Full wwPDB EM Validation Report ⓘ

Apr 24, 2025 – 01:38 PM EDT

PDB ID	:	9BMN / pdb_00009bmn
EMDB ID	:	EMD-44704
Title	:	State-5 of motor domain from full-length human dynein-1 in 5mM AMPPNP
Authors	:	Chai, P.; Zhang, K.
Deposited on	:	2024-05-02
Resolution	:	3.80 Å(reported)

This is a Full wwPDB EM Validation 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:

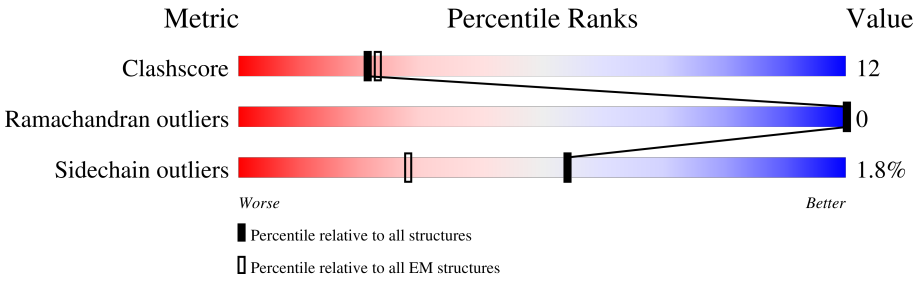
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	4646	9% 42% 16% • 42%

2 Entry composition

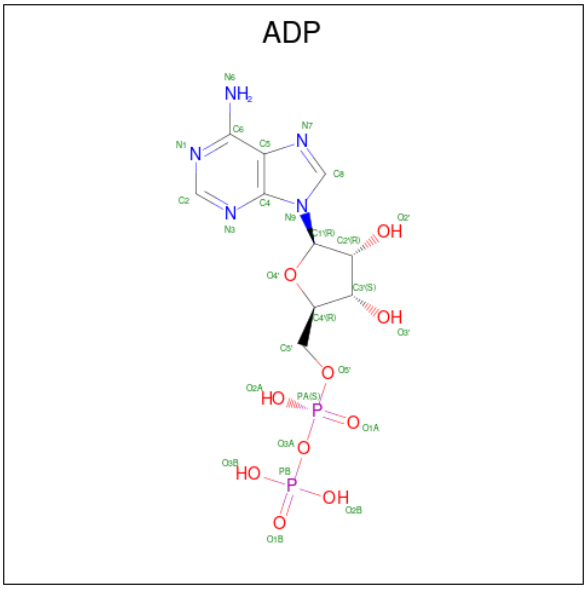
There are 3 unique types of molecules in this entry. The entry contains 21867 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cytoplasmic dynein 1 heavy chain 1.

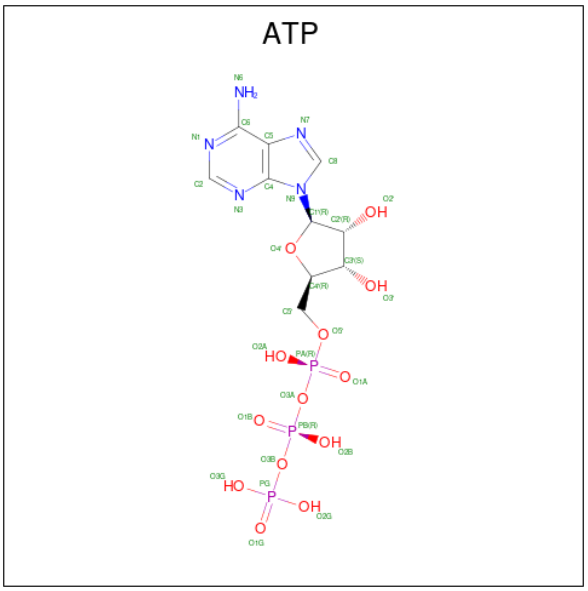
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2711	21755	13852	3757	4035	111	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



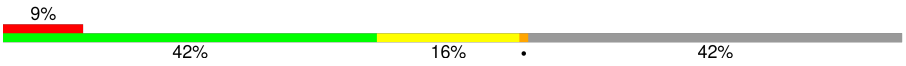
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

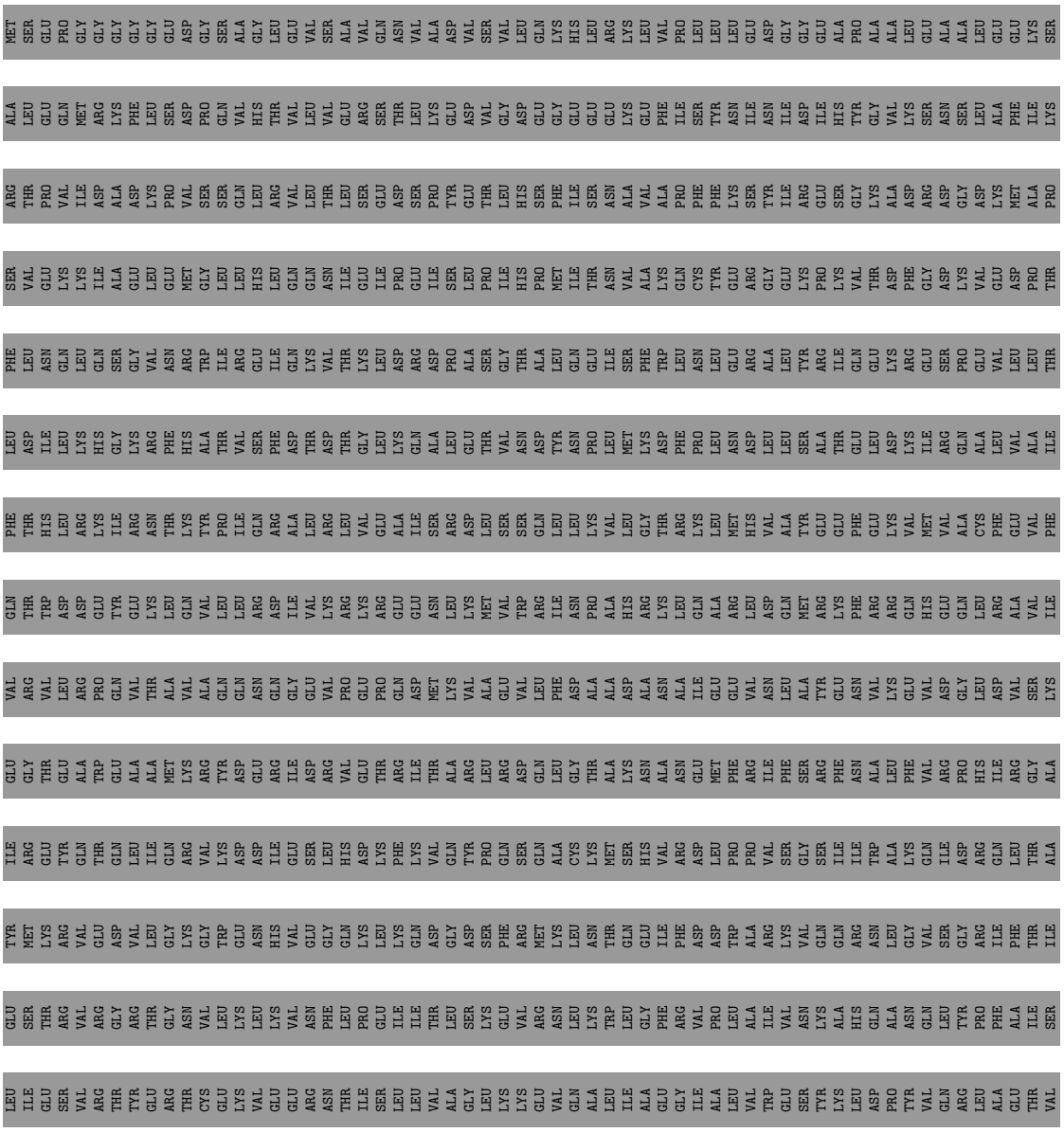
3 Residue-property plots (i)

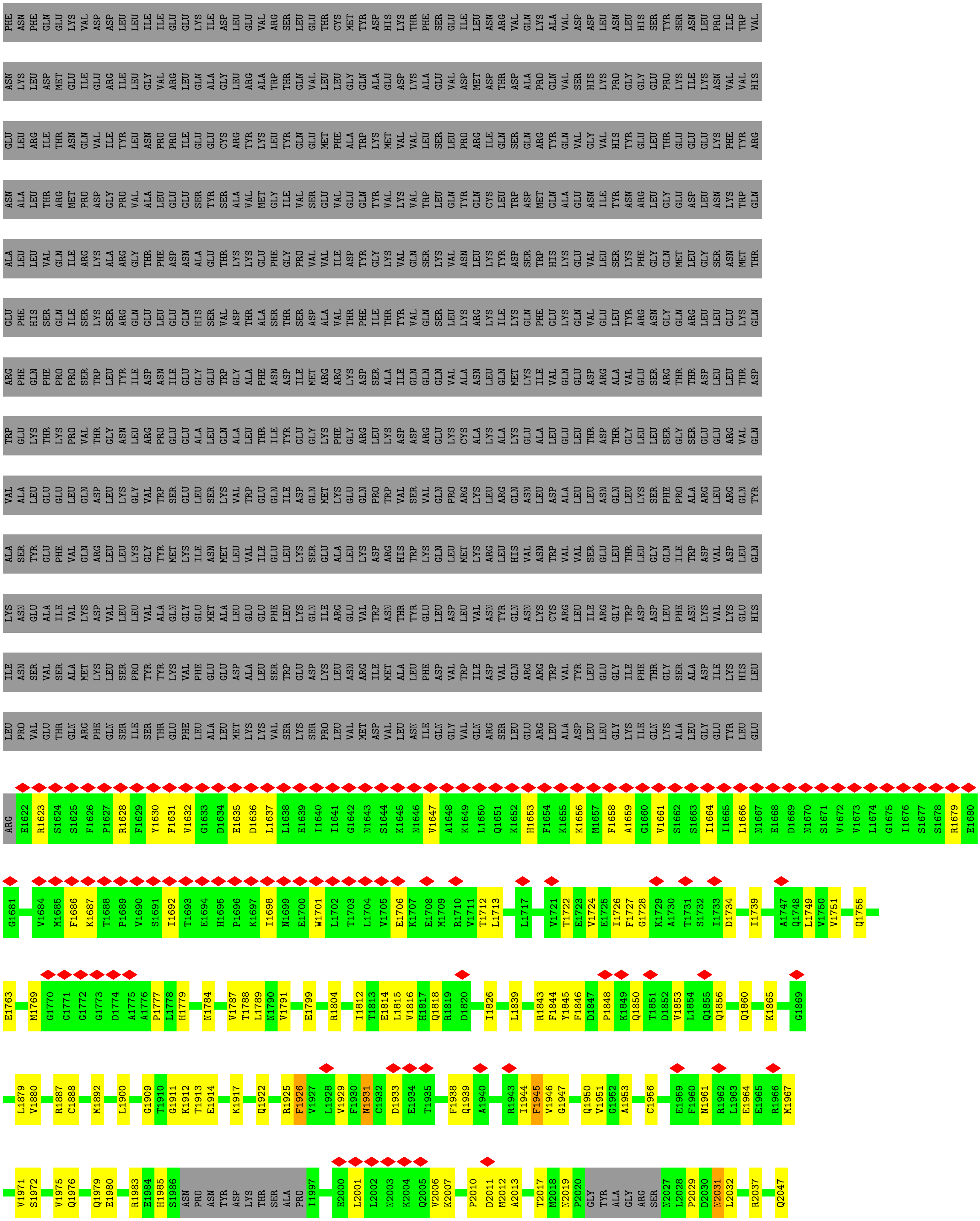
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

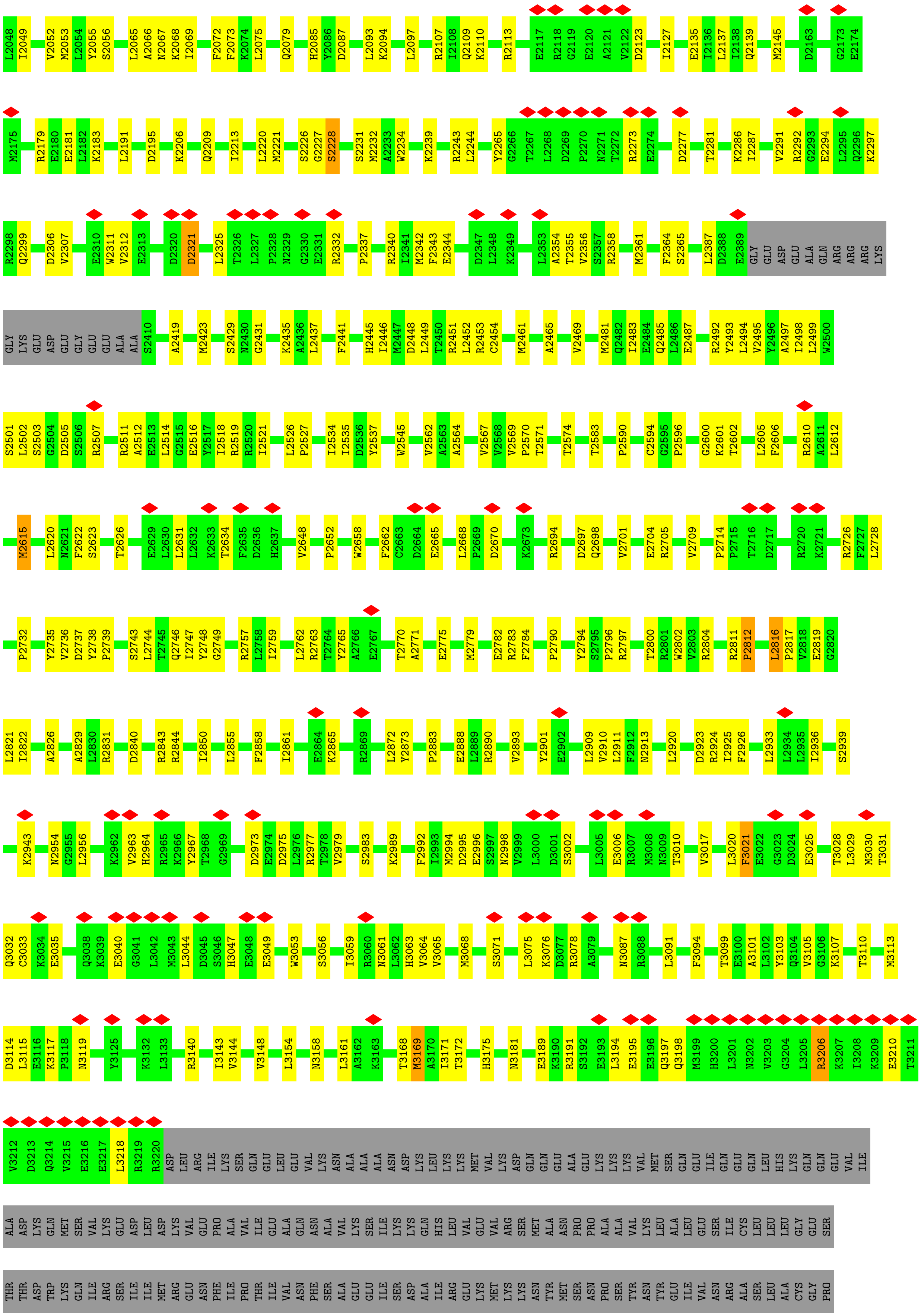
• Molecule 1: Cytoplasmic dynein 1 heavy chain 1

