# wwPDB EM Validation Summary Report

Feb 22, 2025 – 01:42 PM EST

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|---|---|---|
| PDB ID | : | 9EAG |
| EMDB ID | : | EMD-47801 |
| Title | : | The Structure of ApoB100 from Human Low-Density Lipoprotein |
| Authors | : | Berndsen, Z.T.; Cassidy, C.K. |
| Deposited on | : | 2024-11-11 |
| Resolution | : | 9.00 Å(reported) |
| Based on initial model | : | . |

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:

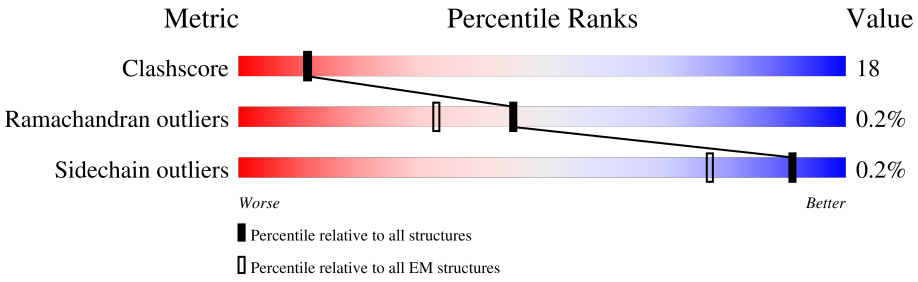
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev117 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.41.4 |

# 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 9.00 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

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 | 4563 | 37% 62% 37% |

## 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 36083 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 Apolipoprotein B 100.

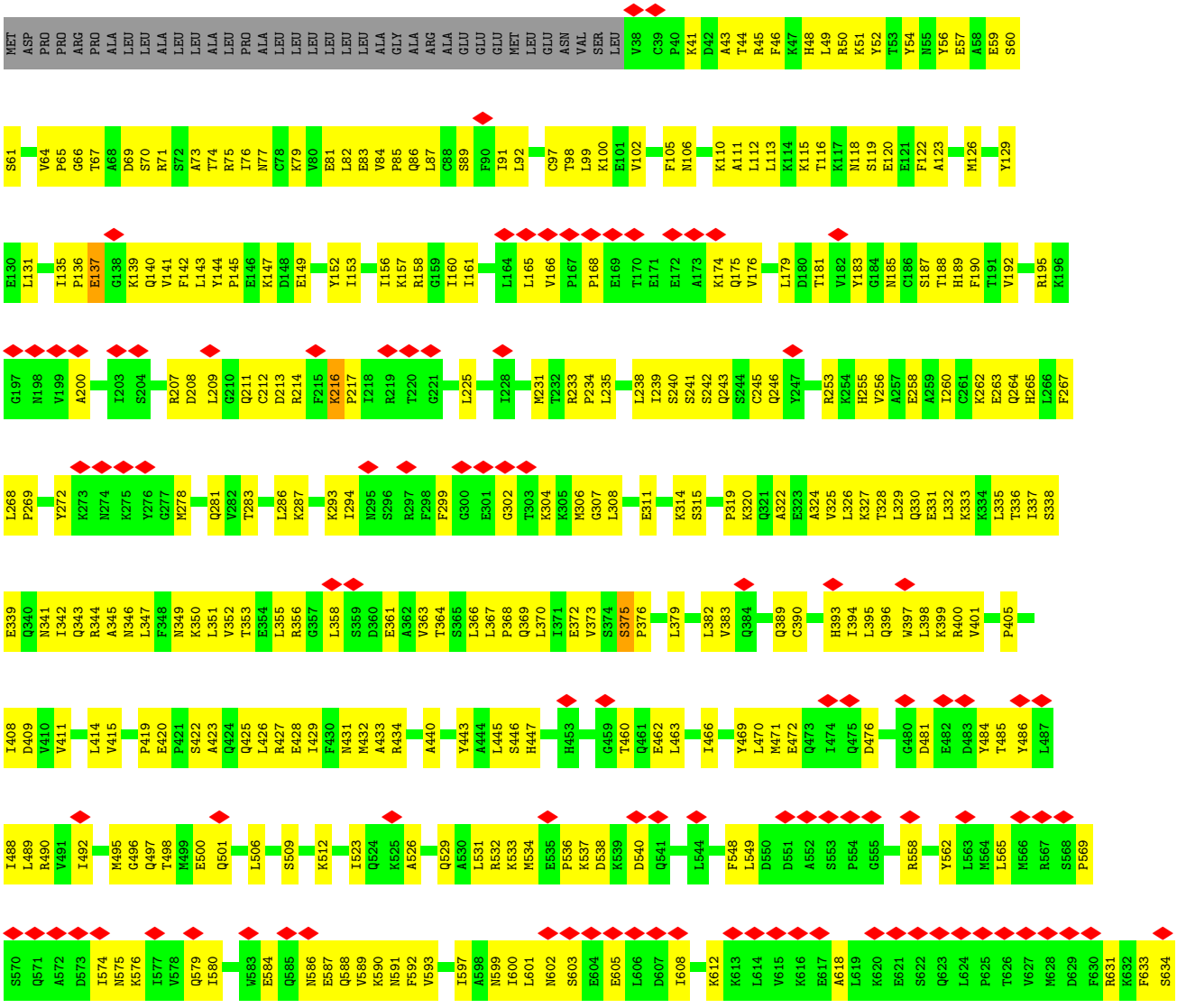
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | A | 4526 | 36083 | 23018 | 6066 | 6897 | 102 | 0 | 0 |

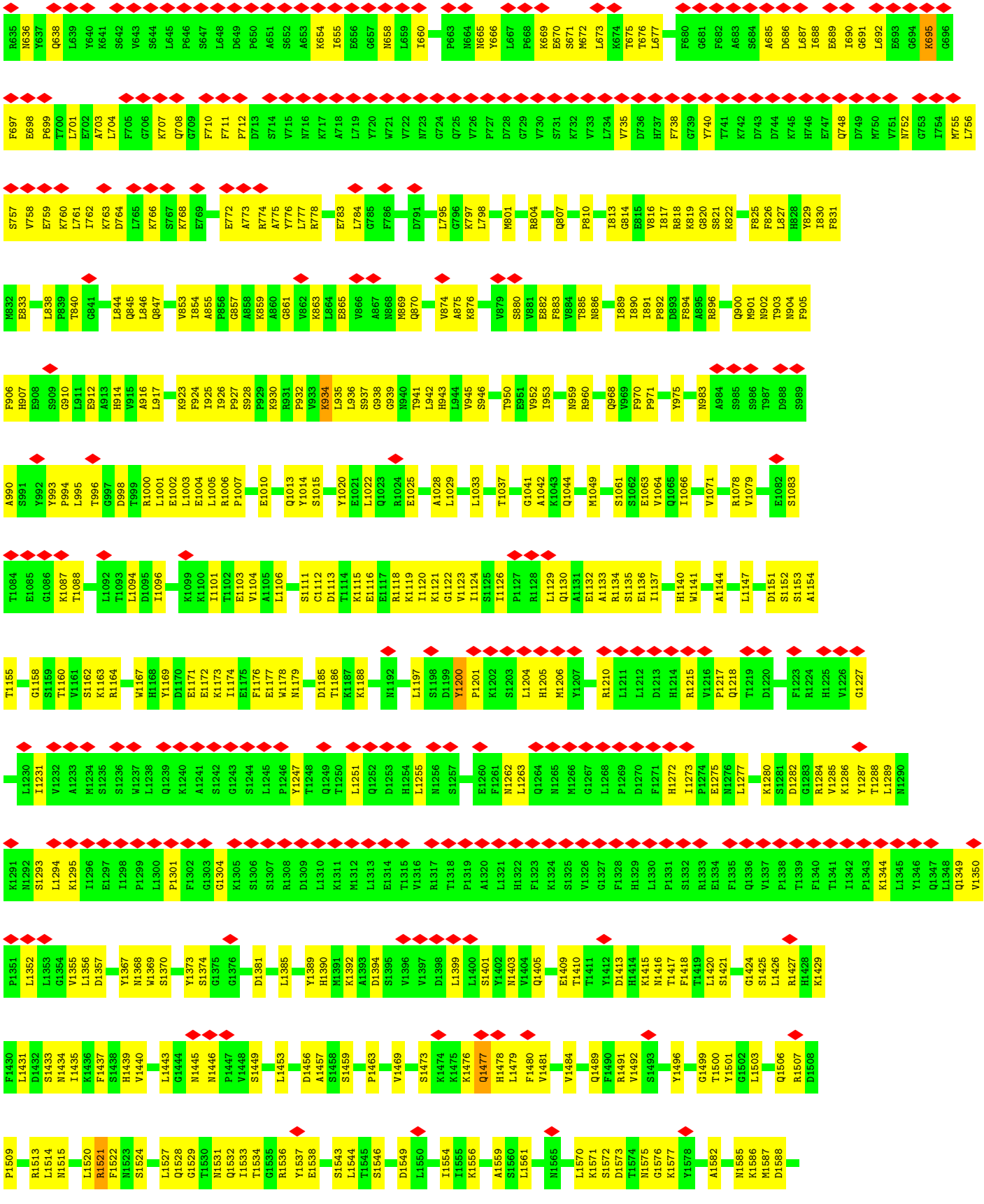
# 3 Residue-property plots (i)

