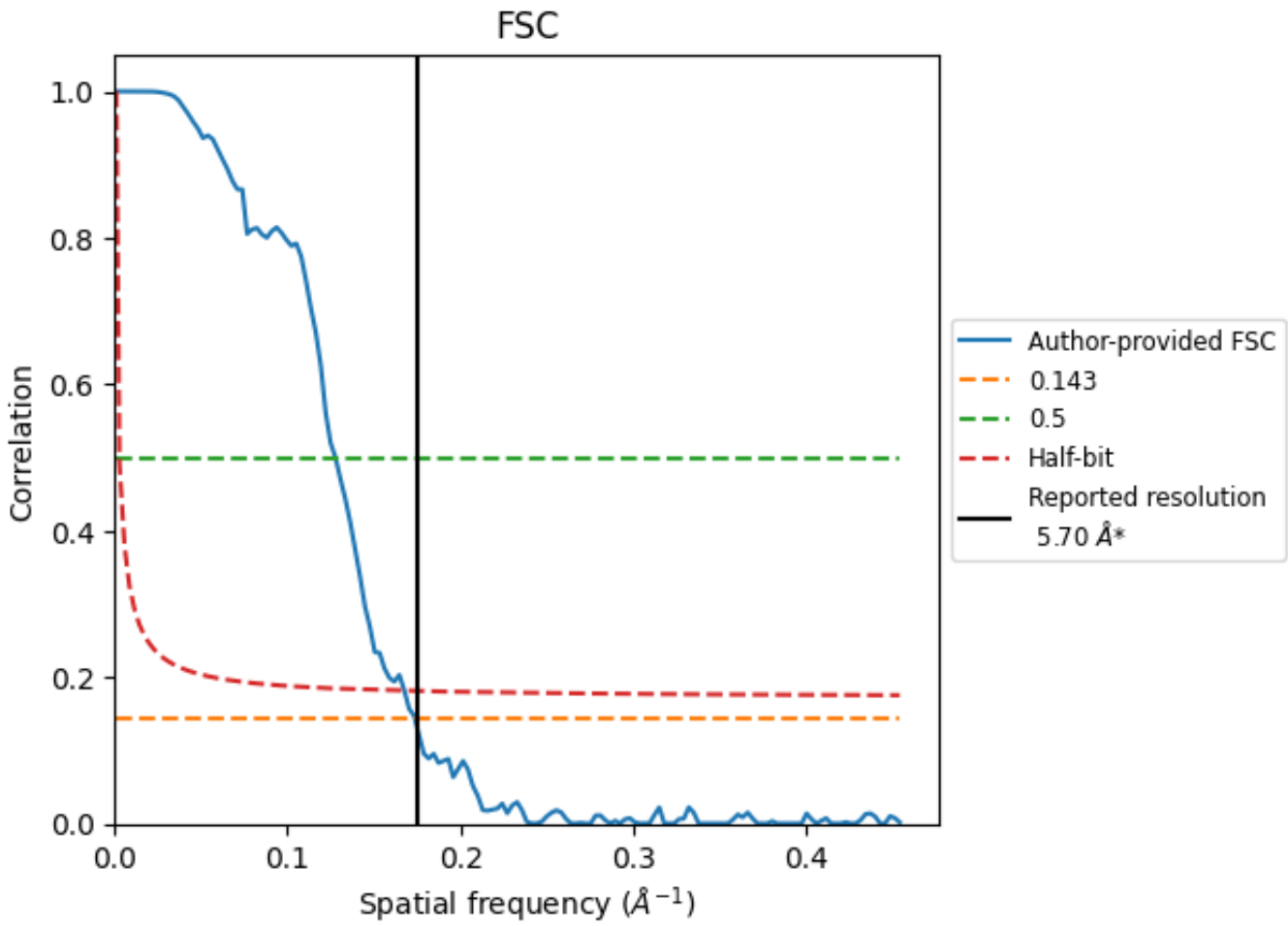



*Reported resolution corresponds to spatial frequency of 0.175 Å$^{-1}$

# 8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

## 8.1 FSC (i)




*Reported resolution corresponds to spatial frequency of 0.175 Å$^{-1}$

## 8.2 Resolution estimates (i)

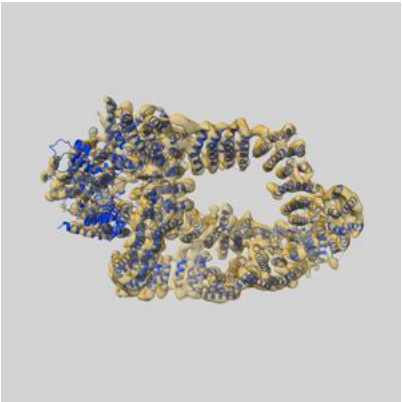
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 5.70 | - | - |
| Author-provided FSC curve | 5.75 | 7.82 | 5.96 |
| Unmasked-calculated* | - | - | - |