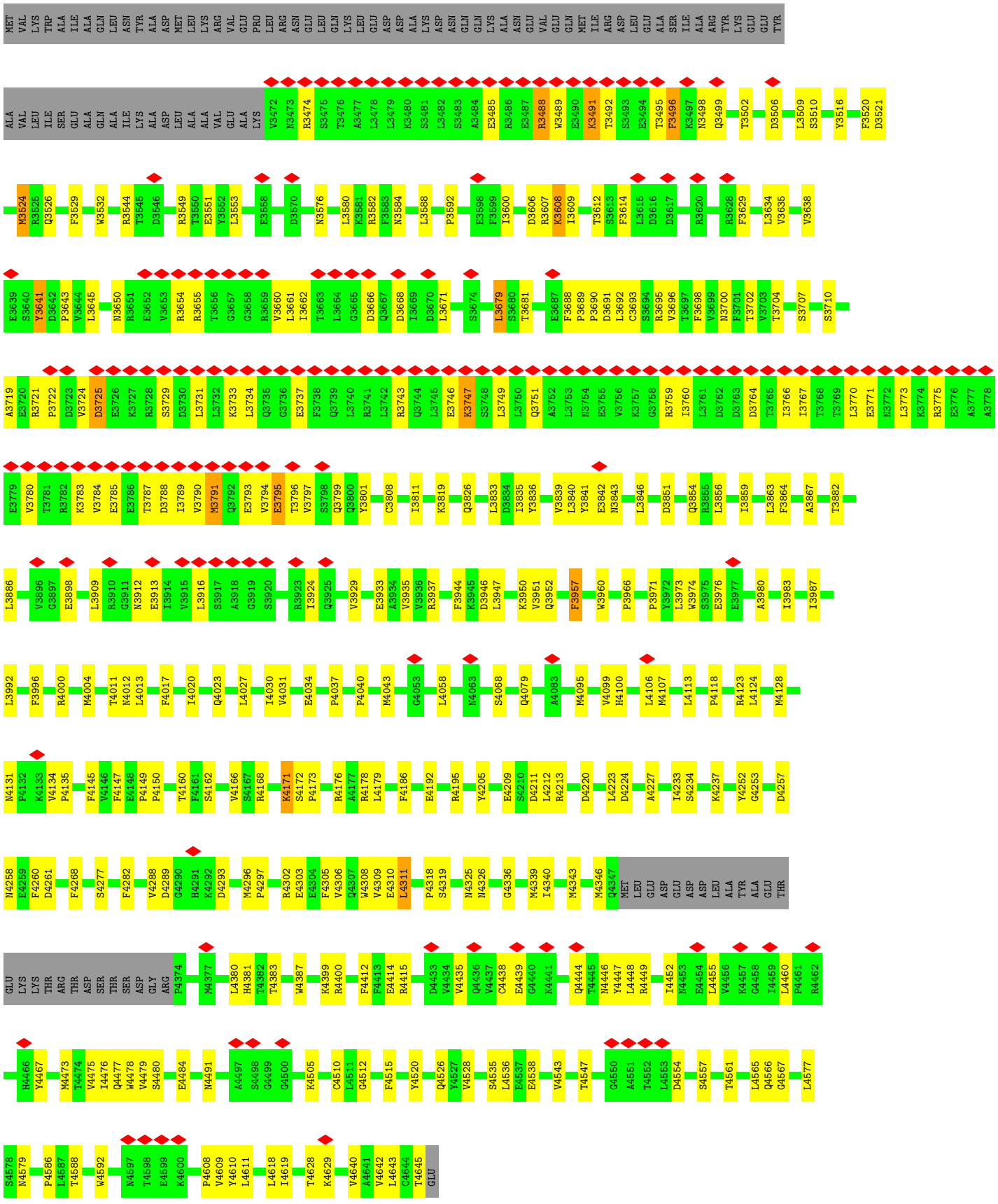
Chain A:








L2048 I2049 V2052 M2053 L2054 Y2055 S2056 L2065 A2066 N2067 K2068 I2069 F2072 F2073 K2074 L2075 Q2079 H2085 Y2086 D2087 L2093 K2094 L2097 R2107 I2108 Q2109 K2110 R2113 E2117 R2118 G2119 E2120 A2121 V2122 D2123 I2127 E2135 I2136 L2137 I2138 Q2139 M2145 D2163 G2173 E2174
M2175 R2179 E2180 E2181 L2182 K2183 L2191 D2195 K2206 Q2209 I2213 L2220 M2221 S2226 G2227 S2228 S2231 M2232 A2233 W2234 K2239 R2243 L2244 Y2265 G2266 T2267 L2268 D2269 P2270 N2271 T2272 R2273 E2274 D2277 T2281 K2286 I2287 V2291 R2292 G2293 E2294 L2295 Q2296 K2297
R2298 Q2299 D2306 V2307 E2310 W2311 V2312 E2313 D2320 D2321 L2325 T2326 L2327 P2328 N2329 G2330 E2331 R2332 P2337 R2340 I2341 M2342 F2343 E2344 D2347 L2348 K2349 L2353 A2354 T2355 V2356 S2357 R2358 M2361 F2364 S2365 L2387 D2388 E2389 GLY GLU ASP GLU ALA GLN ARG ARG ARG LYS
GLY LYS GLU ASP GLU GLY GLU GLU ALA ALA S2410 A2419 M2423 S2429 N2430 G2431 K2435 A2436 L2437 F2441 H2445 I2446 M2447 D2448 L2449 T2450 R2451 L2452 R2453 C2454 M2461 A2465 V2469 M2481 Q2482 I2483 E2484 Q2485 L2486 E2487 R2492 Y2493 L2494 V2495 Y2496 A2497 I2498 L2499 W2500
S2501 L2502 S2503 G2504 D2505 S2506 R2507 R2511 A2512 E2513 L2514 G2515 E2516 Y2517 I2518 R2519 R2520 I2521 L2526 P2527 I2534 I2535 D2536 Y2537 W2545 V2562 A2563 A2564 V2567 V2568 V2569 P2570 T2571 T2574 T2583 P2590 C2594 G2595 P2596 G2600 K2601 T2602 L2605 F2606 R2610 A2611 L2612
M2615 L2620 N2621 F2622 S2623 T2626 E2629 L2630 L2631 L2632 K2633 T2634 F2635 D2636 H2637 V2648 P2652 W2658 F2662 C2663 D2664 E2665 L2668 P2669 D2670 K2673 R2694 D2697 Q2698 V2701 E2704 R2705 V2709 P2714 P2715 T2716 D2717 R2720 K2721 R2726 F2727 L2728
P2732 Y2735 V2736 D2737 Y2738 P2739 S2743 L2744 T2745 Q2746 I2747 Y2748 G2749 R2757 L2758 I2759 L2762 R2763 T2764 Y2765 A2766 E2767 T2770 A2771 E2775 M2779 E2782 R2783 F2784 P2790 Y2794 S2795 P2796 R2797 T2800 R2801 W2802 V2803 R2804 R2811 P2812 L2816 P2817 V2818 E2819 G2820
L2821 I2822 A2826 A2829 L2830 R2831 D2840 R2843 R2844 I2850 L2855 F2858 I2861 E2864 K2865 R2869 L2872 Y2873 P2883 E2888 L2889 R2890 V2893 Y2901 E2902 L2909 V2910 L2911 F2912 N2913 L2920 D2923 R2924 I2925 F2926 L2933 L2934 L2935 I2936 S2939
K2943 N2954 G2955 L2956 K2962 V2963 H2964 R2965 K2966 Y2967 T2968 G2969 D2973 E2974 D2975 L2976 R2977 T2978 V2979 S2983 K2989 F2992 I2993 M2994 D2995 E2996 S2997 N2998 V2999 L3000 D3001 S3002 L3005 E3006 R3007 M3008 N3009 T3010 V3017 L3020 F3021 E3022 G3023 D3024 E3025 T3028 L3029 M3030 T3031
Q3032 C3033 K3034 E3035 Q3038 K3039 E3040 G3041 L3042 M3043 L3044 D3045 S3046 H3047 E3048 E3049 W3053 S3056 I3059 R3060 N3061 L3062 H3063 V3064 V3065 M3068 S3071 L3075 K3076 D3077 R3078 A3079 N3087 R3088 L3091 F3094 T3099 E3100 A3101 L3102 Y3103 Q3104 V3105 G3106 K3107 T3110 M3113
D3114 L3115 E3116 K3117 P3118 N3119 Y3125 K3132 L3133 R3140 I3143 V3144 V3148 L3154 N3158 L3161 A3162 K3163 T3168 M3169 A3170 I3171 T3172 H3175 N3181 E3189 K3190 R3191 S3192 E3193 L3194 E3195 E3196 Q3197 Q3198 M3199 H3200 L3201 N3202 V3203 G3204 L3205 R3206 K3207 I3208 K3209 E3210 T3211
V3212 D3213 Q3214 V3215 E3216 E3217 L3218 R3219 R3220 ASP LEU ARG ILE LYS SER GLN GLU LEU GLU VAL LYS ASN ALA ALA ALA ASN ASP LYS LEU LYS LYS MET VAL LYS ASP GLN GLN GLU ALA GLU LYS LYS LYS VAL MET SER GLN GLU ILE GLN GLU GLN LEU HIS LYS GLN GLN GLU VAL ILE
ALA ASP LYS GLN MET SER VAL LYS GLU ASP LEU ASP LYS VAL GLU PRO ALA VAL ILE GLU ALA GLN ASN ALA VAL LYS SER ILE LYS LYS GLN HIS LEU VAL GLU VAL ARG SER MET ALA ASN PRO PRO ALA ALA VAL LYS LEU ALA LEU GLU SER ILE CYS LEU LEU LEU GLY GLU SER
THR THR ASP TRP LYS GLN ILE ARG SER ILE ILE MET ARG GLU ASN PHE ILE PRO THR ILE VAL ASN PHE SER ALA GLU GLU ILE SER ASP ALA ILE ARG GLU LYS MET LYS LYS ASN TYR MET SER ASN PRO SER TYR ASN TYR GLU ILE VAL ASN ARG ALA SER LEU ALA CYS GLY PRO


MET VAL LYS TRP ALA ILE ALA GLN LEU ASN TYR ALA ASP MET LEU LYS ARG VAL GLU PRO LEU ARG ASN GLU LEU GLN LYS LEU GLU ASP ASP ALA LYS ASP ASN GLN GLN LYS ALA ASN GLU VAL GLU GLN MET ILE ARG ASP LEU GLU GLU ALA SER ILE ALA ARG TYR LYS GLU GLU TYR
ALA VAL LEU ILE SER GLU ALA GLN ALA ILE LYS ALA ASP LEU ALA ALA VAL GLU ALA LYS V3472 N3473 R3474 S3475 T3476 A3477 L3478 L3479 K3480 S3481 L3482 S3483 A3484 E3485 R3486 E3487 R3488 W3489 E3490 K3491 T3492 S3493 E3494 T3495 F3496 K3497 N3498 Q3499 T3502 D3506 L3509 S3510 Y3516 F3520 D3521
M3524 R3525 Q3526 F3529 W3532 R3544 T3545 D3546 R3549 T3550 E3551 Y3552 L3553 E3558 D3570 N3576 L3580 K3581 R3582 F3583 N3584 L3588 P3592 E3598 F3599 I3600 D3606 R3607 K3608 I3609 T3612 S3613 F3614 L3615 D3616 D3617 R3620 R3628 F3629 L3634 V3635 V3638
E3639 S3640 Y3641 D3642 P3643 V3644 L3645 N3650 R3651 E3652 V3653 R3654 R3655 T3656 G3657 G3658 R3659 V3660 L3661 I3662 T3663 L3664 G3665 D3666 Q3667 D3668 I3669 D3670 L3671 S3674 L3679 S3680 T3681 E3687 F3688 P3689 P3690 D3691 L3692 C3693 S3694 R3695 V3696 T3697 F3698 V3699 N3700 F3701 T3702 V3703 T3704 S3707 S3710
A3719 E3720 R3721 P3722 D3723 V3724 D3725 E3726 K3727 R3728 S3729 D3730 L3731 L3732 K3733 L3734 Q3735 G3736 E3737 F3738 Q3739 L3740 R3741 L3742 R3743 Q3744 L3745 E3746 K3747 S3748 L3749 L3750 Q3751 A3752 L3753 N3754 E3755 V3756 K3757 G3758 R3759 I3760 L3761 D3762 D3763 D3764 T3765 I3766 I3767 T3768 T3769 L3770 E3771 N3772 L3773 K3774 R3775 E3776 A3777 A3778
E3779 V3780 T3781 R3782 K3783 V3784 E3785 E3786 T3787 D3788 I3789 V3790 N3791 Q3792 E3793 V3794 E3795 T3796 V3797 S3798 Q3799 Q3800 Y3801 C3808 I3811 K3819 Q3826 L3833 D3834 I3835 Y3836 V3839 L3840 Y3841 E3842 N3843 L3846 D3851 Q3854 R3855 L3856 I3859 L3863 F3864 A3867 T3882
L3886 V3896 G3897 E3898 L3909 R3910 G3911 N3912 E3913 I3914 V3915 L3916 S3917 A3918 G3919 S3920 R3923 I3924 Q3925 V3929 E3933 A3934 V3935 V3936 R3937 F3944 K3945 D3946 L3947 K3950 V3951 Q3952 F3957 W3960 P3966 P3971 Y3972 L3973 W3974 S3975 E3976 E3977 A3980 I3983 I3987
L3992 F3996 R4000 M4004 T4011 N4012 L4013 F4017 I4020 Q4023 L4027 I4030 V4031 E4034 P4037 P4040 M4043 G4053 L4058 M4063 S4068 Q4079 A4083 M4095 V4099 H4100 L4106 M4107 L4113 P4118 R4123 L4124 M4128
N4131 P4132 K4133 V4134 P4135 F4145 V4146 F4147 E4148 P4149 P4150 T4160 F4161 S4162 V4166 S4167 R4168 K4171 S4172 P4173 R4176 A4177 R4178 L4179 F4186 E4192 R4195 Y4205 E4209 S4210 D4211 L4212 R4213 D4220 L4223 D4224 A4227 I4233 S4234 K4237 Y4252 G4253 D4257
N4258 E4259 F4260 D4261 F4268 S4277 F4282 V4288 D4289 G4290 H4291 K4292 D4293 M4296 P4297 R4302 E4303 E4304 F4305 V4306 Q4307 W4308 V4309 E4310 L4311 P4318 S4319 N4325 N4326 G4336 M4339 I4340 M4343 M4346 Q4347 MET LEU GLU ASP GLU ASP LEU ALA TYR ALA GLU THR
GLU LYS LYS THR ARG THR ASP SER THR SER ASP GLY ARG P4374 M4377 L4380 H4381 T4382 T4383 W4387 K4399 R4400 F4412 F4413 E4414 R4415 D4433 V4434 V4435 Q4436 V4437 C4438 E4439 G4440 K4441 Q4444 T4445 N4446 Y4447 L4448 R4449 I4452 N4453 E4454 L4455 V4456 K4457 G4458 I4459 L4460 P4461 R4462
H4466 Y4467 M4473 T4474 V4475 I4476 Q4477 W4478 V4479 S4480 E4484 N4491 A4497 S4498 G4499 G4500 K4505 C4510 L4511 G4512 F4515 Y4520 Q4526 Y4527 V4528 S4535 L4536 E4537 E4538 V4543 T4547 G4550 A4551 T4552 L4553 D4554 S4557 T4561 L4565 Q4566 G4567 L4577
S4578 N4579 P4586 L4587 T4588 W4592 N4597 T4598 E4599 K4600 P4608 V4609 Y4610 L4611 L4618 I4619 T4628 K4629 V4640 A4641 V4642 L4643 C4644 T4645 GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58149	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.938	Depositor
Minimum map value	-0.536	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	333.312, 333.312, 333.312	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.302, 1.302, 1.302	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ATP

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	0.27	0/22220	0.51	6/30121 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2812	PRO	CA-N-CD	-8.55	99.53	111.50
1	A	4311	LEU	CA-CB-CG	6.43	130.09	115.30
1	A	1848	PRO	CA-N-CD	-5.80	103.37	111.50
1	A	4113	LEU	CA-CB-CG	5.53	128.03	115.30
1	A	3791	MET	CA-CB-CG	5.18	122.10	113.30
1	A	2816	LEU	CA-CB-CG	5.01	126.83	115.30

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	21755	0	21789	507	0
2	A	81	0	36	10	0
3	A	31	0	12	1	0
All	All	21867	0	21837	507	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 12.