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: Apolipoprotein B 100

Chain A: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F697 E698 P699 T700 L701 E702 A703 L704 F705 G706 K707 Q708 G709 F710 F711 P712 D713 S714 V715 N716 K717 A718 L719 Y720 W721 V722 N723 G724 Q725 V726 P727 D728 G729 V730 S731 K732 V733 L734 V735 D736 H737 F738 G739 Y740 T741 K742 D743 D744 K745 H746 E747 Q748 D749 M750 V751 N752 G753 I754 M755 L756
S757 V758 E759 K760 L761 I762 K763 D764 L765 K766 S767 K768 E769 E772 A773 R774 A775 Y776 L777 R778 E783 L784 G785 F786 D791 L795 G796 K797 L798 M801 R804 Q807 P810 I813 G814 E815 V816 I817 R818 K819 G820 S821 K822 F825 F826 L827 H828 Y829 I830 F831
M832 E833 L838 P839 T840 G841 L844 Q845 L846 Q847 V853 I854 A855 P856 G857 A858 K859 A860 G861 V862 K863 L864 E865 V866 A867 N868 M869 Q870 V874 A875 K876 V879 S880 V881 E882 F883 V884 T885 N886 I889 I890 I891 P892 D893 F894 A895 R896 Q900 M901 N902 T903 N904 F905
F906 H907 E908 S909 G910 L911 E912 A913 H914 V915 A916 L917 K923 F924 I925 I926 P927 S928 P929 K930 R931 P932 V933 K934 L935 L936 S937 G938 G939 N940 T941 L942 H943 L944 V945 S946 T950 E951 V952 I953 N959 R960 Q968 V969 F970 P971 Y975 N983 A984 S985 S986 T987 D988 S989
A990 S991 Y992 Y993 P994 L995 T996 G997 D998 T999 R1000 L1001 E1002 L1003 E1004 L1005 R1006 P1007 E1010 Q1013 Y1014 S1015 Y1020 E1021 L1022 Q1023 R1024 E1025 A1028 L1029 L1033 T1037 G1041 A1042 K1043 Q1044 M1049 S1061 S1062 E1063 V1064 Q1065 I1066 V1071 R1078 V1079 E1082 S1083
T1084 E1085 G1086 K1087 T1088 L1092 T1093 L1094 D1095 I1096 K1099 K1100 I1101 T1102 E1103 V1104 A1105 L1106 S1111 C1112 D1113 T1114 K1115 E1116 E1117 R1118 K1119 I1120 K1121 G1122 V1123 I1124 S1125 I1126 P1127 R1128 L1129 Q1130 A1131 E1132 A1133 R1134 S1135 E1136 I1137 H1140 W1141 A1144 L1147 D1151 S1152 S1153 A1154
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L1230 I1231 V1232 A1233 M1234 S1235 S1236 W1237 L1238 Q1239 K1240 A1241 S1242 G1243 S1244 L1245 P1246 Y1247 T1248 Q1249 T1250 L1251 Q1252 D1253 H1254 L1255 N1256 S1257 E1260 F1261 N1262 L1263 Q1264 N1265 M1266 G1267 L1268 P1269 D1270 F1271 H1272 I1273 P1274 E1275 N1276 L1277 K1280 S1281 D1282 G1283 R1284 V1285 K1286 Y1287 T1288 L1289 N1290
K1291 N1292 S1293 L1294 K1295 I1296 E1297 I1298 P1299 L1300 P1301 F1302 G1303 G1304 K1305 S1306 S1307 R1308 D1309 L1310 K1311 M1312 L1313 E1314 T1315 V1316 R1317 T1318 P1319 A1320 L1321 H1322 F1323 K1324 S1325 V1326 G1327 F1328 H1329 L1330 P1331 S1332 R1333 E1334 F1335 Q1336 V1337 P1338 T1339 F1340 T1341 I1342 P1343 K1344 L1345 Y1346 Q1347 L1348 Q1349 V1350
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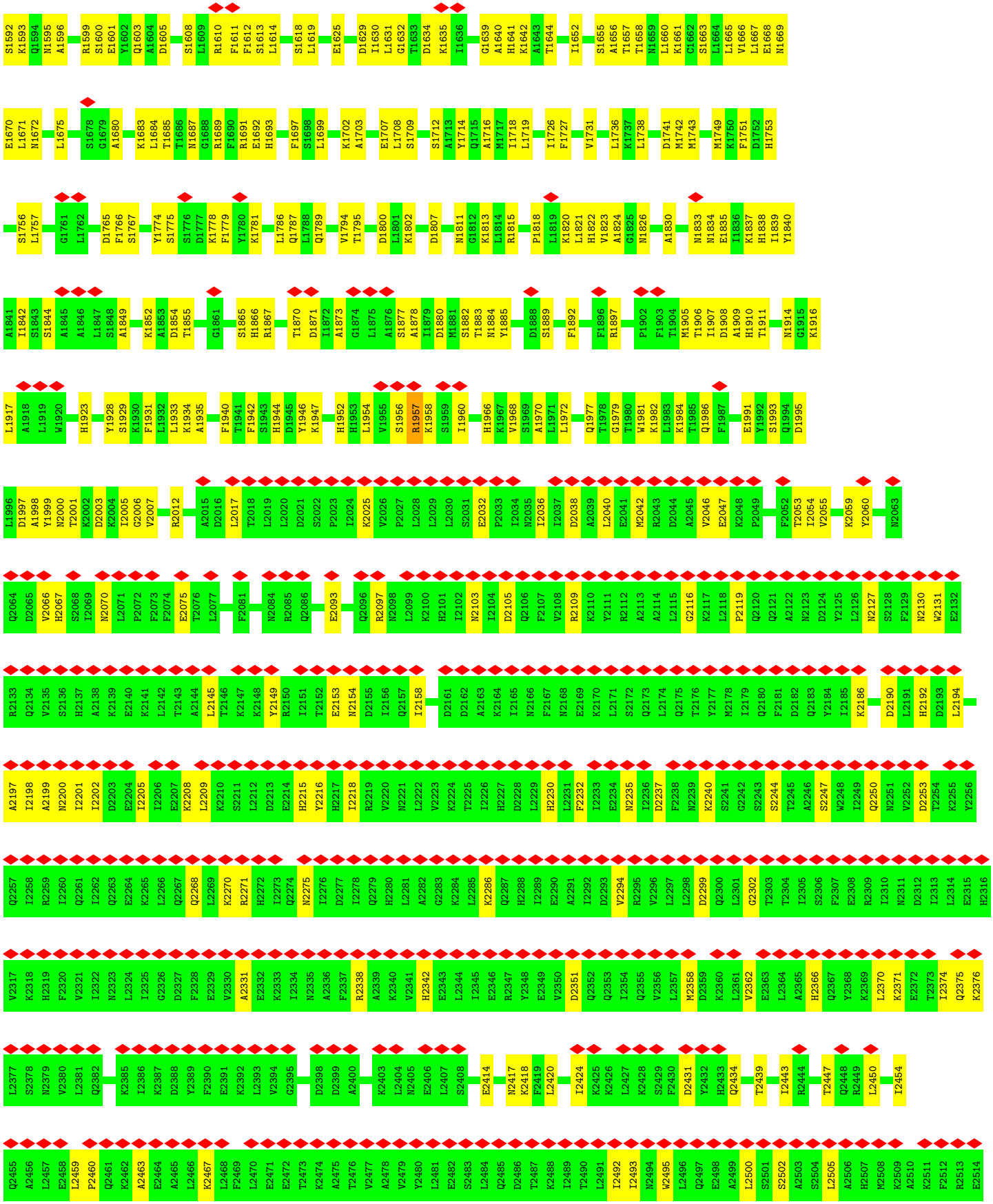
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L1786 Q1787 L1788 Q1789
V1794 T1795
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D1807
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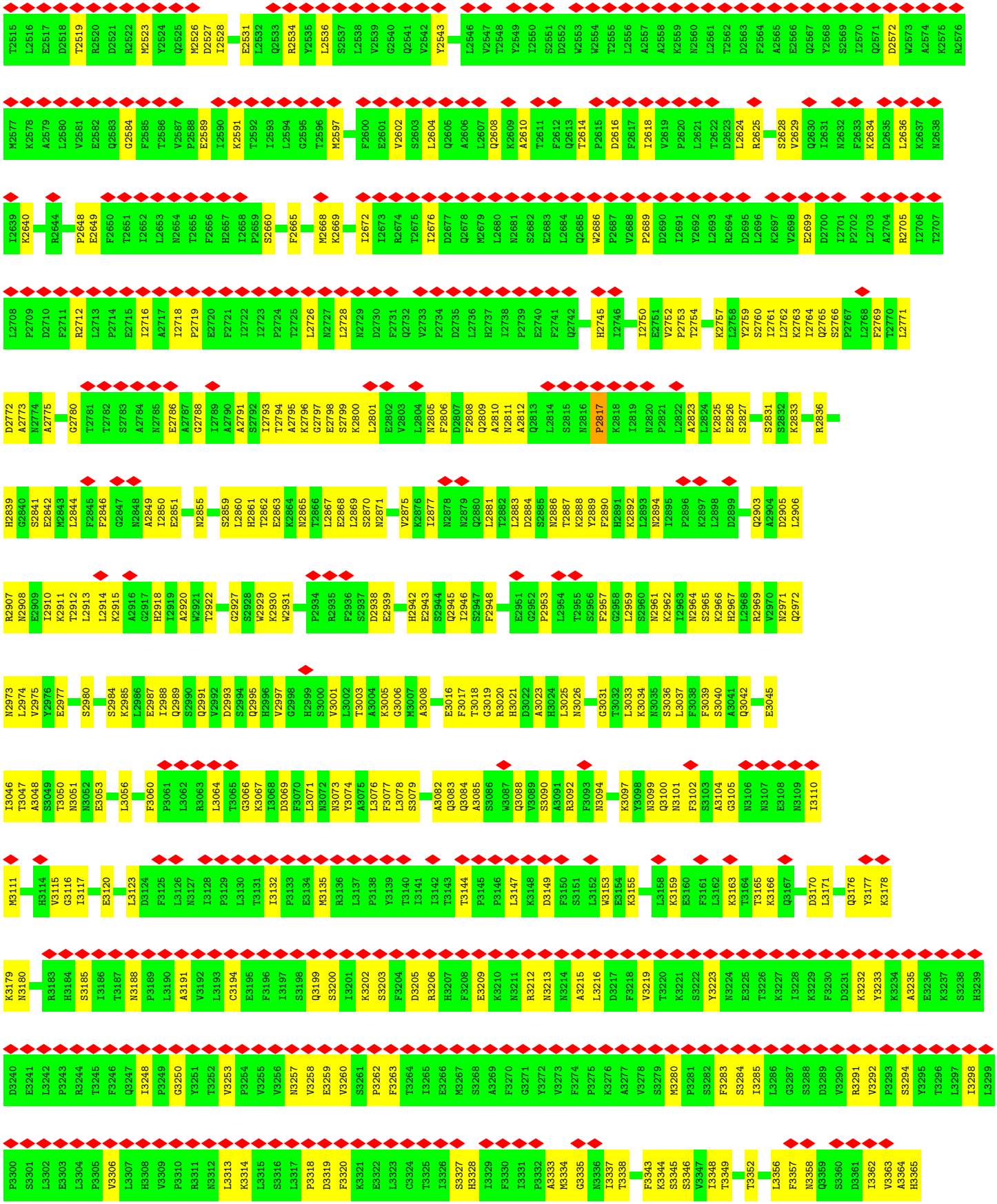
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D3240 E3241 L3242 P3243 R3244 T3245 F3246 Q3247 I3248 P3249 G3250 Y3251 T3252 V3253 P3254 V3255 V3256 N3257 V3258 E3259 V3260 S3261 P3262 F3263 T3264 I3265 E3266 M3267 S3268 A3269 F3270 G3271 Y3272 V3273 F3274 P3275 K3276 A3277 V3278 S3279 M3280 P3281 S3282 F3283 S3284 I3285 L3286 G3287 S3288 D3289 V3290 R3291 V3292 P3293 S3294 Y3295 T3296 L3297 I3298 L3299
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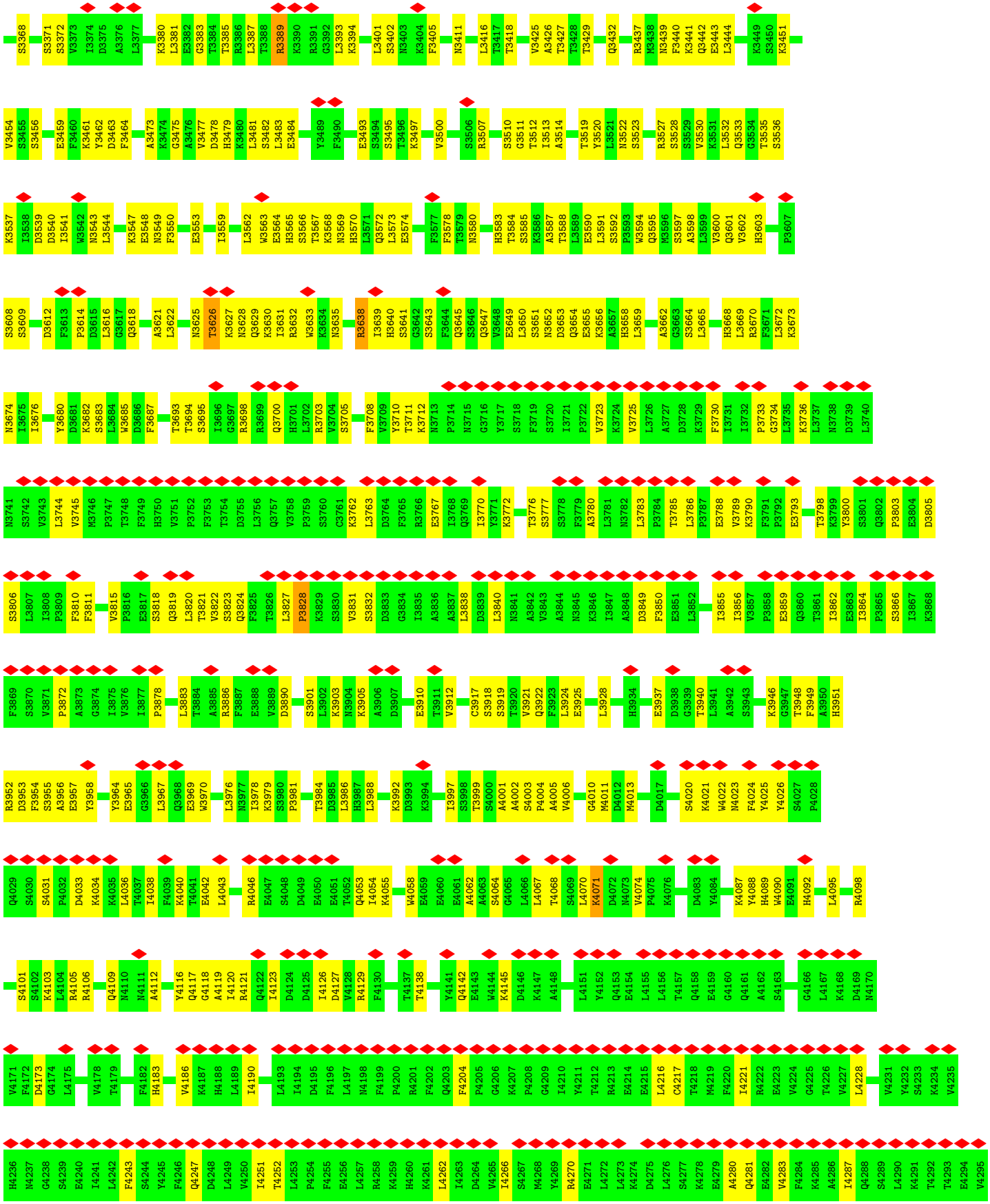
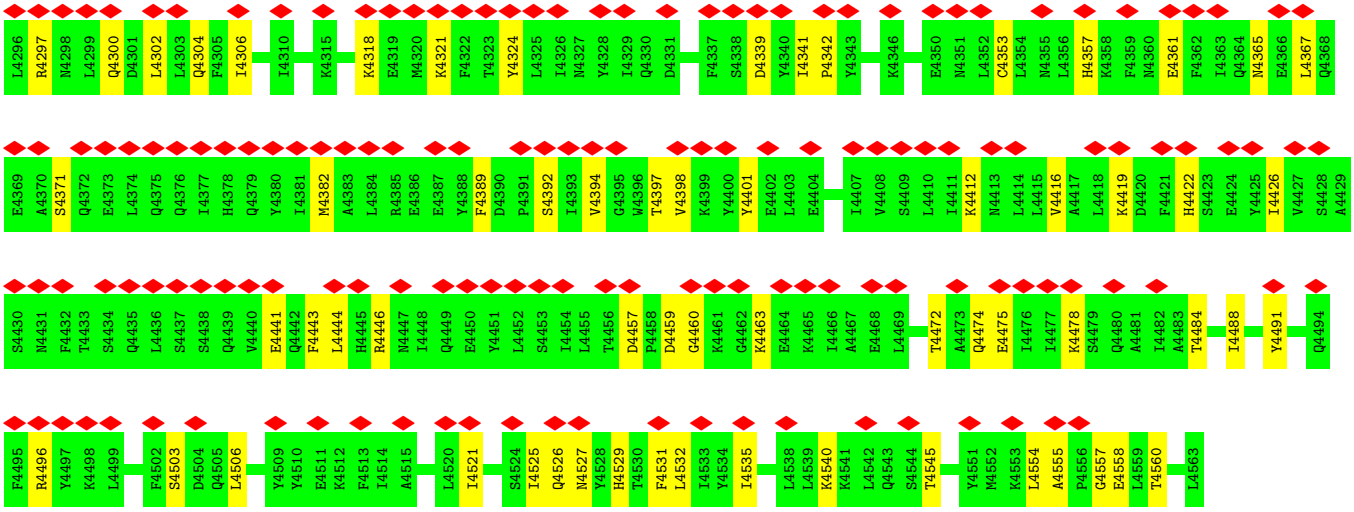