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

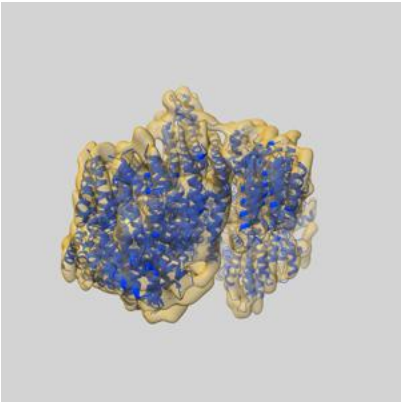
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3790 and PDB model 5OEJ. Per-residue inclusion information can be found in section 3 on page 4.

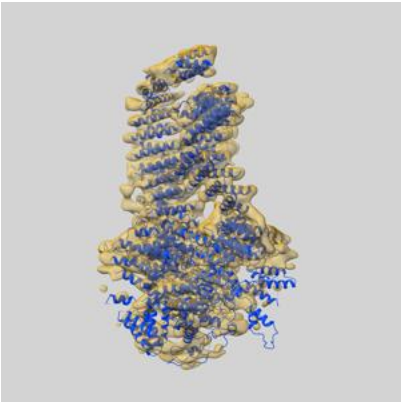
## 9.1 Map-model overlay (i)



X



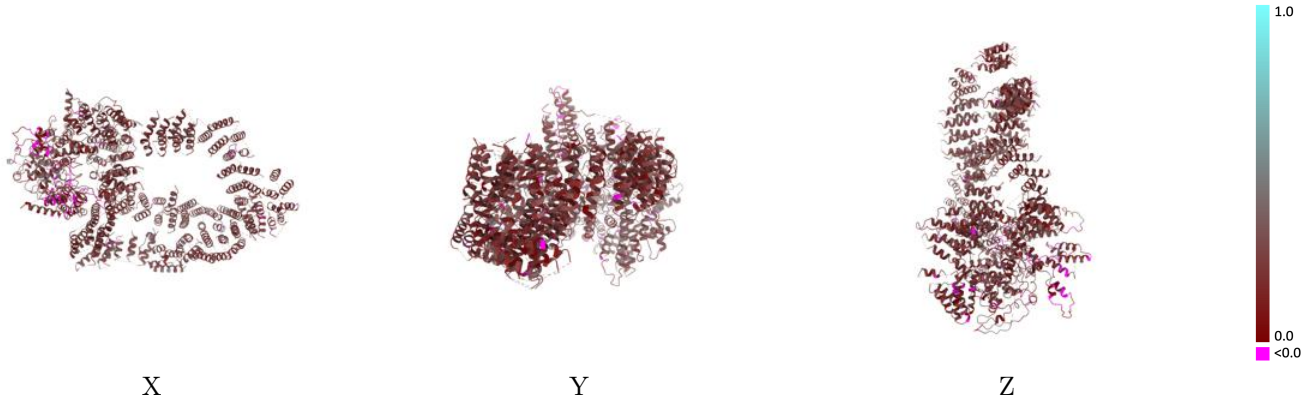
Y



Z

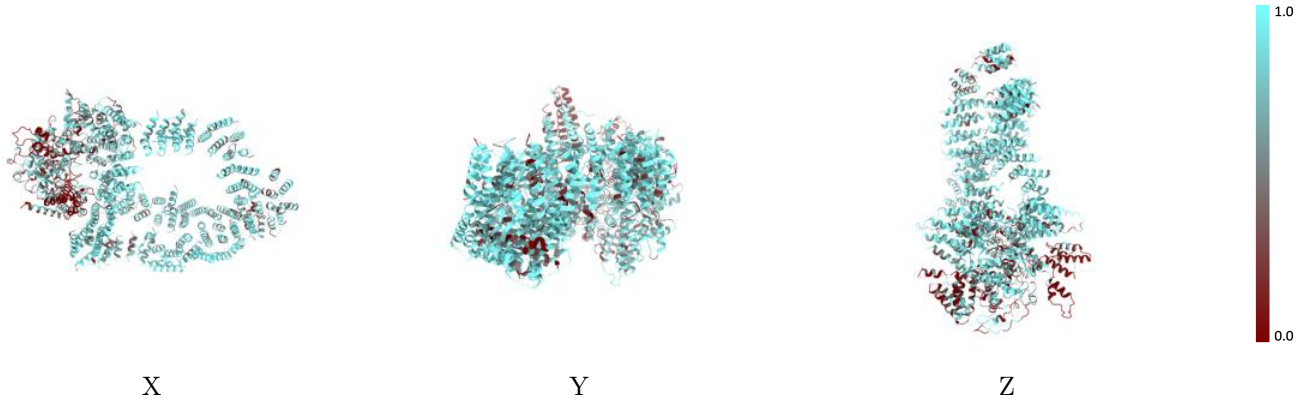
The images above show the 3D surface view of the map at the recommended contour level 0.0429 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