All (507) 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:3662:ILE:HD11	1:A:3671:LEU:HB2	1.54	0.88
1:A:3790:VAL:HG13	1:A:3794:VAL:HB	1.56	0.86
1:A:3661:LEU:HD11	1:A:3668:ASP:HB3	1.61	0.83
1:A:3731:LEU:HD12	1:A:3790:VAL:HG21	1.66	0.78
1:A:2925:ILE:HG21	1:A:2933:LEU:HG	1.67	0.77
1:A:4176:ARG:NH1	1:A:4220:ASP:OD1	2.18	0.77
1:A:4040:PRO:HB3	1:A:4124:LEU:HD23	1.67	0.76
1:A:3992:LEU:O	1:A:3996:PHE:HB2	1.87	0.74
1:A:2494:LEU:O	1:A:2498:ILE:HD12	1.90	0.72
1:A:1950:GLN:HG2	1:A:2006:VAL:HG13	1.71	0.71
1:A:1635:GLU:HB3	1:A:2273:ARG:HB3	1.71	0.71
1:A:2910:VAL:HG11	1:A:3105:VAL:HG22	1.71	0.70
1:A:3198:GLN:HE22	1:A:3496:PHE:HD1	1.37	0.69
1:A:4303:GLU:OE1	1:A:4303:GLU:N	2.26	0.68
1:A:1925:ARG:HH12	1:A:2011:ASP:HB3	1.57	0.68
1:A:2933:LEU:HB2	1:A:3065:VAL:HG23	1.74	0.68
1:A:3983:ILE:HG13	1:A:4011:THR:HG22	1.74	0.68
1:A:3733:LYS:O	1:A:3737:GLU:N	2.19	0.68
1:A:3496:PHE:HA	1:A:3499:GLN:OE1	1.94	0.67
1:A:2499:LEU:HD21	1:A:2518:ILE:HG21	1.75	0.67
1:A:2287:ILE:HA	1:A:2294:GLU:HG3	1.78	0.66
1:A:2446:ILE:HD11	1:A:2714:PRO:HB3	1.78	0.66
1:A:3689:PRO:HG2	1:A:3692:LEU:HD23	1.78	0.66
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.29	0.66
1:A:1964:GLU:HG2	1:A:1967:MET:H	1.61	0.65
1:A:1679:ARG:HH21	1:A:2332:ARG:HH12	1.44	0.65
1:A:3526:GLN:OE1	1:A:3549:ARG:NH2	2.29	0.65
1:A:1961:ASN:ND2	1:A:2019:ASN:O	2.29	0.64
1:A:3691:ASP:O	1:A:3695:ARG:HG2	1.98	0.64
1:A:2615:MET:HG3	1:A:2658:TRP:HB2	1.80	0.64
1:A:1913:THR:O	1:A:1917:LYS:HG3	1.97	0.64
1:A:3576:ASN:ND2	1:A:3700:ASN:O	2.29	0.64
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.80	0.64
1:A:2923:ASP:OD1	1:A:2954:ASN:ND2	2.31	0.63
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.79	0.63
1:A:1799:GLU:OE1	1:A:2109:GLN:NE2	2.32	0.62
1:A:2226:SER:HB2	1:A:2726:ARG:HG2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3010:THR:HG22	1:A:3017:VAL:HG22	1.82	0.62
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.80	0.62
1:A:2605:LEU:HD11	1:A:2709:VAL:HG11	1.80	0.62
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.81	0.62
1:A:2073:PHE:HE2	1:A:2093:LEU:HA	1.64	0.62
1:A:1912:LYS:HE2	1:A:2017:THR:HB	1.82	0.61
1:A:2453:ARG:NH1	1:A:2505:ASP:OD2	2.32	0.61
1:A:3021:PHE:CE1	1:A:3029:LEU:HB2	2.36	0.61
1:A:4043:MET:HG2	1:A:4147:PHE:HE2	1.65	0.61
1:A:4297:PRO:HG3	1:A:4308:TRP:CG	2.35	0.61
1:A:4305:PHE:O	1:A:4309:VAL:HG23	2.00	0.61
1:A:1931:ASN:O	1:A:1931:ASN:ND2	2.32	0.61
1:A:2419:ALA:O	1:A:2423:MET:HG3	2.01	0.61
1:A:3650:ASN:OD1	1:A:3695:ARG:NH1	2.33	0.61
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.34	0.60
1:A:2893:VAL:HG13	1:A:2911:LEU:HD11	1.83	0.60
1:A:1755:GLN:HG2	1:A:1814:GLU:OE1	2.00	0.60
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.83	0.60
1:A:4027:LEU:HB3	1:A:4058:LEU:HD22	1.84	0.60
1:A:2888:GLU:N	1:A:2888:GLU:OE1	2.33	0.60
1:A:2220:LEU:HB2	1:A:2342:MET:HG2	1.83	0.59
1:A:2483:ILE:O	1:A:2487:GLU:HG3	2.03	0.59
1:A:3028:THR:HG22	1:A:3032:GLN:HE21	1.66	0.59
1:A:1913:THR:OG1	2:A:4701:ADP:O1A	2.20	0.59
1:A:2826:ALA:HA	1:A:2850:ILE:HD11	1.84	0.59
1:A:2179:ARG:NH1	1:A:2195:ASP:OD1	2.35	0.59
1:A:3743:ARG:NH1	1:A:3743:ARG:O	2.35	0.59
1:A:2047:GLN:NE2	1:A:2067:ASN:OD1	2.36	0.59
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.32	0.59
1:A:3749:LEU:HD11	1:A:3770:LEU:HD23	1.85	0.58
1:A:1812:ILE:HG21	1:A:2056:SER:HA	1.86	0.58
1:A:2995:ASP:OD1	1:A:2996:GLU:N	2.37	0.58
1:A:3882:THR:HG22	1:A:4339:MET:HG3	1.85	0.58
1:A:4400:ARG:NH1	1:A:4414:GLU:OE2	2.37	0.58
1:A:2694:ARG:O	1:A:2698:GLN:HA	2.04	0.58
1:A:3733:LYS:HD3	1:A:3737:GLU:HG3	1.86	0.58
1:A:4543:VAL:HG13	1:A:4588:THR:HG23	1.86	0.58
1:A:4037:PRO:HB2	1:A:4118:PRO:HG2	1.86	0.58
1:A:3107:LYS:HG3	1:A:3144:VAL:HG21	1.85	0.58
1:A:2606:PHE:O	1:A:2610:ARG:HG2	2.04	0.57
1:A:3031:THR:O	1:A:3035:GLU:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3835:ILE:HD13	1:A:3867:ALA:HA	1.86	0.57
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.85	0.57
1:A:3947:LEU:HA	1:A:3950:LYS:HD2	1.85	0.57
1:A:3175:HIS:HB3	1:A:3516:TYR:HE1	1.69	0.57
1:A:2461:MET:HG2	1:A:2583:THR:HG21	1.87	0.57
1:A:3913:GLU:OE2	1:A:3913:GLU:N	2.38	0.57
1:A:3499:GLN:HA	1:A:3502:THR:HG22	1.86	0.57
1:A:3789:ILE:O	1:A:3793:GLU:N	2.32	0.56
1:A:3843:ASN:HB3	1:A:3846:LEU:HD12	1.87	0.56
1:A:2623:SER:O	1:A:2626:THR:OG1	2.23	0.56
1:A:2816:LEU:HD23	1:A:2817:PRO:O	2.06	0.56
1:A:3746:GLU:HG2	1:A:3773:LEU:HD13	1.87	0.56
1:A:3898:GLU:OE1	1:A:3983:ILE:HD13	2.06	0.56
1:A:3951:VAL:HG22	1:A:3957:PHE:HE2	1.69	0.56
1:A:2797:ARG:NH1	1:A:3087:ASN:OD1	2.37	0.56
1:A:3553:LEU:O	1:A:3582:ARG:NH1	2.37	0.56
1:A:1961:ASN:HD21	1:A:2019:ASN:HB3	1.70	0.56
1:A:2085:HIS:HB2	1:A:2361:MET:HG2	1.88	0.56
1:A:3654:ARG:HG3	1:A:3661:LEU:HB3	1.87	0.55
1:A:2612:LEU:HB3	1:A:2615:MET:CE	2.36	0.55
1:A:2840:ASP:OD1	1:A:2843:ARG:NH2	2.39	0.55
1:A:2936:ILE:HD11	1:A:3091:LEU:HD12	1.87	0.55
1:A:3654:ARG:HH11	1:A:3661:LEU:HG	1.71	0.55
1:A:3946:ASP:HB2	1:A:3950:LYS:HE2	1.87	0.55
1:A:1860:GLN:HG2	1:A:1865:LYS:HG2	1.88	0.55
1:A:2967:TYR:OH	1:A:2975:ASP:OD2	2.16	0.55
1:A:2321:ASP:OD2	1:A:2321:ASP:N	2.34	0.55
1:A:3729:SER:O	1:A:3733:LYS:HG2	2.05	0.55
1:A:1979:GLN:O	1:A:1983:ARG:HG3	2.06	0.55
1:A:1724:VAL:O	1:A:1728:GLY:N	2.38	0.55
1:A:2065:LEU:HD13	1:A:2137:LEU:HD22	1.88	0.55
1:A:3488:ARG:O	1:A:3491:LYS:HG3	2.05	0.55
1:A:3886:LEU:HD11	1:A:4346:MET:HG3	1.88	0.55
1:A:4460:LEU:HD21	1:A:4478:TRP:CD1	2.41	0.55
1:A:3614:PHE:HZ	1:A:3645:LEU:HD11	1.72	0.55
1:A:4209:GLU:OE1	1:A:4213:ARG:NH2	2.40	0.55
1:A:2068:LYS:NZ	1:A:4535:SER:OG	2.40	0.54
1:A:3189:GLU:OE2	1:A:3582:ARG:NH2	2.39	0.54
1:A:2569:VAL:HG11	1:A:2747:ILE:HA	1.88	0.54
1:A:3113:MET:HG3	1:A:3115:LEU:HD11	1.88	0.54
1:A:3721:ARG:O	1:A:3725:ASP:N	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1816:VAL:HG11	1:A:2052:VAL:HG22	1.90	0.54
1:A:2759:ILE:HD12	1:A:2762:LEU:HD23	1.89	0.54
1:A:1687:LYS:HG2	1:A:1712:THR:HG22	1.89	0.54
1:A:3017:VAL:HB	1:A:3020:LEU:HD23	1.90	0.54
1:A:3030:MET:HG3	1:A:3047:HIS:CD2	2.43	0.54
1:A:4510:CYS:HG	1:A:4561:THR:HG1	1.55	0.54
1:A:3021:PHE:CD1	1:A:3025:GLU:HG3	2.42	0.54
1:A:4192:GLU:OE1	1:A:4195:ARG:NH1	2.40	0.54
1:A:3655:ARG:NE	1:A:3660:VAL:HG22	2.22	0.54
1:A:3661:LEU:HD12	1:A:3662:ILE:H	1.72	0.54
1:A:3721:ARG:HB3	1:A:3724:VAL:HB	1.90	0.54
1:A:1631:PHE:HE2	1:A:1656:LYS:HB3	1.73	0.54
1:A:3759:ARG:HG3	1:A:3760:ILE:HG12	1.89	0.54
1:A:1647:VAL:HG11	1:A:1692:ILE:HD13	1.89	0.54
1:A:2784:PHE:HB2	1:A:2794:TYR:HE2	1.72	0.54
1:A:1763:GLU:OE1	1:A:1845:TYR:OH	2.22	0.53
1:A:1788:THR:O	1:A:1791:VAL:HG12	2.08	0.53
1:A:4475:VAL:O	1:A:4479:VAL:HG23	2.08	0.53
1:A:4512:GLY:HA3	1:A:4645:THR:HG23	1.89	0.53
1:A:2110:LYS:HA	1:A:2113:ARG:NH1	2.23	0.53
1:A:2445:HIS:CD2	1:A:2449:LEU:HD22	2.43	0.53
1:A:3929:VAL:O	1:A:3933:GLU:HG3	2.08	0.53
1:A:4260:PHE:HE2	1:A:4618:LEU:HD11	1.74	0.53
1:A:2665:GLU:HB3	1:A:2668:LEU:HB2	1.90	0.53
1:A:4186:PHE:HE1	1:A:4268:PHE:HB3	1.73	0.53
1:A:4526:GLN:HA	1:A:4536:LEU:HD21	1.91	0.53
1:A:1900:LEU:HD21	1:A:2037:ARG:HH21	1.73	0.53
1:A:1713:LEU:HD22	1:A:1749:LEU:HD21	1.91	0.53
1:A:2757:ARG:HA	1:A:2763:ARG:HH21	1.74	0.53
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.91	0.53
1:A:3588:LEU:HD23	1:A:3698:PHE:HE1	1.74	0.52
1:A:2569:VAL:HB	1:A:2747:ILE:HG13	1.91	0.52
1:A:3506:ASP:OD2	1:A:3544:ARG:HD2	2.09	0.52
1:A:3722:PRO:HA	1:A:3725:ASP:HB3	1.91	0.52
1:A:2737:ASP:OD2	1:A:2738:TYR:N	2.40	0.52
1:A:2901:TYR:OH	1:A:2909:LEU:N	2.36	0.52
1:A:1945:PHE:HE1	1:A:1975:VAL:HG12	1.74	0.52
1:A:1972:SER:HB2	1:A:2031:ASN:HD21	1.74	0.52
1:A:2811:ARG:HB3	1:A:2812:PRO:HD2	1.92	0.52
1:A:1628:ARG:HA	1:A:1951:VAL:HG22	1.91	0.52
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3495:THR:O	1:A:3498:ASN:HB3	2.10	0.52
1:A:2449:LEU:HA	1:A:2453:ARG:HH21	1.75	0.52
1:A:1630:TYR:HD1	1:A:1947:GLY:HA2	1.75	0.52
1:A:2992:PHE:HB3	1:A:3064:VAL:HA	1.92	0.52
1:A:1931:ASN:HD22	1:A:1931:ASN:C	2.12	0.52
1:A:4554:ASP:N	1:A:4557:SER:OG	2.43	0.52
1:A:1814:GLU:OE1	1:A:1818:GLN:NE2	2.39	0.52
1:A:1971:VAL:O	1:A:1975:VAL:HG13	2.10	0.52
1:A:3971:PRO:HG2	1:A:3973:LEU:HD11	1.91	0.51
1:A:4444:GLN:O	1:A:4449:ARG:NH1	2.43	0.51
1:A:2481:MET:HG3	1:A:2485:GLN:NE2	2.26	0.51
1:A:2622:PHE:HZ	1:A:2631:LEU:HD21	1.75	0.51
1:A:3734:LEU:HD22	1:A:3783:LYS:HB3	1.91	0.51
1:A:3944:PHE:CE1	1:A:3974:TRP:HB3	2.45	0.51
1:A:2441:PHE:HA	1:A:2449:LEU:HD23	1.91	0.51
1:A:3808:CYS:HG	1:A:3836:TYR:HE2	1.56	0.51
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.92	0.51
1:A:1784:ASN:O	1:A:1787:VAL:HG12	2.11	0.51
1:A:3044:LEU:HB3	1:A:3049:GLU:HG3	1.92	0.51
1:A:1909:GLY:N	2:A:4701:ADP:O2B	2.43	0.51
1:A:2469:VAL:HG22	1:A:2481:MET:HE1	1.92	0.51
1:A:3030:MET:HA	1:A:3030:MET:HE3	1.93	0.50
1:A:3114:ASP:OD2	1:A:3114:ASP:N	2.44	0.50
1:A:3796:THR:HA	1:A:3799:GLN:HG3	1.93	0.50
1:A:4068:SER:HA	1:A:4095:MET:HB3	1.93	0.50
1:A:4311:LEU:O	1:A:4311:LEU:HD23	2.11	0.50
1:A:4567:GLY:HA3	1:A:4640:VAL:HG22	1.92	0.50
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.44	0.50
1:A:1686:PHE:HA	1:A:1712:THR:HG21	1.93	0.50
1:A:2297:LYS:HB2	1:A:2299:GLN:HE22	1.77	0.50
1:A:4100:HIS:HB2	1:A:4131:ASN:HD21	1.76	0.50
1:A:1880:VAL:HG21	1:A:2049:ILE:HG12	1.93	0.50
1:A:3690:PRO:HA	1:A:3693:CYS:SG	2.51	0.50
1:A:3783:LYS:O	1:A:3787:THR:HG23	2.11	0.50
1:A:4387:TRP:HZ3	1:A:4455:LEU:HD21	1.75	0.50
1:A:2461:MET:CE	1:A:2497:ALA:HA	2.42	0.50
1:A:2446:ILE:HG22	1:A:2505:ASP:O	2.11	0.50
1:A:4566:GLN:O	1:A:4640:VAL:HA	2.12	0.50
1:A:1853:VAL:HA	1:A:1856:GLN:HG3	1.94	0.50
1:A:3609:ILE:HD11	1:A:3634:LEU:HB2	1.94	0.50
1:A:3791:MET:O	1:A:3795:GLU:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2518:ILE:HA	1:A:2521:ILE:HG12	1.94	0.50
1:A:2865:LYS:O	1:A:2865:LYS:NZ	2.40	0.50
1:A:2872:LEU:HD12	1:A:2920:LEU:HD12	1.93	0.50
1:A:3071:SER:O	1:A:3075:LEU:N	2.38	0.50
1:A:4179:LEU:HD12	1:A:4223:LEU:HD11	1.94	0.50
1:A:2049:ILE:HD11	2:A:4701:ADP:C6	2.47	0.49
1:A:2694:ARG:O	1:A:2698:GLN:CA	2.60	0.49
1:A:3161:LEU:HB3	1:A:3168:THR:HG22	1.95	0.49
1:A:4277:SER:HA	1:A:4282:PHE:CG	2.47	0.49
1:A:3785:GLU:O	1:A:3789:ILE:HG13	2.12	0.49
1:A:3158:ASN:ND2	1:A:3169:MET:O	2.36	0.49
1:A:4171:LYS:HG3	1:A:4172:SER:H	1.76	0.49
1:A:4387:TRP:HZ2	1:A:4476:ILE:HG13	1.77	0.49
1:A:2562:VAL:O	1:A:2804:ARG:NH1	2.46	0.49
1:A:3101:ALA:O	1:A:3105:VAL:HG23	2.12	0.49
1:A:3169:MET:HE1	1:A:3688:PHE:H	1.76	0.49
1:A:3661:LEU:HD12	1:A:3662:ILE:N	2.27	0.49
1:A:1939:GLN:H	1:A:1939:GLN:CD	2.15	0.49
1:A:3040:GLU:OE1	1:A:3053:TRP:NE1	2.46	0.49
1:A:4306:VAL:O	1:A:4310:GLU:HG2	2.13	0.49
1:A:4381:HIS:NE2	1:A:4439:GLU:OE2	2.45	0.49
1:A:1653:HIS:HA	1:A:1656:LYS:HD2	1.93	0.49
1:A:4610:TYR:HB2	1:A:4643:LEU:HD22	1.95	0.49
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	1.95	0.49
1:A:1722:THR:O	1:A:1726:ILE:HG12	2.12	0.48
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.95	0.48
1:A:2601:LYS:HG2	1:A:2736:VAL:HB	1.94	0.48
1:A:3974:TRP:NE1	1:A:3976:GLU:OE2	2.46	0.48
1:A:4336:GLY:O	1:A:4340:ILE:HG12	2.12	0.48
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.95	0.48
1:A:1912:LYS:NZ	2:A:4701:ADP:O3B	2.45	0.48
1:A:3771:GLU:O	1:A:3775:ARG:HG2	2.13	0.48
1:A:2123:ASP:O	1:A:2127:ILE:HG13	2.14	0.48
1:A:3021:PHE:CE1	1:A:3025:GLU:HG3	2.48	0.48
1:A:3115:LEU:HD22	1:A:3143:ILE:HG13	1.96	0.48
1:A:2511:ARG:HB3	1:A:2535:ILE:CD1	2.43	0.48
1:A:1844:PHE:HZ	1:A:1922:GLN:HE21	1.60	0.48
1:A:4013:LEU:HD23	1:A:4017:PHE:CZ	2.48	0.48
1:A:2228:SER:HB3	1:A:2364:PHE:HB3	1.94	0.48
1:A:2694:ARG:O	1:A:2698:GLN:N	2.47	0.48
1:A:3916:LEU:HD21	1:A:3937:ARG:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2312:VAL:HG21	1:A:2355:THR:HG21	1.95	0.48
1:A:2977:ARG:HG3	1:A:3020:LEU:HB3	1.95	0.48
1:A:2623:SER:HA	1:A:2668:LEU:HD23	1.95	0.48
1:A:2771:ALA:O	1:A:2775:GLU:N	2.38	0.48
1:A:3197:GLN:OE1	1:A:3496:PHE:HE1	1.97	0.48
1:A:2511:ARG:HB3	1:A:2535:ILE:HD13	1.96	0.48
1:A:2519:ARG:HG2	1:A:2526:LEU:HD13	1.96	0.48
1:A:2819:GLU:HA	1:A:2861:ILE:HD11	1.95	0.48
1:A:3154:LEU:HD21	1:A:3532:TRP:HZ2	1.77	0.47