S3368 S3371 S3372 V3373 I3374 D3375 A3376 L3377 K3380 L3381 E3382 G3383 T3384 T3385 R3386 L3387 T3388 R3389 K3390 R3391 G3392 L3393 K3394 L3401 S3402 N3403 K3404 F3405 N3411 L3416 T3417 T3418 V3425 A3426 T3427 T3428 T3429 Q3432 R3437 M3438 N3439 F3440 K3441 Q3442 E3443 L3444 K3449 S3450 K3451
V3454 S3455 S3456 E3459 F3460 K3461 Y3462 D3463 F3464 A3473 K3474 G3475 A3476 V3477 D3478 H3479 K3480 L3481 S3482 L3483 E3484 Y3489 F3490 E3493 S3494 S3495 T3496 K3497 V3500 S3506 R3507 S3510 G3511 T3512 I3513 A3514 T3519 Y3520 L3521 N3522 S3523 R3527 S3528 S3529 V3530 K3531 L3532 Q3533 G3534 T3535 S3536
K3537 T3538 D3539 D3540 T3541 W3542 N3543 L3544 K3547 E3548 N3549 F3550 E3553 I3559 L3562 W3563 E3564 H3565 S3566 T3567 K3568 N3569 H3570 L3571 Q3572 L3573 E3574 F3577 F3578 T3579 N3580 H3583 T3584 S3585 K3586 A3587 T3588 L3589 E3590 L3591 S3592 P3593 W3594 Q3595 M3596 S3597 A3598 L3599 V3600 Q3601 V3602 H3603 P3607
S3608 S3609 D3612 F3613 P3614 D3615 L3616 G3617 Q3618 A3621 L3622 N3625 T3626 K3627 N3628 Q3629 K3630 I3631 R3632 W3633 K3634 N3635 R3638 I3639 H3640 S3641 G3642 S3643 F3644 Q3645 S3646 Q3647 V3648 E3649 L3650 S3651 N3652 D3653 Q3654 E3655 K3656 A3657 H3658 L3659 A3662 G3663 S3664 L3665 H3668 L3669 R3670 F3671 L3672 K3673
N3674 I3675 I3676 Y3680 D3681 K3682 S3683 L3684 W3685 D3686 F3687 T3693 T3694 S3695 I3696 G3697 R3698 R3699 Q3700 H3701 L3702 R3703 V3704 S3705 F3708 V3709 Y3710 T3711 K3712 N3713 P3714 N3715 G3716 Y3717 S3718 F3719 S3720 I3721 P3722 V3723 K3724 V3725 L3726 A3727 D3728 K3729 F3730 I3731 I3732 P3733 G3734 L3735 K3736 L3737 N3738 D3739 L3740
N3741 S3742 V3743 L3744 V3745 M3746 P3747 T3748 F3749 H3750 V3751 P3752 F3753 T3754 D3755 L3756 Q3757 V3758 P3759 S3760 C3761 K3762 L3763 D3764 F3765 R3766 E3767 I3768 Q3769 I3770 Y3771 K3772 T3776 S3777 S3778 F3779 A3780 L3781 N3782 L3783 P3784 T3785 L3786 P3787 E3788 V3789 K3790 F3791 P3792 E3793 T3798 K3799 Y3800 S3801 Q3802 P3803 E3804 D3805
S3806 L3807 I3808 P3809 F3810 F3811 V3815 P3816 E3817 S3818 Q3819 L3820 T3821 V3822 S3823 Q3824 F3825 T3826 L3827 P3828 K3829 S3830 V3831 S3832 D3833 G3834 I3835 A3836 A3837 L3838 D3839 L3840 N3841 A3842 V3843 A3844 N3845 K3846 I3847 A3848 D3849 F3850 E3851 L3852 I3855 I3856 V3857 P3858 E3859 Q3860 T3861 I3862 E3863 I3864 P3865 S3866 I3867 K3868
F3869 S3870 V3871 P3872 A3873 G3874 I3875 V3876 I3877 P3878 L3883 T3884 A3885 R3886 F3887 E3888 V3889 D3890 S3901 L3902 K3903 N3904 K3905 A3906 D3907 E3910 T3911 V3912 C3917 S3918 S3919 T3920 V3921 Q3922 F3923 L3924 E3925 L3928 H3934 E3937 D3938 Q3939 T3940 L3941 A3942 S3943 K3946 G3947 T3948 F3949 A3950 H3951
R3952 D3953 F3954 S3955 A3956 E3957 Y3958 Y3964 E3965 G3966 L3967 Q3968 E3969 W3970 L3976 N3977 I3978 K3979 S3980 P3981 T3984 D3985 L3986 H3987 L3988 K3992 D3993 K3994 I3997 S3998 T3999 S4000 A4001 A4002 S4003 P4004 A4005 V4006 G4010 M4011 D4012 M4013 D4017 S4020 K4021 W4022 N4023 F4024 Y4025 Y4026 S4027 P4028
Q4029 S4030 S4031 P4032 D4033 K4034 K4035 L4036 T4037 I4038 F4039 K4040 T4041 E4042 L4043 R4046 E4047 S4048 D4049 E4050 E4051 T4052 Q4053 I4054 K4055 W4058 E4059 E4060 E4061 A4062 A4063 S4064 G4065 L4066 L4067 T4068 S4069 L4070 K4071 D4072 N4073 V4074 P4075 K4076 D4083 Y4084 K4087 Y4088 H4089 W4090 E4091 H4092 L4095 R4098
S4101 S4102 K4103 L4104 R4105 R4106 Q4109 N4110 N4111 A4112 Y4116 Q4117 G4118 A4119 I4120 R4121 Q4122 I4123 D4124 D4125 I4126 D4127 V4128 R4129 F4130 T4137 T4138 Y4141 Q4142 E4143 W4144 K4145 D4146 K4147 A4148 L4151 Y4152 Q4153 E4154 L4155 L4156 T4157 Q4158 E4159 G4160 Q4161 A4162 S4163 G4166 L4167 K4168 D4169 N4170
V4171 F4172 D4173 G4174 L4175 V4178 T4179 F4182 H4183 V4186 K4187 H4188 L4189 I4190 L4193 I4194 D4195 F4196 L4197 N4198 F4199 P4200 R4201 F4202 Q4203 F4204 P4205 G4206 K4207 P4208 G4209 I4210 Y4211 T4212 R4213 E4214 E4215 L4216 C4217 T4218 M4219 F4220 I4221 R4222 E4223 V4224 G4225 T4226 V4227 L4228 V4231 Y4232 S4233 K4234 V4235
H4236 N4237 G4238 S4239 E4240 I4241 L4242 F4243 S4244 Y4245 F4246 Q4247 D4248 L4249 V4250 I4251 T4252 L4253 P4254 F4255 E4256 L4257 R4258 K4259 H4260 K4261 L4262 I4263 D4264 V4265 I4266 S4267 M4268 Y4269 R4270 E4271 L4272 L4273 K4274 D4275 L4276 S4277 K4278 E4279 A4280 Q4281 E4282 V4283 F4284 K4285 A4286 I4287 Q4288 S4289 L4290 K4291 T4292 T4293 E4294 V4295