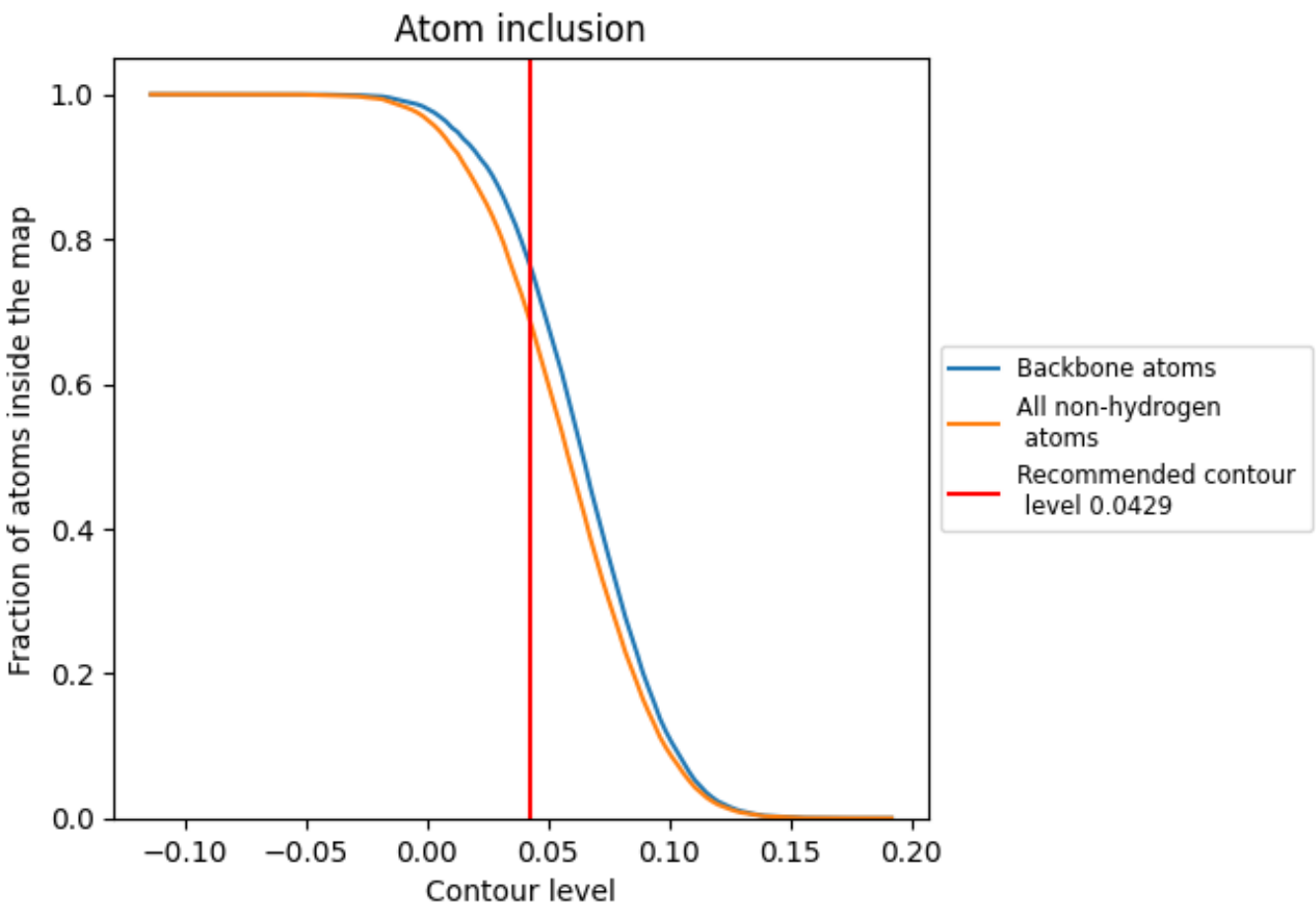

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model (i)




The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0429).

## 9.4 Atom inclusion (i)




At the recommended contour level, 76% of all backbone atoms, 68% 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 (0.0429) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.6830 | 0.2190 |
| B | 0.6830 | 0.2190 |