1:A:3629:PHE:CD1	1:A:3629:PHE:N	2.82	0.47
1:A:4176:ARG:NH2	1:A:4224:ASP:OD1	2.44	0.47
1:A:2963:VAL:HG21	1:A:2998:ASN:HB3	1.95	0.47
1:A:4013:LEU:HD23	1:A:4017:PHE:CE2	2.50	0.47
1:A:4387:TRP:CZ3	1:A:4455:LEU:HD21	2.50	0.47
1:A:4381:HIS:HD2	1:A:4438:CYS:HB3	1.78	0.47
1:A:2448:ASP:O	1:A:2453:ARG:NH2	2.47	0.47
1:A:4166:VAL:HG12	1:A:4302:ARG:HH12	1.79	0.47
1:A:2231:SER:OG	1:A:2344:GLU:OE2	2.31	0.47
1:A:3206:ARG:O	1:A:3210:GLU:HG2	2.13	0.47
1:A:1632:VAL:HB	1:A:1636:ASP:HB2	1.96	0.47
1:A:1976:GLN:HG2	1:A:1980:GLU:OE2	2.15	0.47
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.49	0.47
1:A:3499:GLN:HA	1:A:3502:THR:CG2	2.45	0.47
1:A:1631:PHE:HA	1:A:1947:GLY:HA3	1.96	0.47
1:A:4565:LEU:HD13	1:A:4642:VAL:HG22	1.97	0.47
1:A:2029:PRO:HG2	1:A:2032:LEU:HD12	1.96	0.47
1:A:2743:SER:O	1:A:2747:ILE:HG22	2.15	0.47
1:A:2956:LEU:HG	1:A:2989:LYS:HB2	1.96	0.47
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	1.97	0.47
1:A:2445:HIS:ND1	1:A:2505:ASP:OD1	2.45	0.47
1:A:2564:ALA:HB3	1:A:2567:VAL:HG22	1.96	0.46
1:A:2964:HIS:HA	1:A:3643:PRO:HD2	1.97	0.46
1:A:3638:VAL:HG11	1:A:3679:LEU:HB3	1.97	0.46
1:A:4031:VAL:HG21	1:A:4058:LEU:HD21	1.95	0.46
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.97	0.46
1:A:3951:VAL:HG22	1:A:3957:PHE:CE2	2.48	0.46
1:A:2354:ALA:HB1	1:A:2358:ARG:HE	1.80	0.46
1:A:4446:ASN:OD1	1:A:4447:TYR:N	2.46	0.46
1:A:2337:PRO:O	1:A:2340:ARG:NH1	2.48	0.46
1:A:2748:TYR:HH	1:A:2800:THR:HG1	1.63	0.46
1:A:3002:SER:O	1:A:3006:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1739:ILE:HG23	1:A:1804:ARG:HD3	1.96	0.46
1:A:2087:ASP:HB2	1:A:2356:VAL:HG12	1.97	0.46
1:A:4257:ASP:OD2	1:A:4258:ASN:N	2.49	0.46
1:A:2107:ARG:NH1	1:A:2135:GLU:OE1	2.48	0.46
1:A:2227:GLY:HA2	1:A:2452:LEU:HD12	1.97	0.46
1:A:2431:GLY:O	1:A:2435:LYS:HE2	2.16	0.46
1:A:2527:PRO:HD2	1:A:2534:ILE:HG22	1.97	0.46
1:A:2797:ARG:NH2	2:A:4703:ADP:O3A	2.48	0.46
1:A:3158:ASN:HD22	1:A:3171:ILE:HG13	1.80	0.46
1:A:3793:GLU:O	1:A:3797:VAL:HG23	2.15	0.46
1:A:4128:MET:SD	1:A:4134:VAL:HG21	2.56	0.46
1:A:1724:VAL:HA	1:A:1727:PHE:HD1	1.80	0.46
1:A:3492:THR:O	1:A:3496:PHE:HB2	2.16	0.46
1:A:3787:THR:O	1:A:3790:VAL:HB	2.16	0.46
1:A:2498:ILE:HG23	1:A:2502:LEU:HD22	1.97	0.45
1:A:2612:LEU:HB3	1:A:2615:MET:HE3	1.97	0.45
1:A:3641:TYR:HD2	1:A:3692:LEU:HD21	1.81	0.45
1:A:1888:CYS:O	1:A:1892:MET:HG2	2.16	0.45
1:A:2890:ARG:NH1	1:A:2911:LEU:O	2.48	0.45
1:A:2939:SER:O	1:A:3172:THR:HB	2.15	0.45
1:A:1769:MET:N	1:A:1769:MET:HE2	2.32	0.45
1:A:1779:HIS:CE1	1:A:1826:ILE:HD12	2.52	0.45
1:A:1946:VAL:HG12	1:A:2001:LEU:HD13	1.98	0.45
1:A:3030:MET:HA	1:A:3033:CYS:SG	2.57	0.45
1:A:3113:MET:HG3	1:A:3115:LEU:CD1	2.46	0.45
1:A:3851:ASP:HB3	1:A:3854:GLN:HG2	1.98	0.45
1:A:2461:MET:CG	1:A:2583:THR:HG21	2.46	0.45
1:A:2495:VAL:HG11	1:A:2526:LEU:HD21	1.99	0.45
1:A:4288:VAL:O	1:A:4319:SER:OG	2.23	0.45
1:A:2512:ALA:O	1:A:2516:GLU:HG2	2.16	0.45
1:A:2739:PRO:HD2	1:A:2796:PRO:HG2	1.99	0.45
1:A:3764:ASP:OD1	1:A:3764:ASP:N	2.48	0.45
1:A:3836:TYR:HE1	1:A:3840:LEU:HD11	1.81	0.45
1:A:2913:ASN:OD1	1:A:2913:ASN:N	2.50	0.45
1:A:2989:LYS:NZ	1:A:3061:ASN:OD1	2.47	0.45
1:A:3485:GLU:O	1:A:3489:TRP:HD1	1.99	0.45
1:A:3641:TYR:CD2	1:A:3692:LEU:HD21	2.52	0.45
1:A:4020:ILE:HA	1:A:4023:GLN:NE2	2.31	0.45
1:A:2307:VAL:HG23	1:A:2311:TRP:CZ2	2.52	0.45
1:A:2694:ARG:NE	1:A:2697:ASP:OD1	2.50	0.45
1:A:4547:THR:HA	1:A:4586:PRO:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1985:HIS:NE2	1:A:2010:PRO:HB3	2.32	0.45
1:A:2615:MET:H	1:A:2615:MET:HE2	1.81	0.45
1:A:2648:VAL:HG13	1:A:2701:VAL:HG22	1.99	0.45
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.52	0.45
1:A:2762:LEU:HD11	1:A:2821:LEU:HD22	1.99	0.44
1:A:2973:ASP:O	1:A:2977:ARG:HD3	2.17	0.44
1:A:3191:ARG:NE	1:A:3195:GLU:OE1	2.50	0.44
1:A:3194:LEU:O	1:A:3198:GLN:HG2	2.17	0.44
1:A:3833:LEU:HD13	1:A:3833:LEU:HA	1.88	0.44
1:A:1658:PHE:CG	1:A:1661:VAL:HB	2.53	0.44
1:A:2079:GLN:O	1:A:4415:ARG:NH2	2.50	0.44
1:A:1850:GLN:HB3	1:A:1856:GLN:HG2	1.99	0.44
1:A:2220:LEU:O	1:A:2342:MET:HA	2.17	0.44
1:A:2449:LEU:HA	1:A:2449:LEU:HD12	1.77	0.44
1:A:3789:ILE:HG22	1:A:3793:GLU:HG2	1.98	0.44
1:A:1879:LEU:HD11	2:A:4701:ADP:C5	2.53	0.44
1:A:4473:MET:HG3	1:A:4477:GLN:HB2	1.99	0.44
1:A:1659:ALA:O	1:A:1679:ARG:NH2	2.51	0.44
1:A:1911:GLY:HA3	2:A:4701:ADP:C2	2.53	0.44
1:A:3218:LEU:HD21	1:A:3760:ILE:O	2.17	0.44
1:A:3960:TRP:CZ3	1:A:3996:PHE:HD2	2.34	0.44
1:A:3983:ILE:HG12	1:A:4012:ASN:OD1	2.18	0.44
1:A:4211:ASP:HB3	1:A:4252:TYR:CE2	2.53	0.44
1:A:3767:ILE:HA	1:A:3770:LEU:HD12	1.99	0.44
1:A:4289:ASP:N	1:A:4289:ASP:OD1	2.50	0.44
1:A:2571:THR:H	1:A:2574:THR:HB	1.82	0.44
1:A:3780:VAL:O	1:A:3784:VAL:HG23	2.18	0.44
1:A:2873:TYR:CZ	1:A:2883:PRO:HD3	2.53	0.44
1:A:2926:PHE:HA	1:A:3063:HIS:CD2	2.52	0.44
1:A:3681:THR:HG21	1:A:3688:PHE:HZ	1.83	0.44
1:A:4260:PHE:CE2	1:A:4608:PRO:HB3	2.53	0.44
1:A:2325:LEU:O	1:A:2332:ARG:HA	2.17	0.44
1:A:3103:TYR:CE2	1:A:3107:LYS:HD2	2.53	0.44
1:A:3117:LYS:HE3	1:A:3119:ASN:ND2	2.32	0.44
1:A:3721:ARG:HH21	1:A:3724:VAL:HG11	1.82	0.44
1:A:4577:LEU:HD23	1:A:4577:LEU:HA	1.79	0.44
1:A:1751:VAL:O	1:A:1755:GLN:HG3	2.19	0.43
1:A:2181:GLU:OE1	1:A:2243:ARG:NH1	2.51	0.43
1:A:2503:SER:HB3	1:A:2514:LEU:HD22	1.99	0.43
1:A:2594:CYS:O	1:A:2735:TYR:HA	2.18	0.43
1:A:2612:LEU:HB3	1:A:2615:MET:HE2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2964:HIS:H	1:A:2967:TYR:HB2	1.83	0.43
1:A:3529:PHE:CE2	1:A:3549:ARG:HD3	2.53	0.43
1:A:1779:HIS:ND1	1:A:1826:ILE:HD12	2.33	0.43
1:A:2053:MET:HE1	1:A:2094:LYS:HA	1.99	0.43
1:A:2239:LYS:HD2	1:A:2239:LYS:HA	1.76	0.43
1:A:2943:LYS:HG3	1:A:3094:PHE:CD2	2.53	0.43
1:A:2979:VAL:HG21	1:A:2992:PHE:CE2	2.53	0.43
1:A:3692:LEU:O	1:A:3696:VAL:HG22	2.18	0.43
1:A:1623:ARG:HB3	1:A:1630:TYR:HD2	1.84	0.43
1:A:2183:LYS:HB2	1:A:2183:LYS:HE2	1.86	0.43
1:A:2497:ALA:O	1:A:2501:SER:HB2	2.17	0.43
1:A:2762:LEU:HD21	1:A:2821:LEU:HB2	2.00	0.43
1:A:2831:ARG:HB3	1:A:2924:ARG:NH2	2.33	0.43
1:A:3655:ARG:HH21	1:A:3660:VAL:HG13	1.84	0.43
1:A:2449:LEU:HD11	1:A:2454:CYS:SG	2.58	0.43
1:A:2865:LYS:HA	1:A:2865:LYS:HD2	1.86	0.43
1:A:3704:THR:H	1:A:3707:SER:HB3	1.83	0.43
1:A:4535:SER:O	1:A:4538:GLU:HG2	2.17	0.43
1:A:2596:PRO:HB2	1:A:2738:TYR:CE1	2.54	0.43
1:A:2191:LEU:HD21	1:A:2232:MET:HE2	2.01	0.43
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.19	0.43
1:A:3846:LEU:HD21	1:A:3859:ILE:HG13	2.00	0.43
1:A:4186:PHE:HE2	1:A:4252:TYR:CD1	2.36	0.43
1:A:1914:GLU:OE1	2:A:4701:ADP:H3'	2.19	0.43
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.53	0.43
1:A:4227:ALA:HB2	1:A:4233:ILE:HD12	2.00	0.43
1:A:4380:LEU:HA	1:A:4383:THR:HG22	2.00	0.43
1:A:1713:LEU:HD23	1:A:1713:LEU:HA	1.89	0.43
1:A:1929:VAL:HG22	1:A:1956:CYS:HB3	2.01	0.43
1:A:1945:PHE:CE1	1:A:1975:VAL:HG12	2.54	0.43
1:A:2073:PHE:HE1	1:A:2145:MET:HE1	1.84	0.43
1:A:3056:SER:O	1:A:3059:ILE:HG22	2.18	0.43
1:A:1950:GLN:NE2	1:A:2007:LYS:H	2.17	0.43
1:A:2602:THR:HG23	1:A:2662:PHE:HE2	1.83	0.43
1:A:2762:LEU:HD12	1:A:2765:TYR:HB2	2.00	0.43
1:A:2779:MET:HA	1:A:2782:GLU:HB3	2.00	0.43
1:A:2873:TYR:CE2	1:A:2883:PRO:HD3	2.54	0.43
1:A:1843:ARG:NH2	1:A:1860:GLN:HB3	2.34	0.42
1:A:2790:PRO:HB3	1:A:3076:LYS:HG3	2.00	0.42
1:A:2943:LYS:HE2	1:A:2943:LYS:HB2	1.84	0.42
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2387:LEU:HD23	1:A:2387:LEU:HA	1.93	0.42
1:A:2492:ARG:HG2	1:A:2545:TRP:NE1	2.34	0.42
1:A:3638:VAL:HG22	1:A:3681:THR:HG22	2.00	0.42
1:A:4168:ARG:NH1	1:A:4220:ASP:OD2	2.43	0.42
1:A:4178:ARG:HD2	1:A:4296:MET:HE1	2.01	0.42
1:A:4178:ARG:NH1	1:A:4296:MET:HE3	2.34	0.42
1:A:4628:THR:O	1:A:4629:LYS:HG2	2.19	0.42
1:A:2286:LYS:NZ	1:A:2291:VAL:HB	2.35	0.42
1:A:2299:GLN:N	1:A:2299:GLN:OE1	2.53	0.42
1:A:3169:MET:SD	1:A:3693:CYS:HB3	2.59	0.42
1:A:4288:VAL:HG23	1:A:4289:ASP:OD1	2.19	0.42
1:A:1664:ILE:HD12	1:A:1666:LEU:HD11	2.01	0.42
1:A:1985:HIS:CD2	1:A:2010:PRO:HB3	2.55	0.42
1:A:2012:MET:SD	1:A:2013:ALA:N	2.93	0.42
1:A:2228:SER:N	3:A:4702:ATP:O1B	2.51	0.42
1:A:2615:MET:SD	1:A:2615:MET:N	2.92	0.42
1:A:3935:VAL:HG13	1:A:3947:LEU:HD23	2.01	0.42
1:A:4234:SER:HB3	1:A:4237:LYS:HG2	2.01	0.42
1:A:1635:GLU:HG2	1:A:1636:ASP:H	1.85	0.42
1:A:2911:LEU:HD23	1:A:2911:LEU:HA	1.76	0.42
1:A:3181:ASN:ND2	1:A:3584:ASN:OD1	2.53	0.42
1:A:4149:PRO:HA	1:A:4150:PRO:HD3	1.94	0.42
1:A:1789:LEU:HD13	1:A:1815:LEU:HB3	2.02	0.42
1:A:1926:PHE:O	1:A:1953:ALA:HB1	2.19	0.42
1:A:1933:ASP:OD1	1:A:1933:ASP:N	2.49	0.42
1:A:2209:GLN:O	1:A:2213:ILE:HG12	2.20	0.42
1:A:2652:PRO:HD2	1:A:2705:ARG:CZ	2.49	0.42
1:A:4205:TYR:OH	1:A:4261:ASP:OD2	2.25	0.42
1:A:1628:ARG:HG3	1:A:1706:GLU:OE1	2.20	0.42
1:A:2206:LYS:HD3	1:A:2206:LYS:HA	1.82	0.42
1:A:3592:PRO:HG3	1:A:3702:THR:HG22	2.02	0.42
1:A:3115:LEU:HD22	1:A:3143:ILE:HG21	2.01	0.42
1:A:3719:ALA:HB3	1:A:3840:LEU:HD13	2.01	0.42
1:A:3747:LYS:O	1:A:3751:GLN:HG2	2.20	0.42
1:A:4173:PRO:HG2	1:A:4176:ARG:HB2	2.02	0.42
1:A:1769:MET:CE	1:A:1777:PRO:HD2	2.50	0.42
1:A:3766:ILE:HD12	1:A:3766:ILE:HA	1.91	0.42
1:A:3787:THR:HA	1:A:3790:VAL:HB	2.00	0.42
1:A:3811:ILE:HD11	1:A:3864:PHE:CE1	2.55	0.42
1:A:3924:ILE:HG23	1:A:3952:GLN:NE2	2.35	0.42
1:A:1944:ILE:HD12	1:A:1944:ILE:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4288:VAL:HG22	1:A:4293:ASP:HA	2.01	0.42
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	2.01	0.42
1:A:1724:VAL:HA	1:A:1727:PHE:CD1	2.54	0.41
1:A:2277:ASP:OD1	1:A:2277:ASP:N	2.53	0.41
1:A:2600:GLY:H	2:A:4703:ADP:H5'2	1.85	0.41
1:A:2992:PHE:HE1	1:A:2994:MET:SD	2.43	0.41
1:A:3801:TYR:CD1	1:A:3856:LEU:HD13	2.54	0.41
1:A:3909:LEU:HD21	1:A:4343:MET:HE2	2.01	0.41
1:A:3808:CYS:SG	1:A:3836:TYR:HE2	2.43	0.41
1:A:2979:VAL:HG21	1:A:2992:PHE:HE2	1.86	0.41
1:A:3154:LEU:HD12	1:A:3171:ILE:HD13	2.02	0.41
1:A:3607:ARG:O	1:A:3608:LYS:HG2	2.20	0.41
1:A:3801:TYR:HD1	1:A:3856:LEU:HD13	1.85	0.41
1:A:4467:TYR:HB3	1:A:4515:PHE:HD2	1.85	0.41
1:A:3606:ASP:N	1:A:3606:ASP:OD1	2.50	0.41
1:A:4031:VAL:O	1:A:4123:ARG:NH2	2.49	0.41
1:A:2527:PRO:HG3	1:A:2545:TRP:CG	2.55	0.41
1:A:2744:LEU:HA	1:A:2747:ILE:HG22	2.02	0.41
1:A:3110:THR:O	1:A:3140:ARG:NH1	2.53	0.41
1:A:3488:ARG:HD2	1:A:3746:GLU:OE1	2.20	0.41
1:A:3976:GLU:OE1	1:A:3980:ALA:HB2	2.20	0.41
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.55	0.41
1:A:4435:VAL:O	1:A:4439:GLU:HG2	2.20	0.41
1:A:1628:ARG:HD3	1:A:1951:VAL:HG13	2.03	0.41
1:A:2620:LEU:HD11	1:A:2634:THR:HG21	2.03	0.41
1:A:2747:ILE:HD12	2:A:4703:ADP:C6	2.56	0.41
1:A:2779:MET:O	1:A:2783:ARG:N	2.53	0.41
1:A:3076:LYS:HB2	1:A:3076:LYS:HE2	1.93	0.41
1:A:4480:SER:O	1:A:4484:GLU:HG2	2.21	0.41
1:A:2265:TYR:O	1:A:2281:THR:OG1	2.29	0.41
1:A:2570:PRO:O	1:A:2746:GLN:NE2	2.54	0.41
1:A:2822:ILE:HD11	1:A:2858:PHE:CD2	2.56	0.41
1:A:2855:LEU:HD13	1:A:2855:LEU:HA	1.87	0.41
1:A:3495:THR:HG23	1:A:3496:PHE:HD2	1.86	0.41
1:A:3509:LEU:HD23	1:A:3509:LEU:HA	1.88	0.41
1:A:4107:MET:HG2	1:A:4135:PRO:HB3	2.02	0.41
1:A:4399:LYS:HA	1:A:4399:LYS:HD3	1.82	0.41
1:A:4448:LEU:O	1:A:4452:ILE:HG12	2.21	0.41
1:A:1887:ARG:NH2	1:A:4253:GLY:O	2.53	0.41
1:A:2072:PHE:HA	1:A:2075:LEU:HD12	2.03	0.41
1:A:2989:LYS:HZ1	1:A:3061:ASN:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3612:THR:O	1:A:3635:VAL:HA	2.20	0.41
1:A:3788:ASP:O	1:A:3791:MET:HB3	2.21	0.41
1:A:1698:ILE:HD12	1:A:1701:TRP:NE1	2.36	0.40
1:A:3521:ASP:N	1:A:3521:ASP:OD1	2.53	0.40
1:A:3841:TYR:O	1:A:3842:GLU:HG2	2.21	0.40
1:A:4297:PRO:HG3	1:A:4308:TRP:CD2	2.56	0.40
1:A:1623:ARG:HE	1:A:1637:LEU:HD22	1.86	0.40
1:A:2107:ARG:HH12	1:A:2135:GLU:CD	2.24	0.40
1:A:2749:GLY:N	1:A:2770:THR:HG21	2.36	0.40
1:A:3819:LYS:HB2	1:A:3826:GLN:OE1	2.21	0.40
1:A:4030:ILE:HG21	1:A:4145:PHE:CZ	2.56	0.40
1:A:4460:LEU:HD12	1:A:4460:LEU:HA	1.88	0.40
1:A:2097:LEU:HD13	1:A:2097:LEU:HA	1.95	0.40
1:A:2286:LYS:HE2	1:A:2292:ARG:NH1	2.35	0.40
1:A:2453:ARG:HD3	1:A:2728:LEU:O	2.21	0.40
1:A:2704:GLU:HG3	1:A:2705:ARG:HG3	2.03	0.40
1:A:1846:PHE:CE2	1:A:1856:GLN:HB3	2.57	0.40
1:A:3666:ASP:OD1	1:A:3666:ASP:N	2.55	0.40
1:A:3983:ILE:O	1:A:3987:ILE:HG22	2.20	0.40