L4296 R4297 M4298 L4299 Q4300 D4301 L4302 L4303 Q4304 F4305 I4306 I4310 K4315 K4318 E4319 M4320 K4321 F4322 T4323 Y4324 L4325 I4326 N4327 Y4328 I4329 Q4330 D4331 F4337 S4338 D4339 Y4340 I4341 P4342 Y4343 K4346 E4350 N4351 L4352 C4353 L4364 N4355 L4356 H4357 K4358 F4359 N4360 E4361 F4362 I4363 Q4364 N4365 E4366 L4367 Q4368
E4369 A4370 S4371 Q4372 E4373 L4374 Q4375 Q4376 I4377 H4378 Q4379 Y4380 I4381 M4382 A4383 L4384 R4385 E4386 E4387 Y4388 F4389 D4390 P4391 S4392 I4393 V4394 G4395 W4396 T4397 V4398 K4399 Y4400 Y4401 E4402 L4403 E4404 I4407 V4408 S4409 L4410 I4411 K4412 N4413 L4414 L4415 V4416 A4417 L4418 K4419 D4420 F4421 H4422 S4423 E4424 Y4425 I4426 V4427 S4428 A4429
S4430 N4431 F4432 T4433 S4434 Q4435 L4436 S4437 S4438 Q4439 V4440 E4441 Q4442 F4443 L4444 H4445 R4446 N4447 I4448 Q4449 E4450 Y4451 L4452 S4453 I4454 L4455 T4456 D4457 P4458 D4459 G4460 K4461 G4462 K4463 E4464 K4465 I4466 A4467 E4468 L4469 T4472 A4473 Q4474 E4475 I4476 I4477 K4478 S4479 Q4480 A4481 I4482 A4483 T4484 I4488 Y4491 Q4494
F4495 R4496 Y4497 K4498 L4499 F4502 S4503 D4504 Q4505 L4506 Y4509 Y4510 E4511 K4512 F4513 I4514 A4515 L4520 I4521 S4524 I4525 Q4526 N4527 Y4528 H4529 T4530 F4531 L4532 I4533 Y4534 I4535 L4538 L4539 K4540 K4541 L4542 Q4543 S4544 T4545 Y4551 M4552 K4553 L4554 A4555 P4556 G4557 E4558 L4559 T4560 L4563

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 52843 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | TFS KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 50 | Depositor |
| Minimum defocus (nm) | 800 | Depositor |
| Maximum defocus (nm) | 2800 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 1.148 | Depositor |
| Minimum map value | -0.560 | Depositor |
| Average map value | -0.000 | Depositor |
| Map value standard deviation | 0.025 | Depositor |
| Recommended contour level | 0.182 | Depositor |
| Map size (Å) | 490.5, 490.5, 490.5 | wwPDB |
| Map dimensions | 450, 450, 450 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.09, 1.09, 1.09 | 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 | 0.26 | 0/36813 | 0.48 | 0/49814 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 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 | 36083 | 0 | 36243 | 1282 | 0 |
| All | All | 36083 | 0 | 36243 | 1282 | 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 18.

The worst 5 of 1282 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:825:PHE:O | 1:A:857:GLY:HA2 | 1.68 | 0.93 |
| 1:A:3918:SER:HA | 1:A:3925:GLU:HG2 | 1.52 | 0.92 |
| 1:A:322:ALA:O | 1:A:325:VAL:HB | 1.70 | 0.92 |
| 1:A:4138:THR:HG22 | 1:A:4142:GLN:HE22 | 1.37 | 0.88 |
| 1:A:3965:GLU:O | 1:A:3969:GLU:HB2 | 1.73 | 0.86 |

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 | 4524/4563 (99%) | 4297 (95%) | 219 (5%) | 8 (0%) | 44 78 |

5 of 8 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 137 | GLU |
| 1 | A | 1477 | GLN |
| 1 | A | 3828 | PRO |
| 1 | A | 375 | SER |
| 1 | A | 1200 | TYR |

### 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 | 4051/4080 (99%) | 4041 (100%) | 10 (0%) | 92 94 |

5 of 10 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 3389 | ARG |
| 1 | A | 3638 | ARG |
| 1 | A | 4071 | LYS |
| 1 | A | 934 | LYS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1215 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 3442 | GLN |
| 1 | A | 3824 | GLN |
| 1 | A | 4526 | GLN |
| 1 | A | 3987 | HIS |
| 1 | A | 3645 | GLN |

#### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry

There are no ligands in this entry.

### 5.7 Other polymers

There are no such residues in this entry.

### 5.8 Polymer linkage issues

There are no chain breaks in this entry.

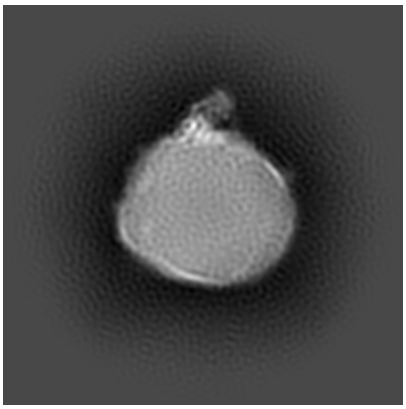
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-47801. These allow visual inspection of the internal detail of the map and identification of artifacts.