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	2699/4646 (58%)	2641 (98%)	58 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	2407/4125 (58%)	2363 (98%)	44 (2%)	54 71

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1734	ASP
1	A	1926	PHE
1	A	1931	ASN
1	A	1938	PHE
1	A	1945	PHE
1	A	2031	ASN
1	A	2055	TYR
1	A	2228	SER
1	A	2306	ASP
1	A	2321	ASP
1	A	2365	SER
1	A	2429	SER
1	A	2507	ARG
1	A	2537	TYR
1	A	2615	MET
1	A	2670	ASP
1	A	2844	ARG
1	A	2983	SER
1	A	3021	PHE
1	A	3068	MET
1	A	3078	ARG
1	A	3169	MET
1	A	3206	ARG
1	A	3474	ARG
1	A	3488	ARG
1	A	3491	LYS
1	A	3496	PHE
1	A	3524	MET
1	A	3551	GLU
1	A	3608	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3641	TYR
1	A	3679	LEU
1	A	3710	SER
1	A	3725	ASP
1	A	3747	LYS
1	A	3795	GLU
1	A	3912	ASN
1	A	3957	PHE
1	A	4004	MET
1	A	4034	GLU
1	A	4079	GLN
1	A	4162	SER
1	A	4171	LYS
1	A	4491	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1922	GLN
1	A	3032	GLN
1	A	3181	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are 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	$\#\|Z\| > 2$
2	ADP	A	4701	-	24,29,29	0.86	0	29,45,45	1.66	4 (13%)
2	ADP	A	4704	-	24,29,29	0.85	0	29,45,45	1.19	2 (6%)
3	ATP	A	4702	-	28,33,33	0.72	0	34,52,52	0.60	1 (2%)
2	ADP	A	4703	-	24,29,29	0.89	0	29,45,45	1.29	3 (10%)

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
2	ADP	A	4701	-	-	0/12/32/32	0/3/3/3
2	ADP	A	4704	-	-	4/12/32/32	0/3/3/3
3	ATP	A	4702	-	-	3/18/38/38	0/3/3/3
2	ADP	A	4703	-	-	4/12/32/32	0/3/3/3

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4701	ADP	O4'-C1'-N9	4.63	114.88	108.75
2	A	4701	ADP	C4'-O4'-C1'	-4.25	106.03	109.92
2	A	4703	ADP	N3-C2-N1	-4.00	123.24	128.67
2	A	4704	ADP	N3-C2-N1	-3.63	123.74	128.67
2	A	4701	ADP	N3-C2-N1	-3.47	123.97	128.67
2	A	4704	ADP	C4-C5-N7	-2.45	106.75	109.34
2	A	4701	ADP	C4-C5-N7	-2.39	106.81	109.34
3	A	4702	ATP	C5-C6-N6	2.34	123.88	120.31
2	A	4703	ADP	C4-C5-N7	-2.29	106.92	109.34
2	A	4703	ADP	C4'-O4'-C1'	2.18	111.93	109.92

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4703	ADP	C5'-O5'-PA-O1A
2	A	4703	ADP	C5'-O5'-PA-O2A
2	A	4703	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	PA-O3A-PB-O2B
2	A	4704	ADP	PA-O3A-PB-O3B
2	A	4704	ADP	C5'-O5'-PA-O1A
3	A	4702	ATP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'
2	A	4704	ADP	C3'-C4'-C5'-O5'
2	A	4703	ADP	O4'-C4'-C5'-O5'
3	A	4702	ATP	PA-O3A-PB-O1B

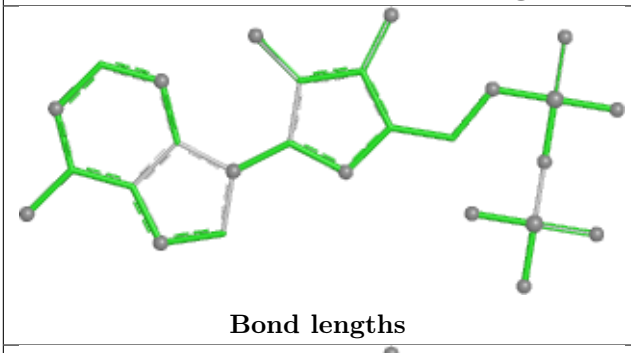
There are no ring outliers.

3 monomers are involved in 11 short contacts:

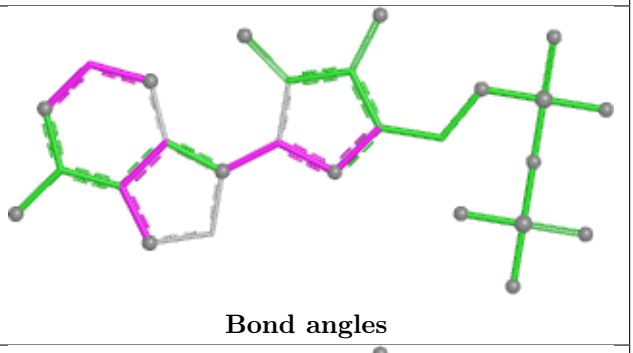
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	7	0
3	A	4702	ATP	1	0
2	A	4703	ADP	3	0

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.