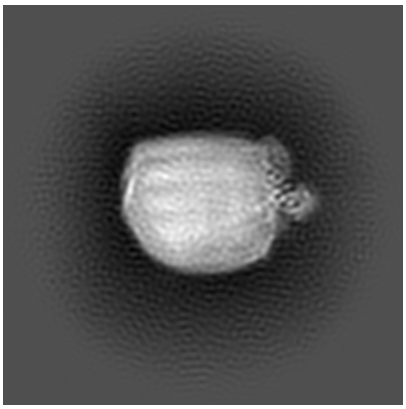
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

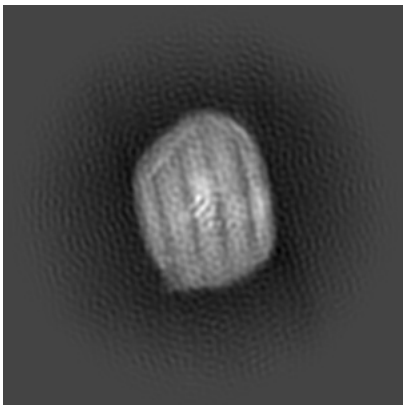
### 6.1.1 Primary map



X

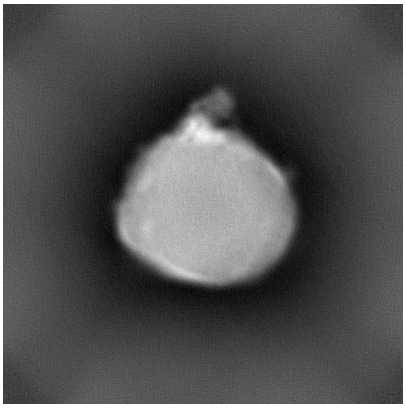


Y

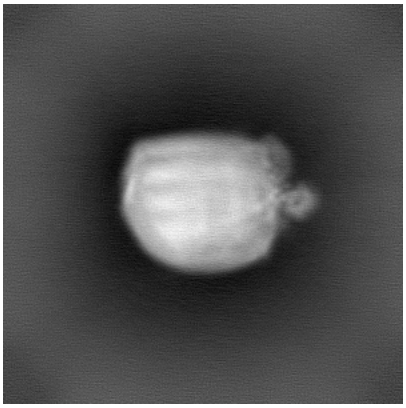


Z

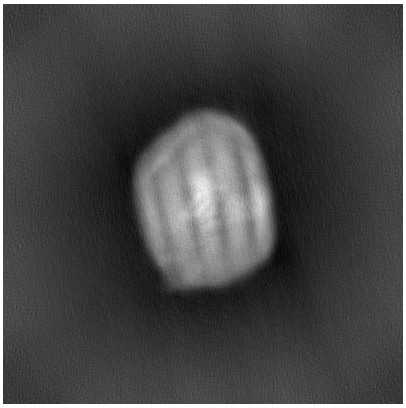
### 6.1.2 Raw map



X



Y

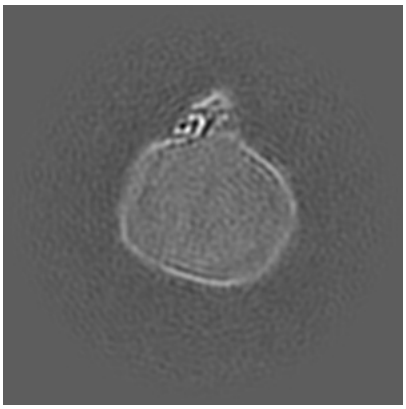


Z

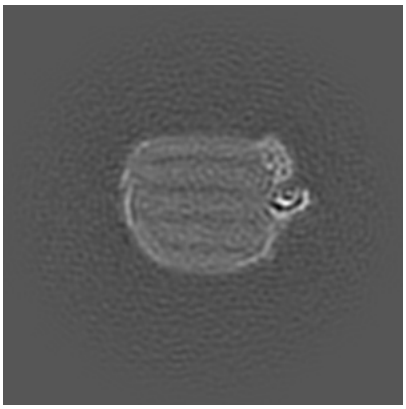
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

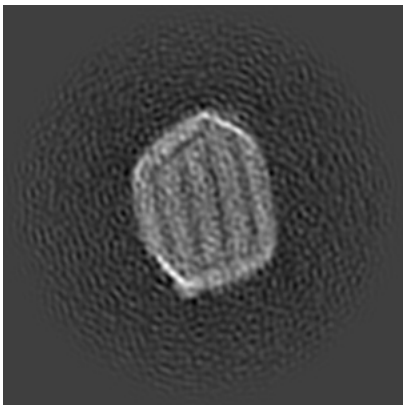
### 6.2.1 Primary map



X Index: 225

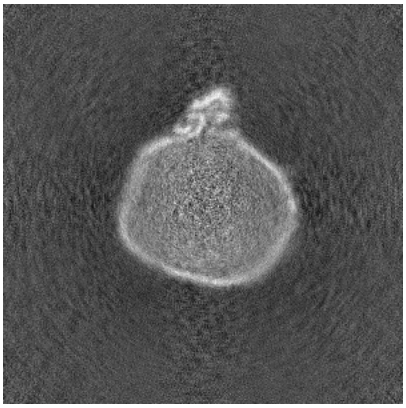


Y Index: 225

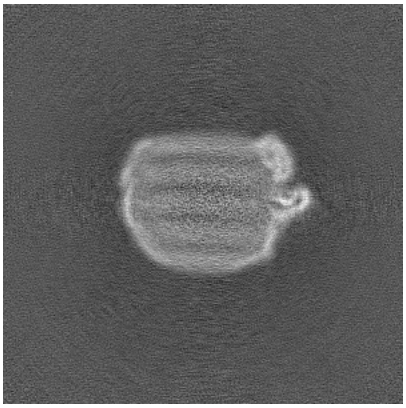


Z Index: 225

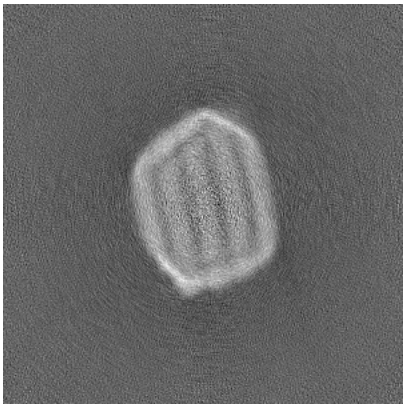
### 6.2.2 Raw map



X Index: 225



Y Index: 225

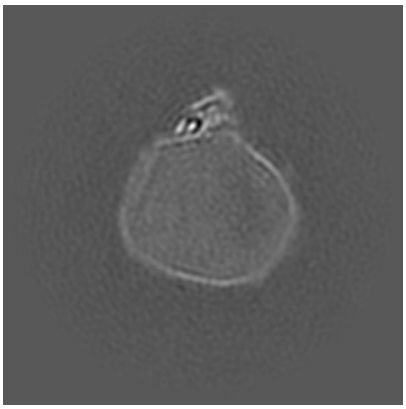


Z Index: 225

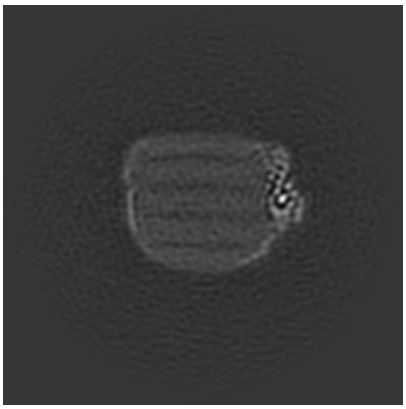
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

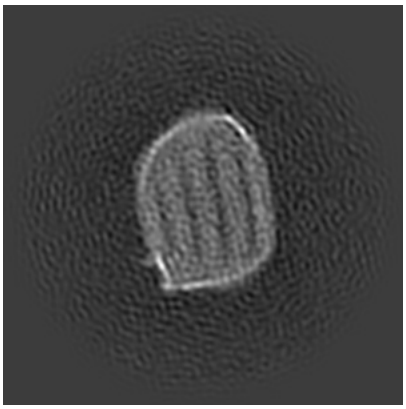
### 6.3.1 Primary map



X Index: 230

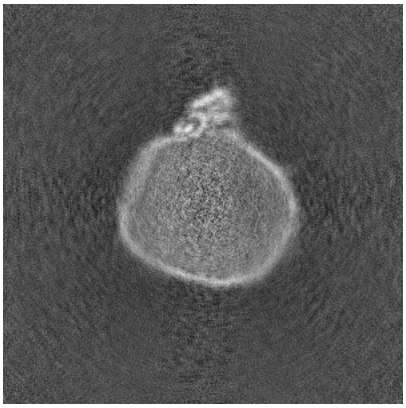


Y Index: 213

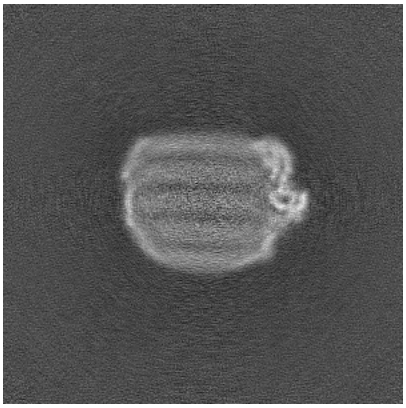


Z Index: 196

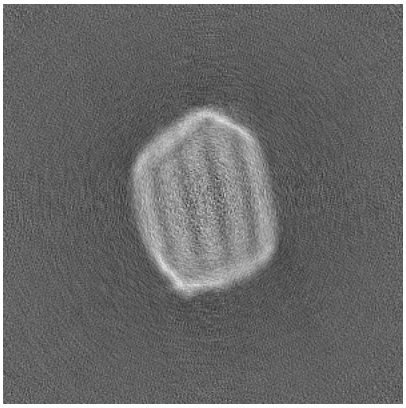
### 6.3.2 Raw map



X Index: 227



Y Index: 219

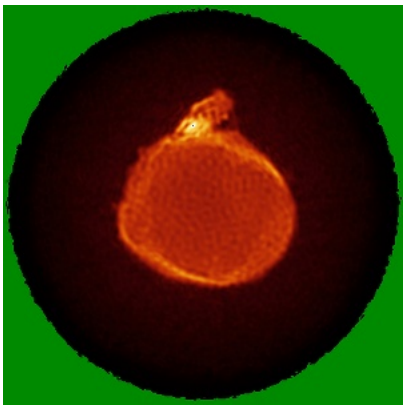


Z Index: 219

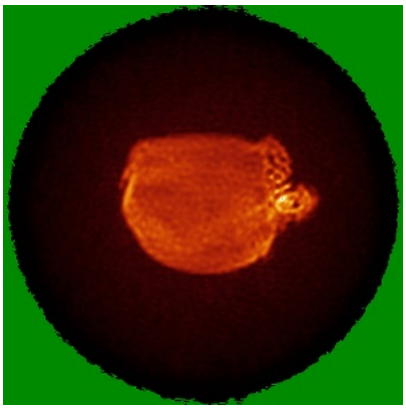
The images above show the largest variance slices of the map in three orthogonal directions.

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

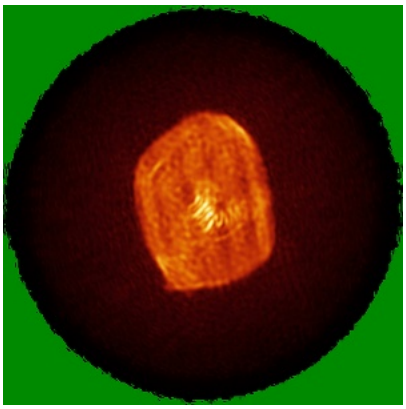
### 6.4.1 Primary map



X

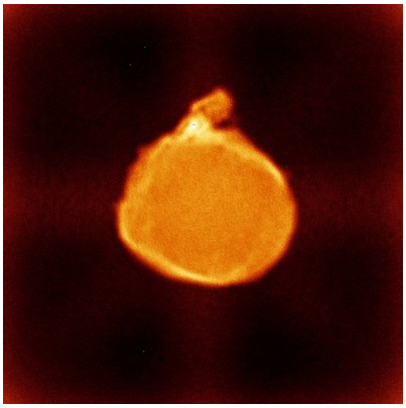


Y

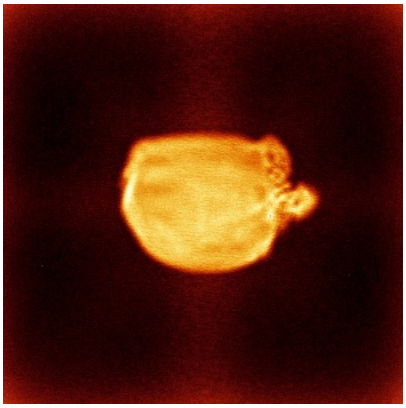


Z

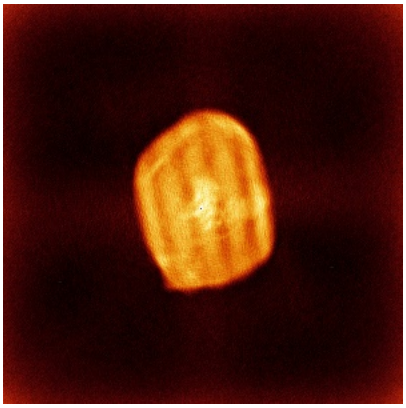
### 6.4.2 Raw map



X



Y

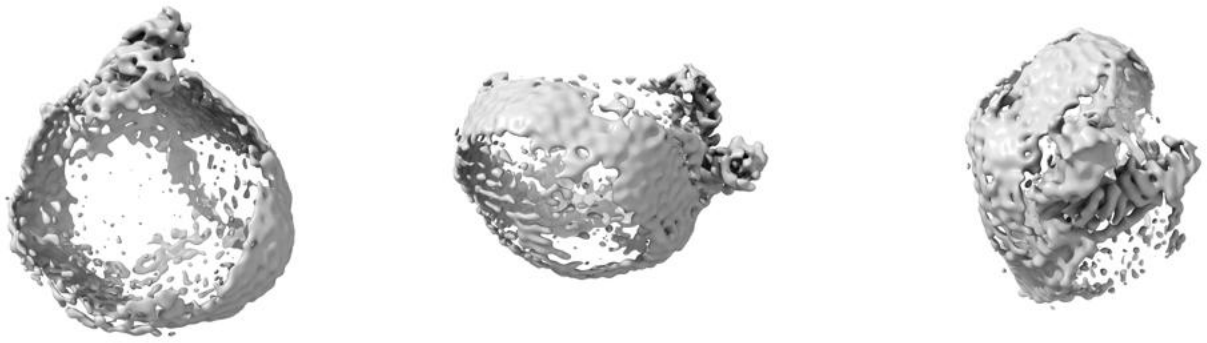


Z

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 0.182. 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.

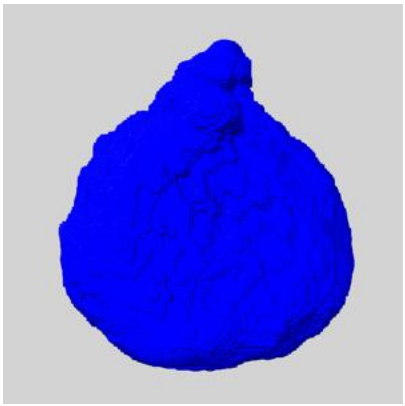
## 6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

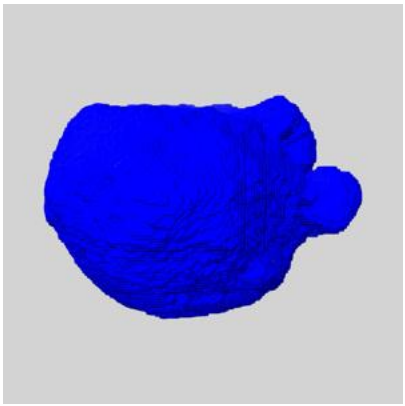
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

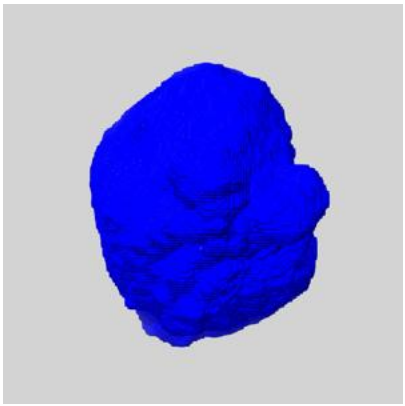
### 6.6.1 emd_47801_msk_1.map (i)