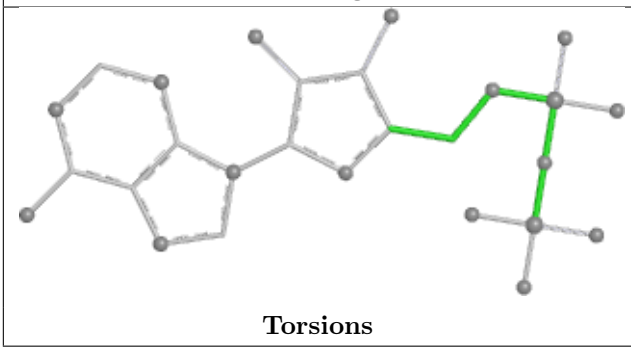
Ligand ADP A 4701



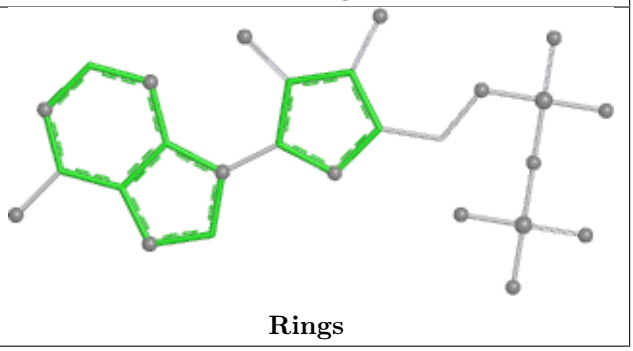
Bond lengths



Bond angles

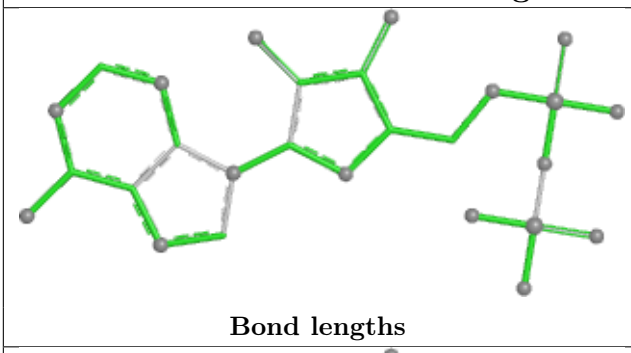


Torsions

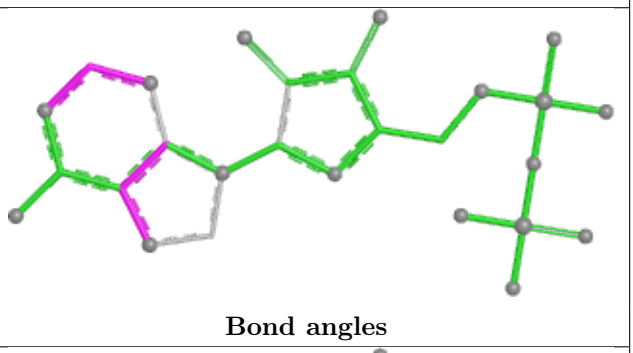


Rings

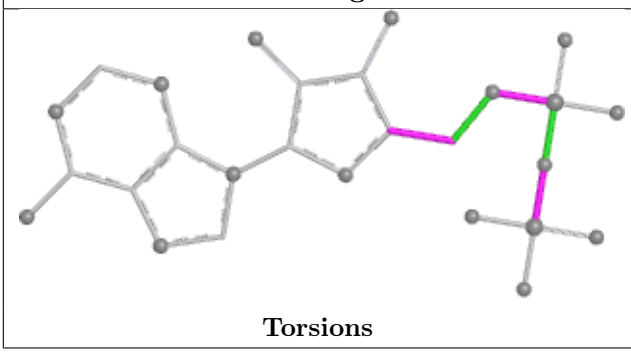
Ligand ADP A 4704



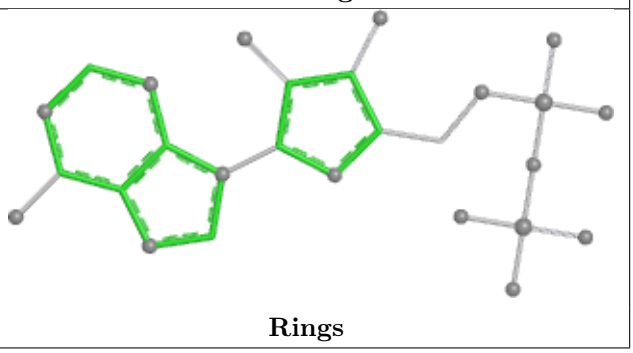
Bond lengths



Bond angles

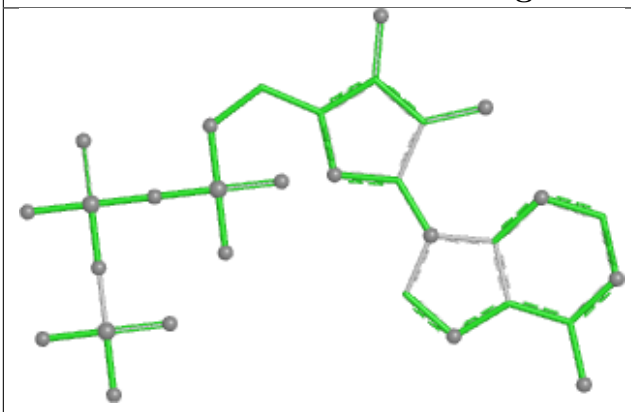


Torsions

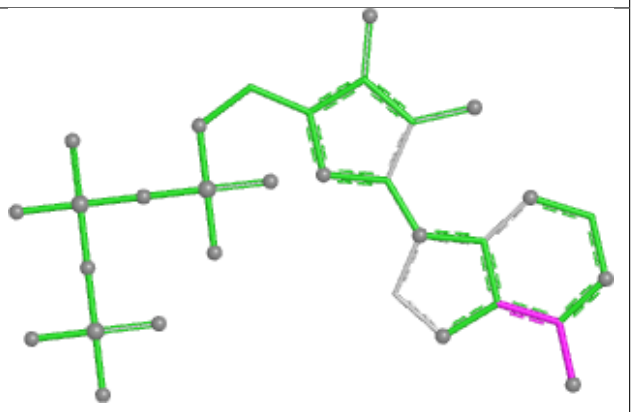


Rings

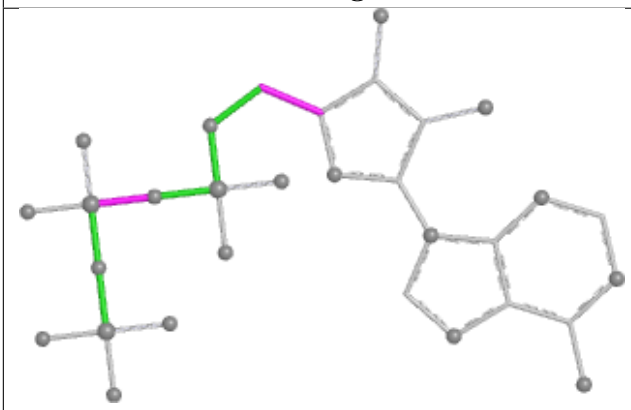
Ligand ATP A 4702



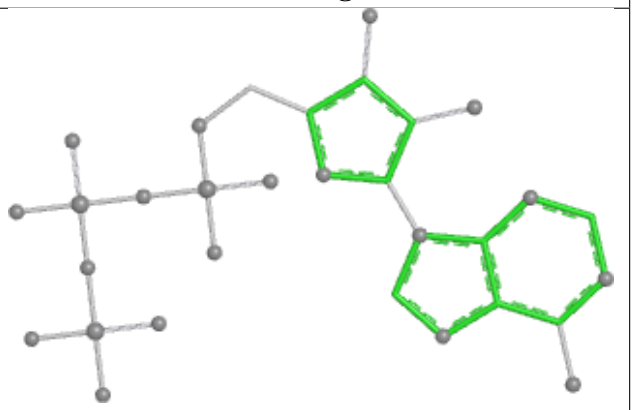
Bond lengths



Bond angles

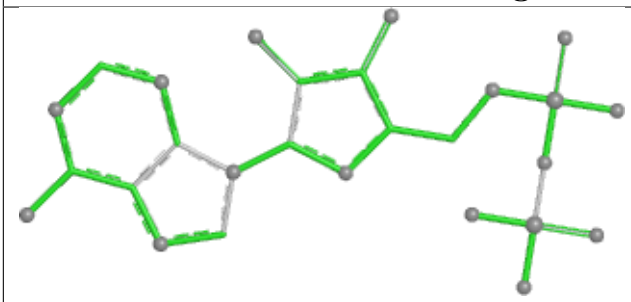


Torsions

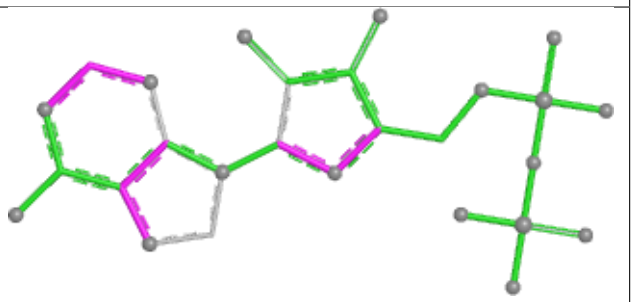


Rings

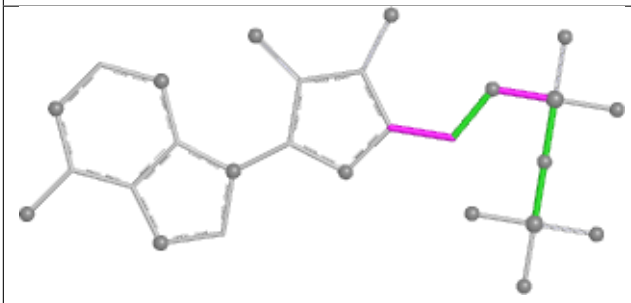
Ligand ADP A 4703



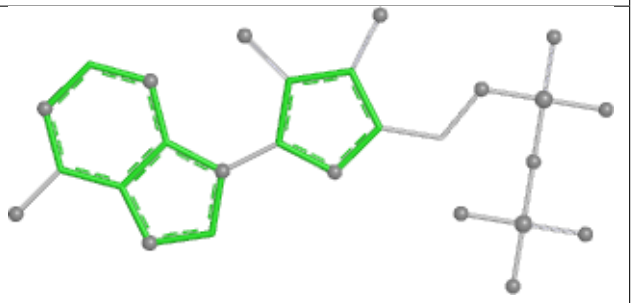
Bond lengths



Bond angles



Torsions



Rings

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.

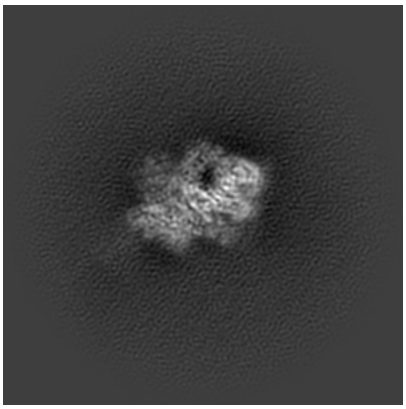
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44704. These allow visual inspection of the internal detail of the map and identification of artifacts.

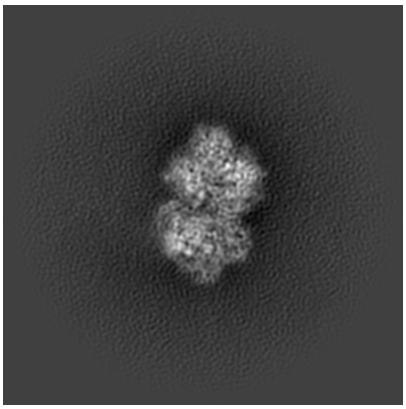
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

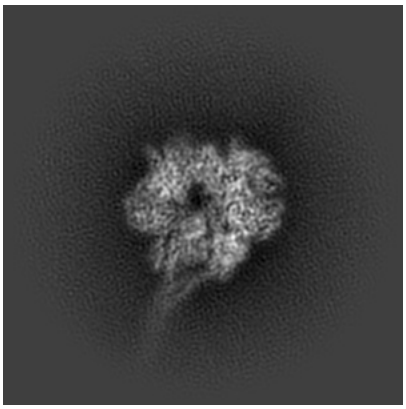
6.1.1 Primary map



X

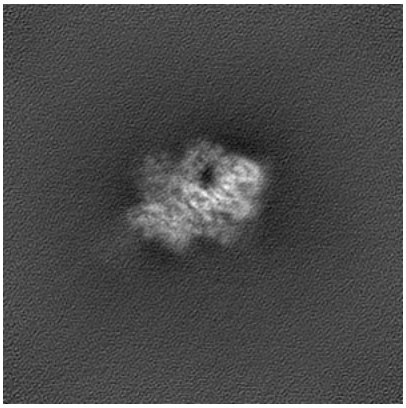


Y

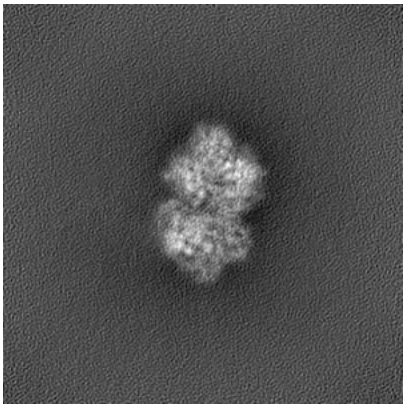


Z

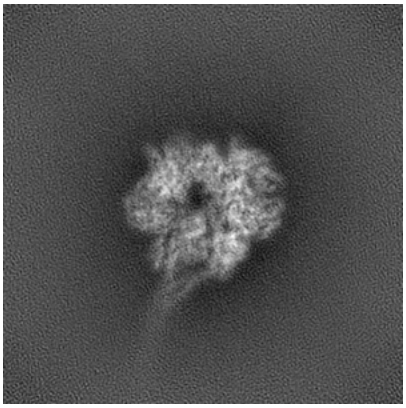
6.1.2 Raw map



X



Y

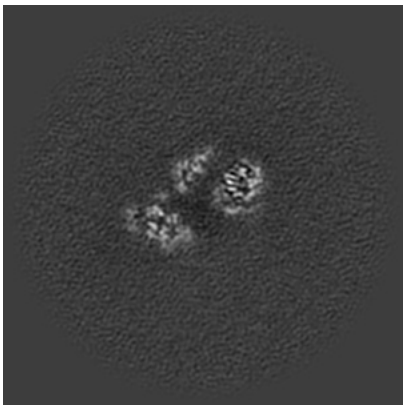


Z

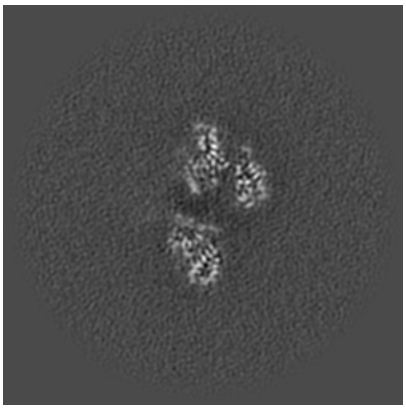
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

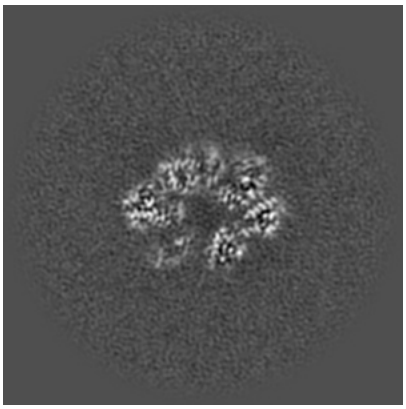
6.2.1 Primary map



X Index: 128



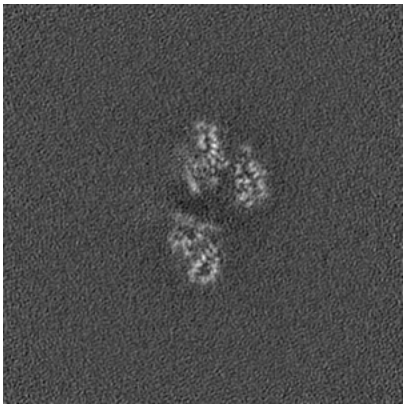
Y Index: 128



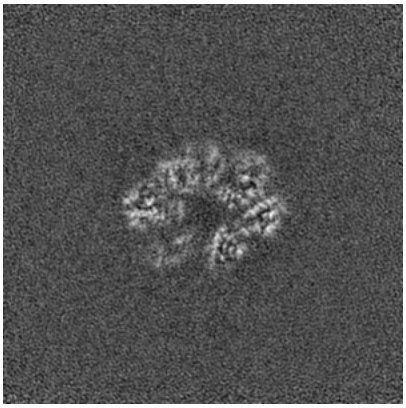
Z Index: 128

6.2.2 Raw map

X Index: 128



Y Index: 128

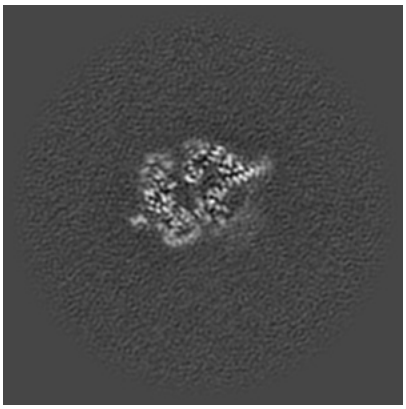


Z Index: 128

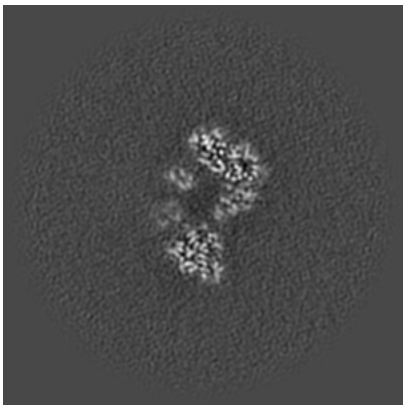
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

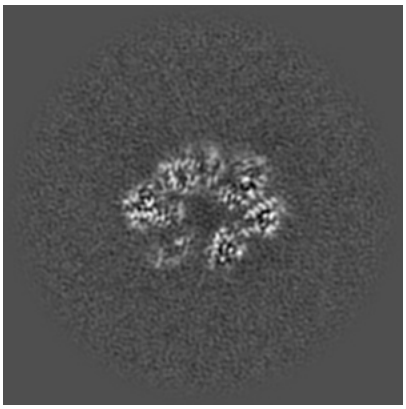
6.3.1 Primary map



X Index: 146

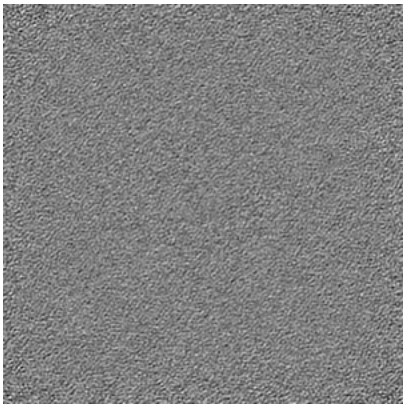


Y Index: 120

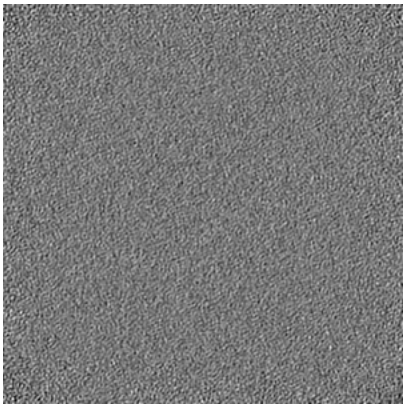


Z Index: 128

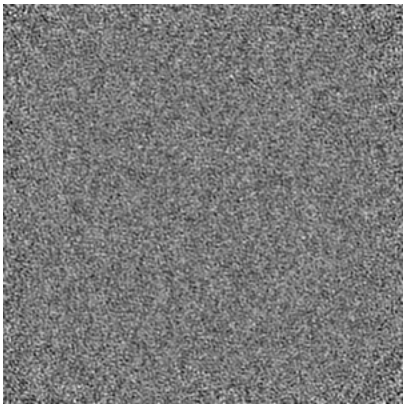
6.3.2 Raw map



X Index: 0



Y Index: 0

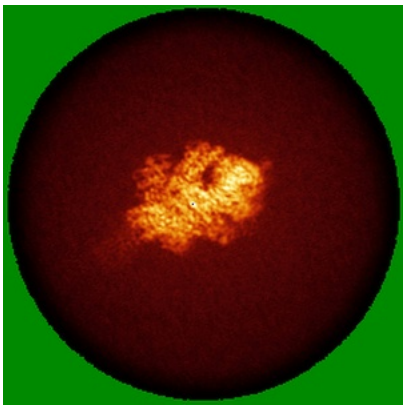


Z Index: 0

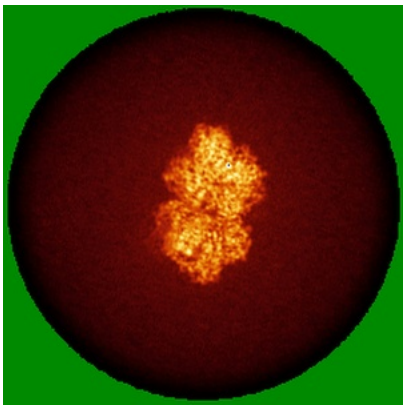
The images above show the largest variance slices of the map in three orthogonal directions.

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

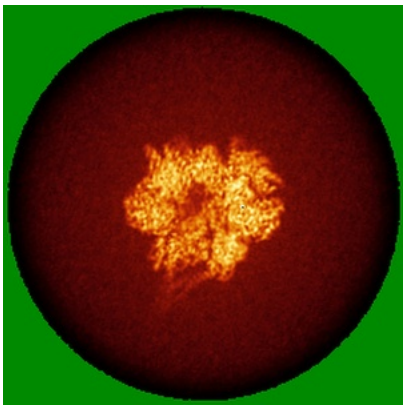
6.4.1 Primary map



X

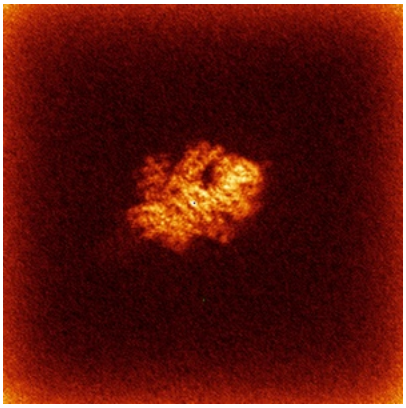


Y

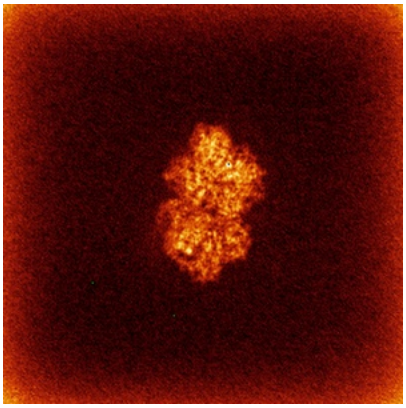


Z

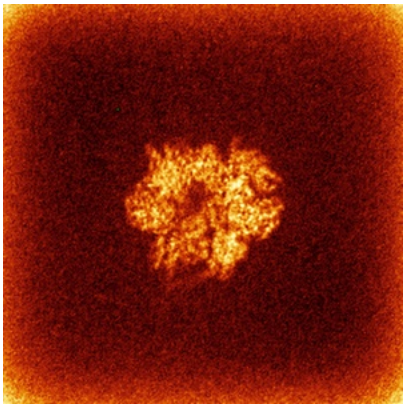
6.4.2 Raw map



X



Y

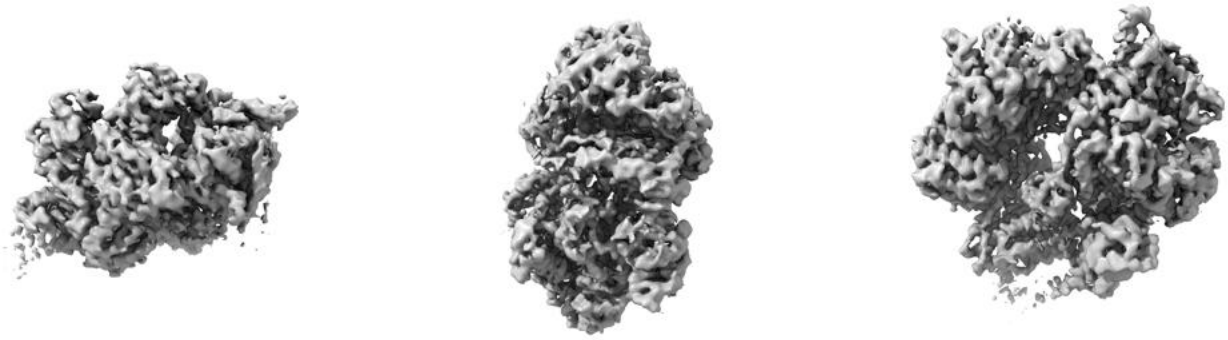


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

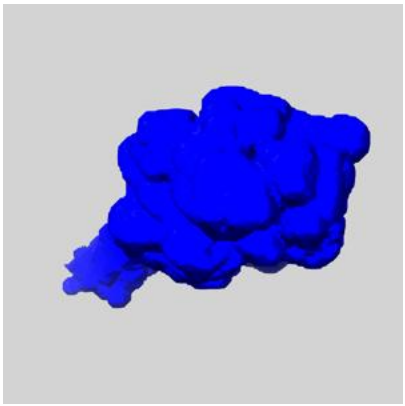
6.6 Mask visualisation (i)

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

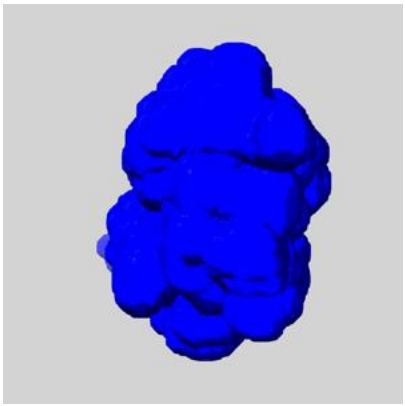
A mask typically either:

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

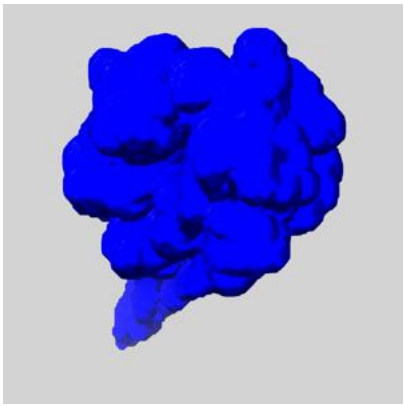
6.6.1 emd_44704_msk_1.map (i)



X



Y

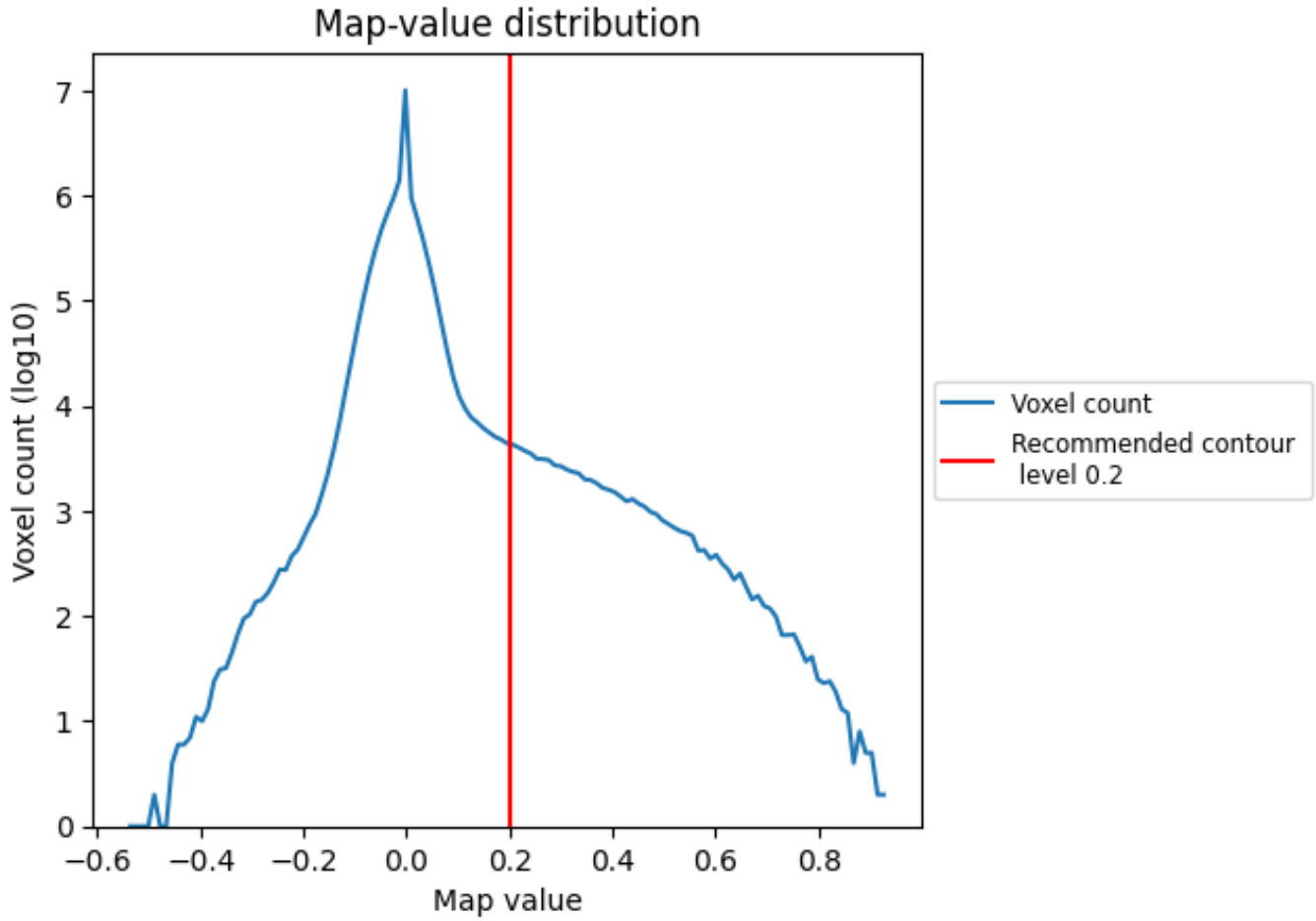


Z

7 Map analysis

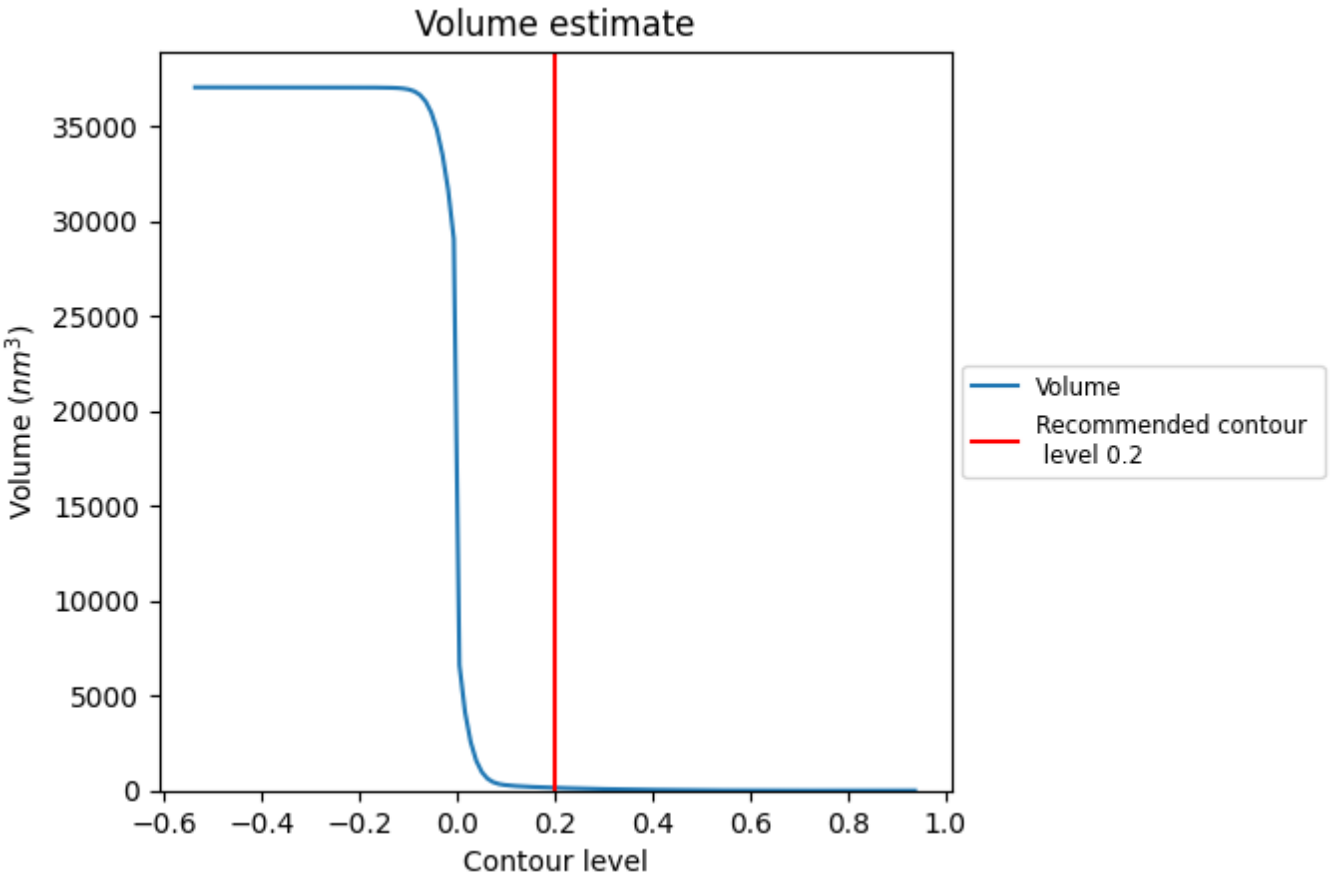
This section contains the results of statistical analysis of the map.

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.