X



Y

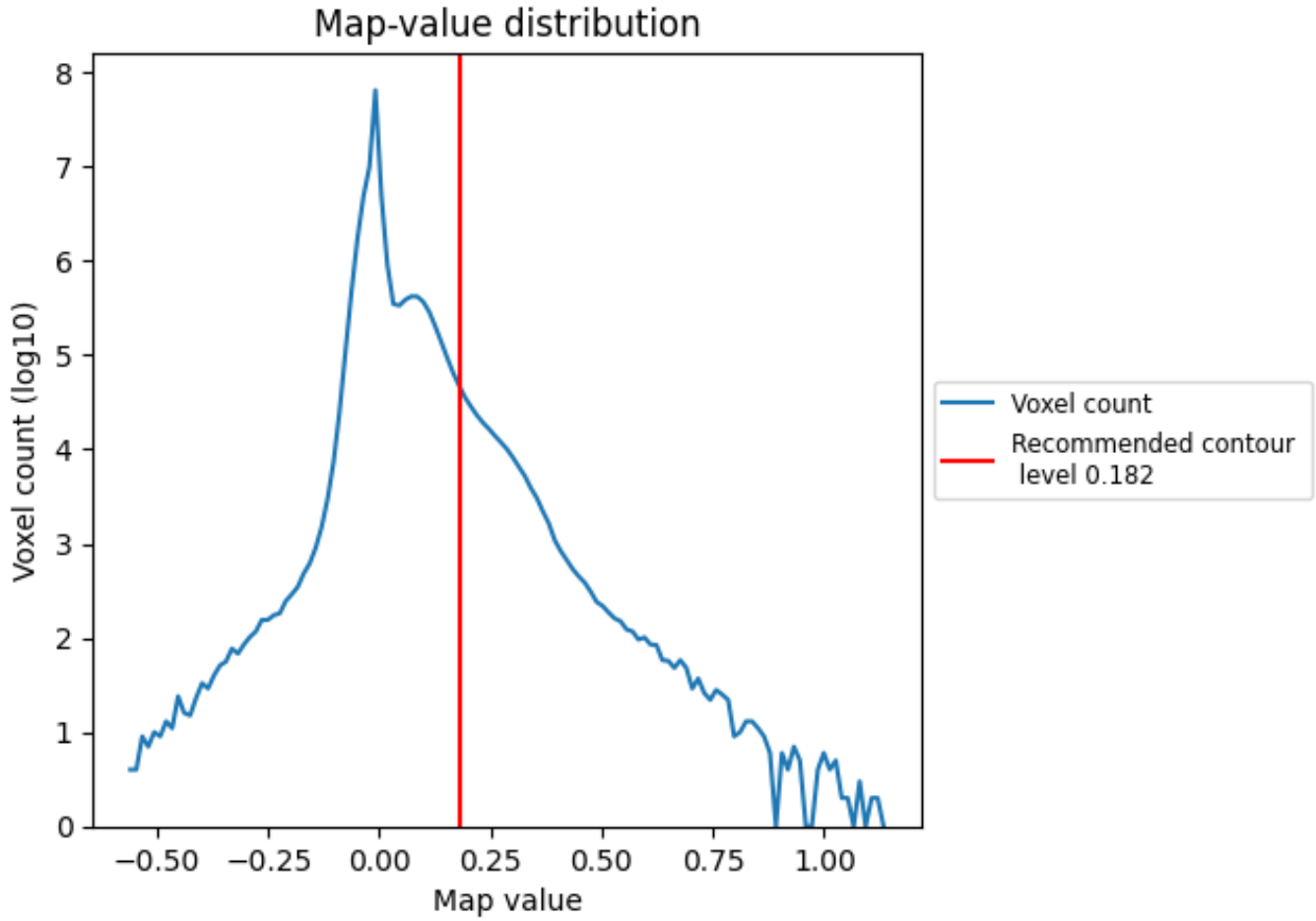


Z

# 7 Map analysis

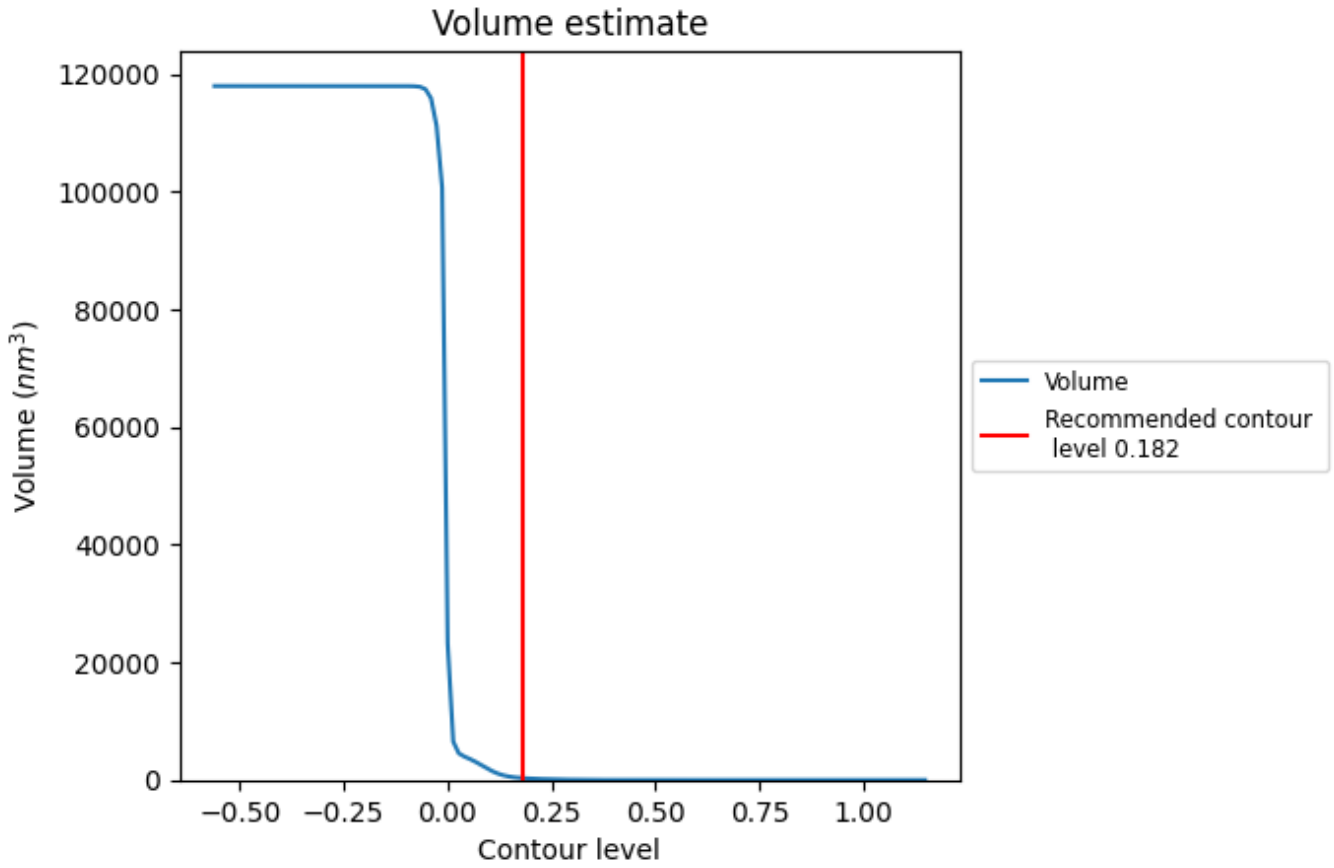
This section contains the results of statistical analysis of the map.

## 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.

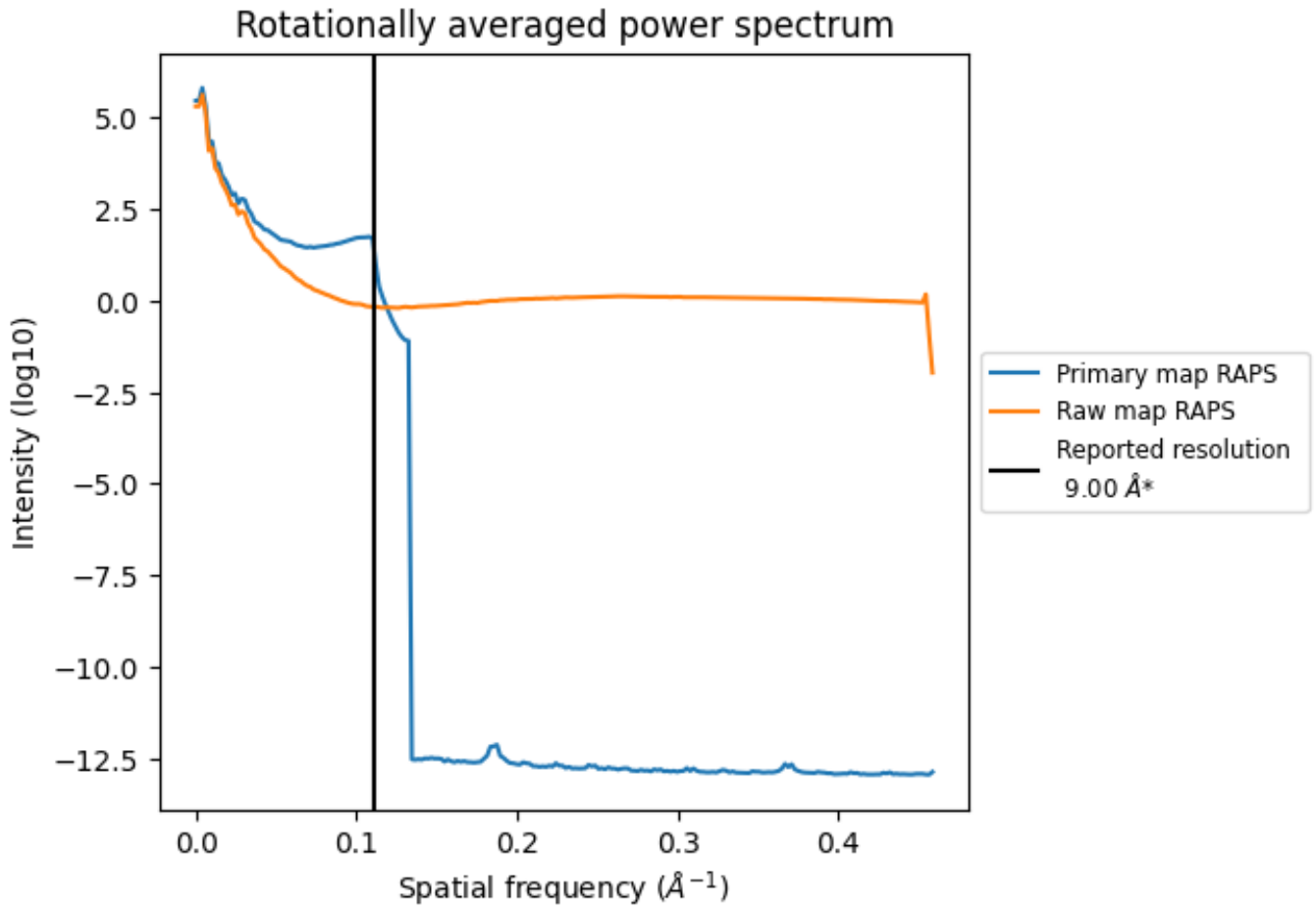
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 304 $nm^3$; this corresponds to an approximate mass of 275 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)