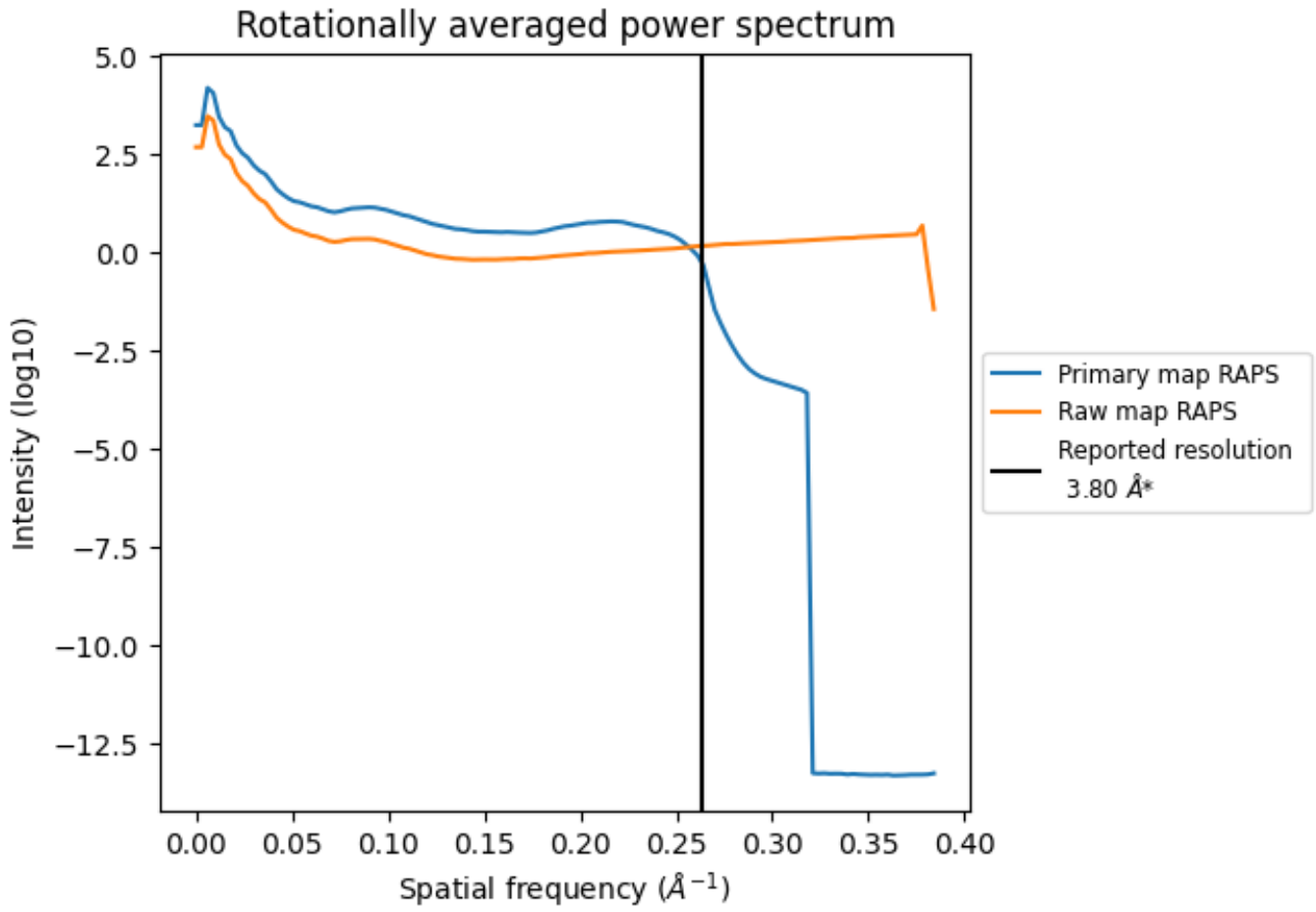
7.2 Volume estimate



The volume at the recommended contour level is 147 nm^3; this corresponds to an approximate mass of 133 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)

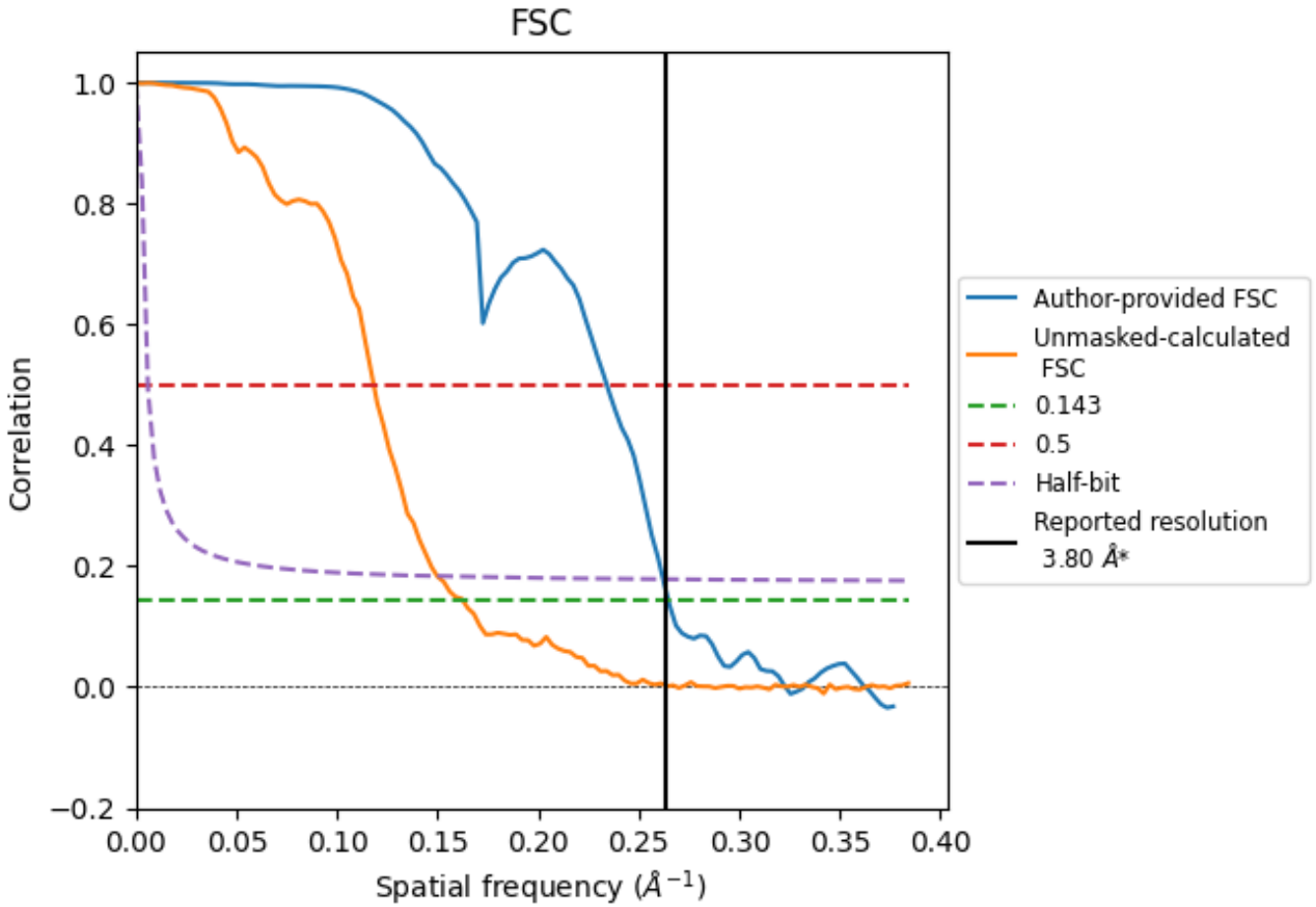


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

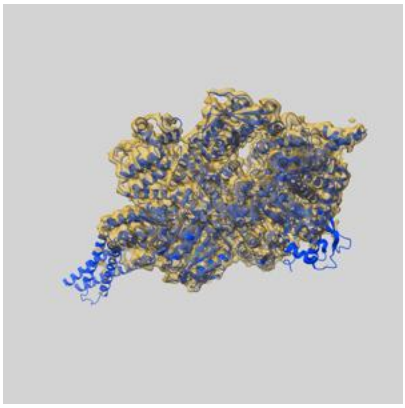
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.78	4.27	3.82
Unmasked-calculated*	6.15	8.45	6.67

*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 6.15 differs from the reported value 3.8 by more than 10 %

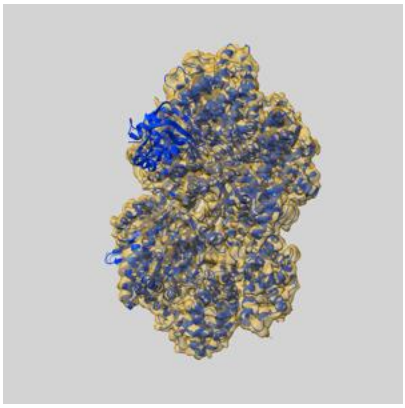
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44704 and PDB model 9BMN. Per-residue inclusion information can be found in section 3 on page 5.

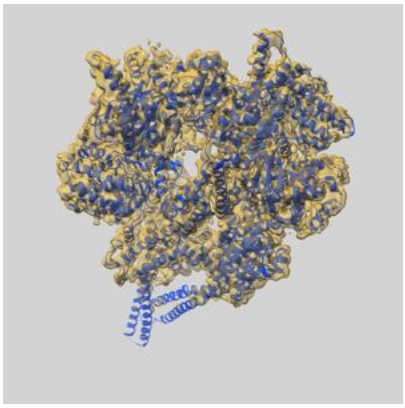
9.1 Map-model overlay



X



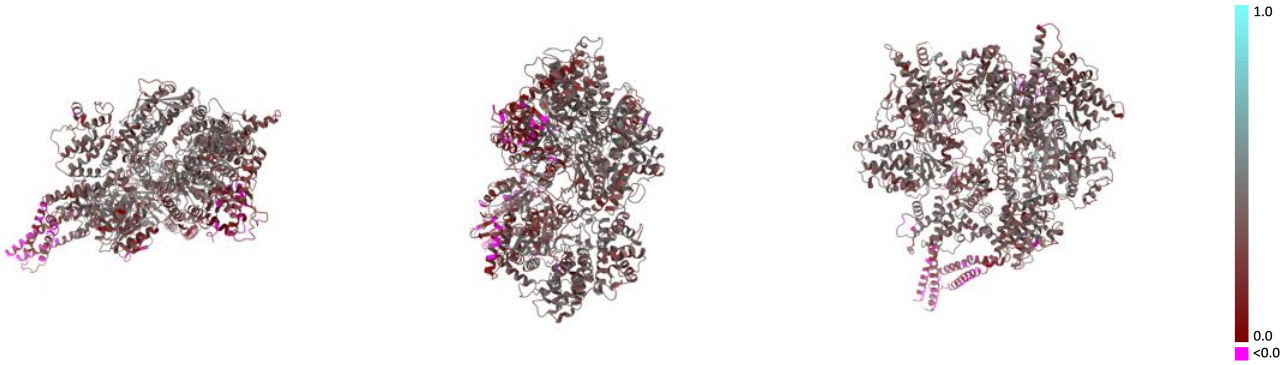
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

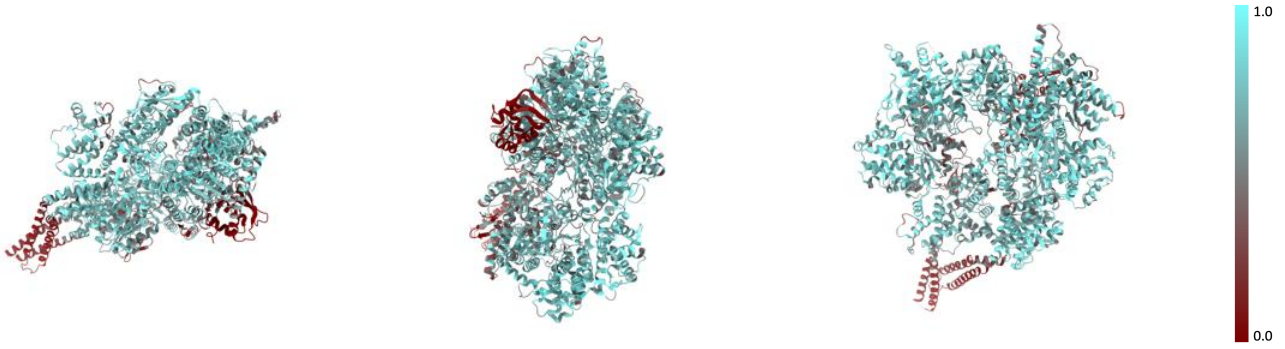
9.2 Q-score mapped to coordinate model (i)



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.

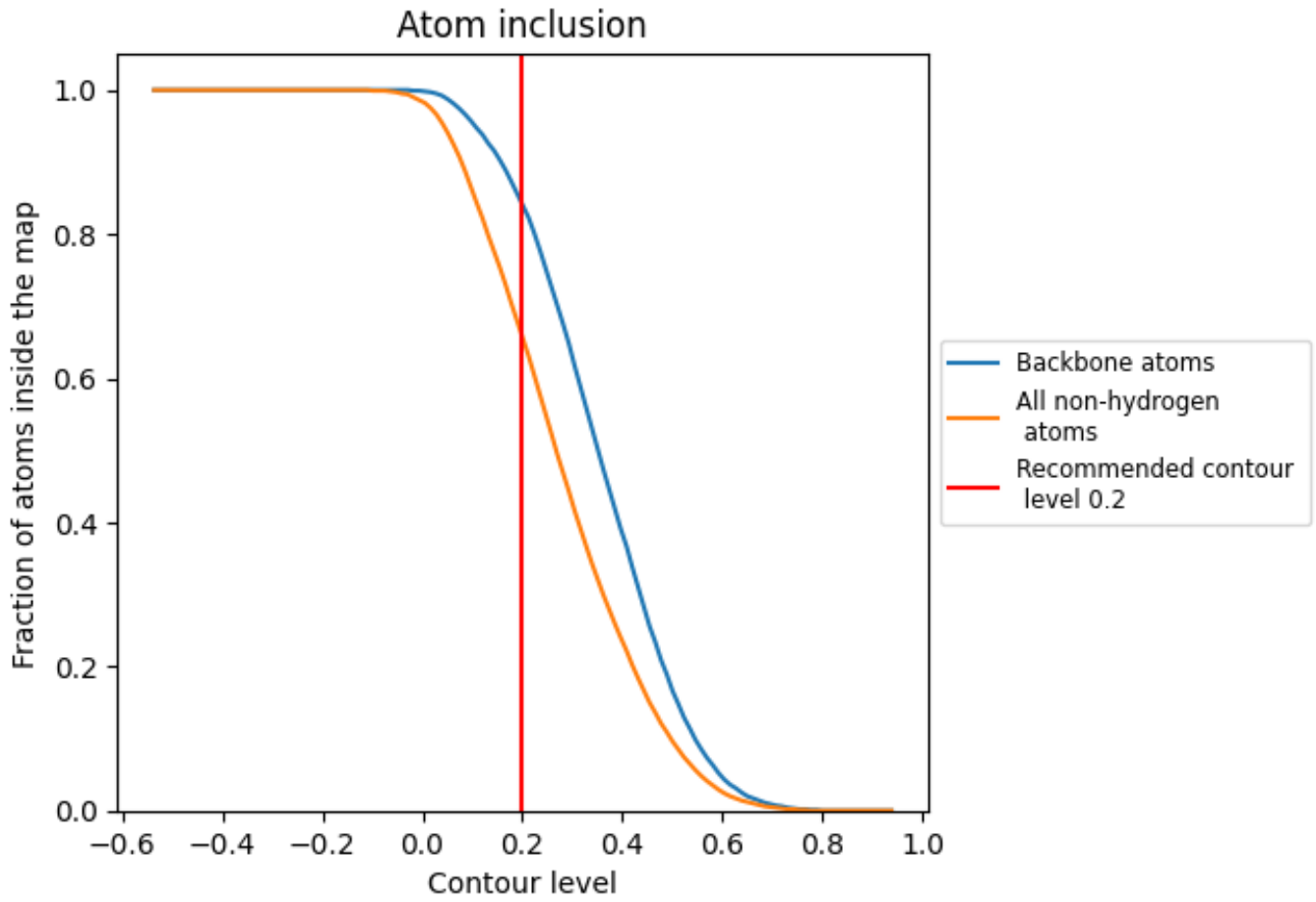
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 66% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6570	0.3320
A	0.6570	0.3320