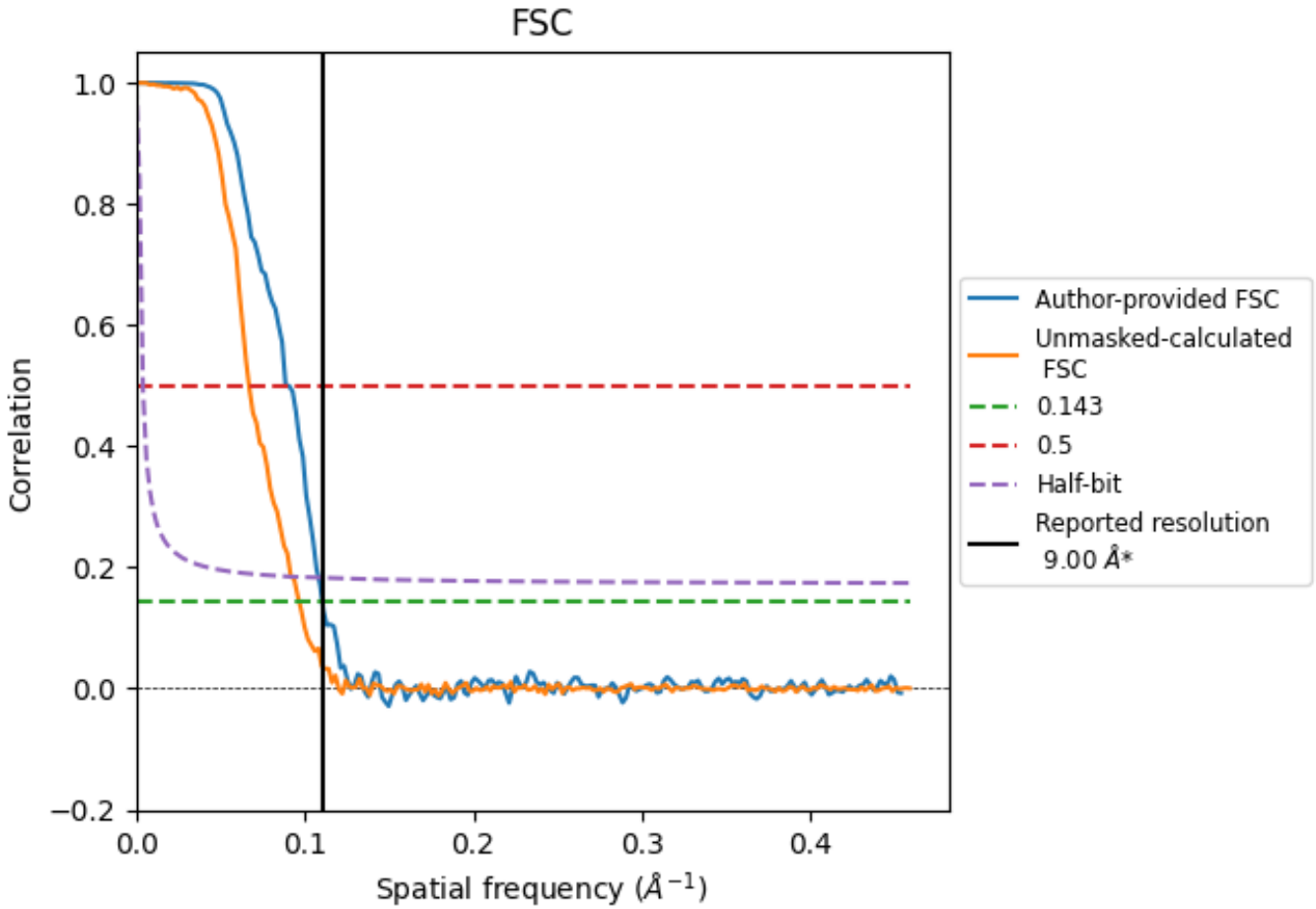



*Reported resolution corresponds to spatial frequency of 0.111 Å$^{-1}$

# 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 0.111 Å$^{-1}$

## 8.2 Resolution estimates (i)

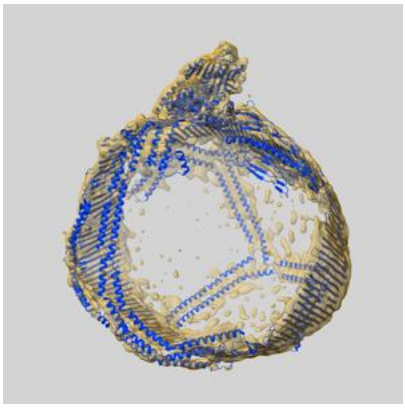
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 9.00 | - | - |
| Author-provided FSC curve | 9.06 | 11.27 | 9.24 |
| Unmasked-calculated* | 10.34 | 14.93 | 10.85 |

*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 10.34 differs from the reported value 9.0 by more than 10 %

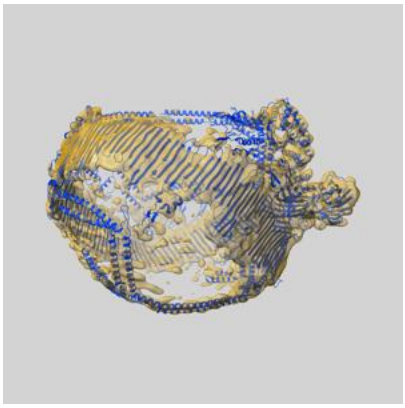
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-47801 and PDB model 9EAG. Per-residue inclusion information can be found in section 3 on page 4.

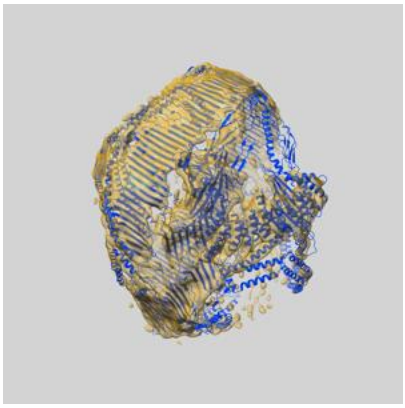
## 9.1 Map-model overlay



X



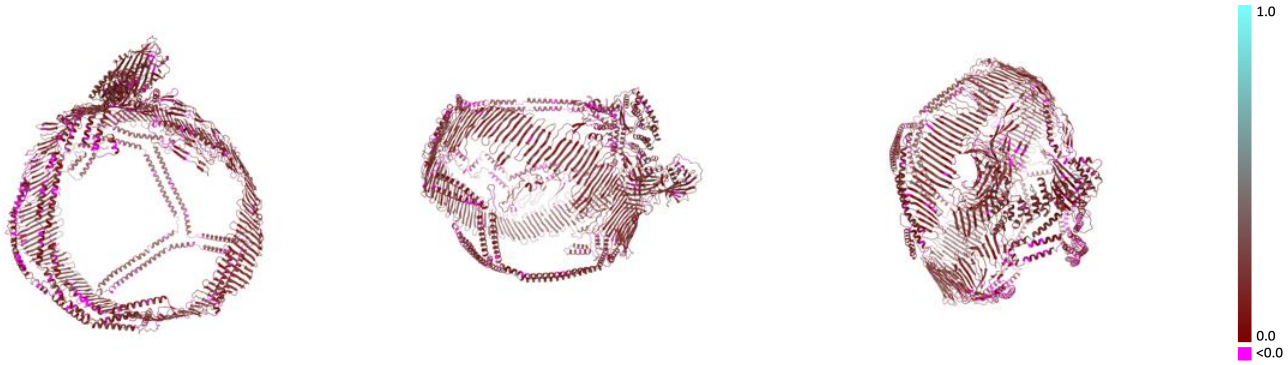
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.182 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.

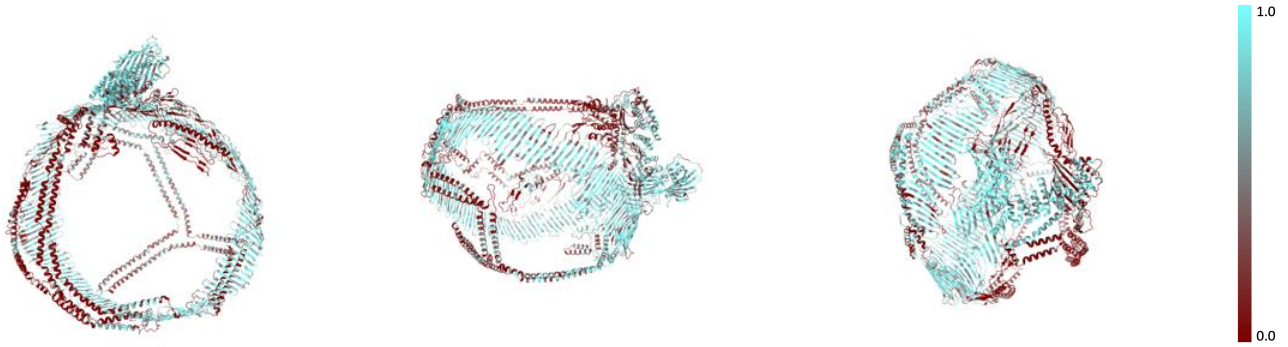
## 9.2 Q-score mapped to coordinate model (i)




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.

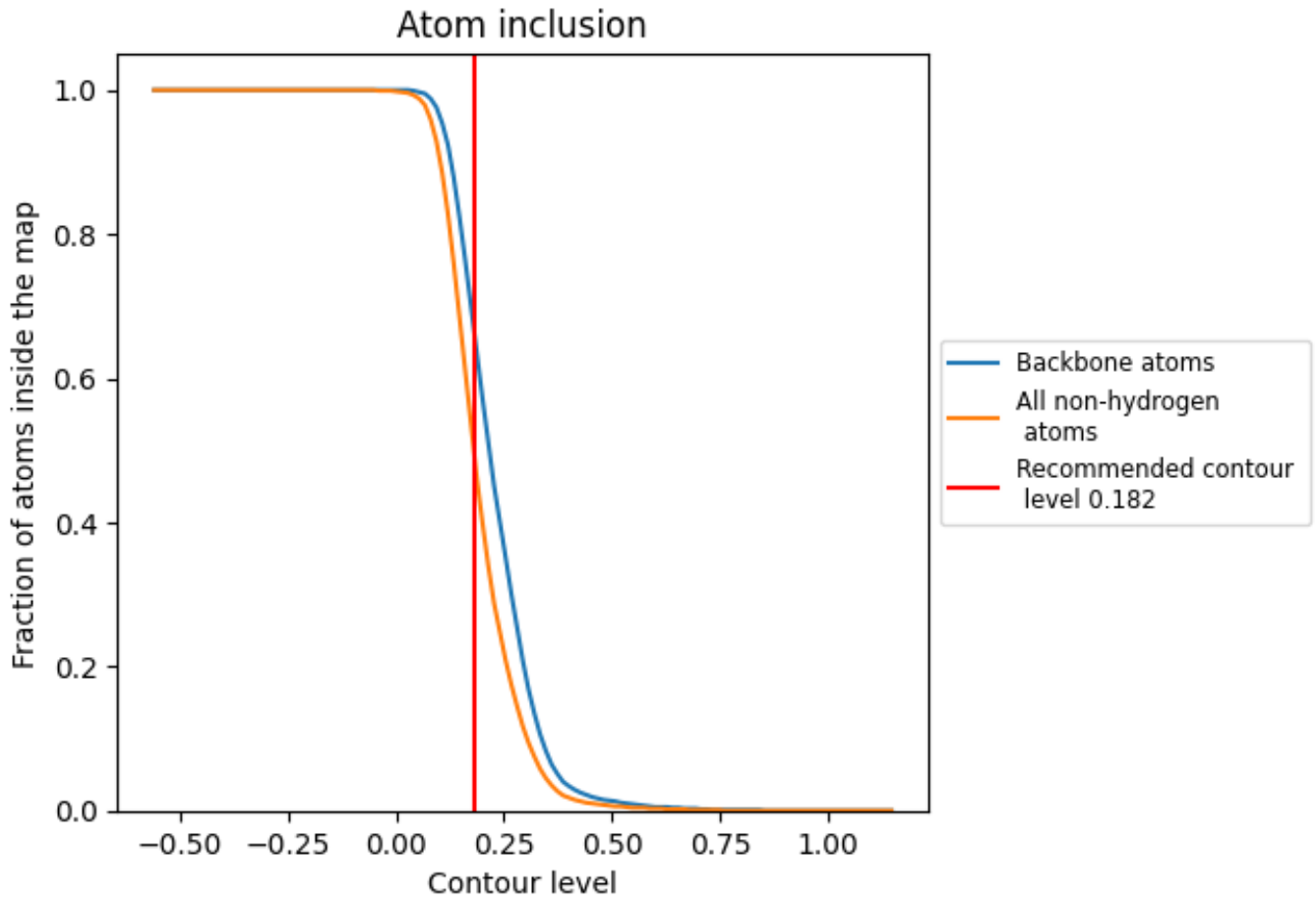
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.182).

## 9.4 Atom inclusion (i)




At the recommended contour level, 66% of all backbone atoms, 49% 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 (0.182) and Q-score for the entire model and for each chain.


| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.4900 | 0.1570 |
| A | 0.4900 | 0.1570 |