Full wwPDB EM Validation Report ⓘ

May 14, 2025 – 04:45 AM EDT

PDB ID	:	9DH8 / pdb_00009dh8
EMDB ID	:	EMD-46859
Title	:	State-5 of the motor domain from full-length human dynein-1 in 5mM AMPPNP with 5mM Mg2+
Authors	:	Chai, P.; Zhang, K.
Deposited on	:	2024-09-03
Resolution	:	3.50 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:

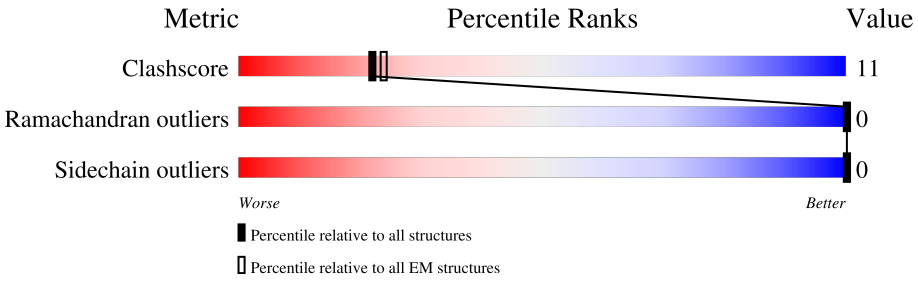
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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	8% 42% 16% 42%

2 Entry composition

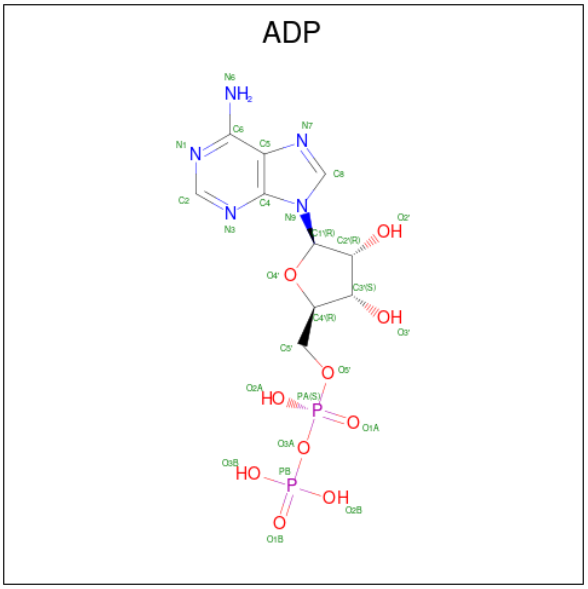
There are 3 unique types of molecules in this entry. The entry contains 21847 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

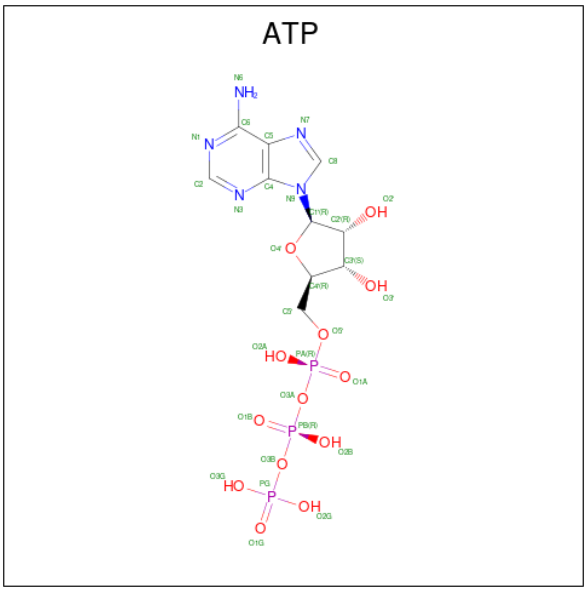
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2709	21735	13841	3752	4031	111	0	0

- 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).



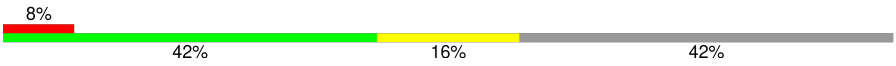
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

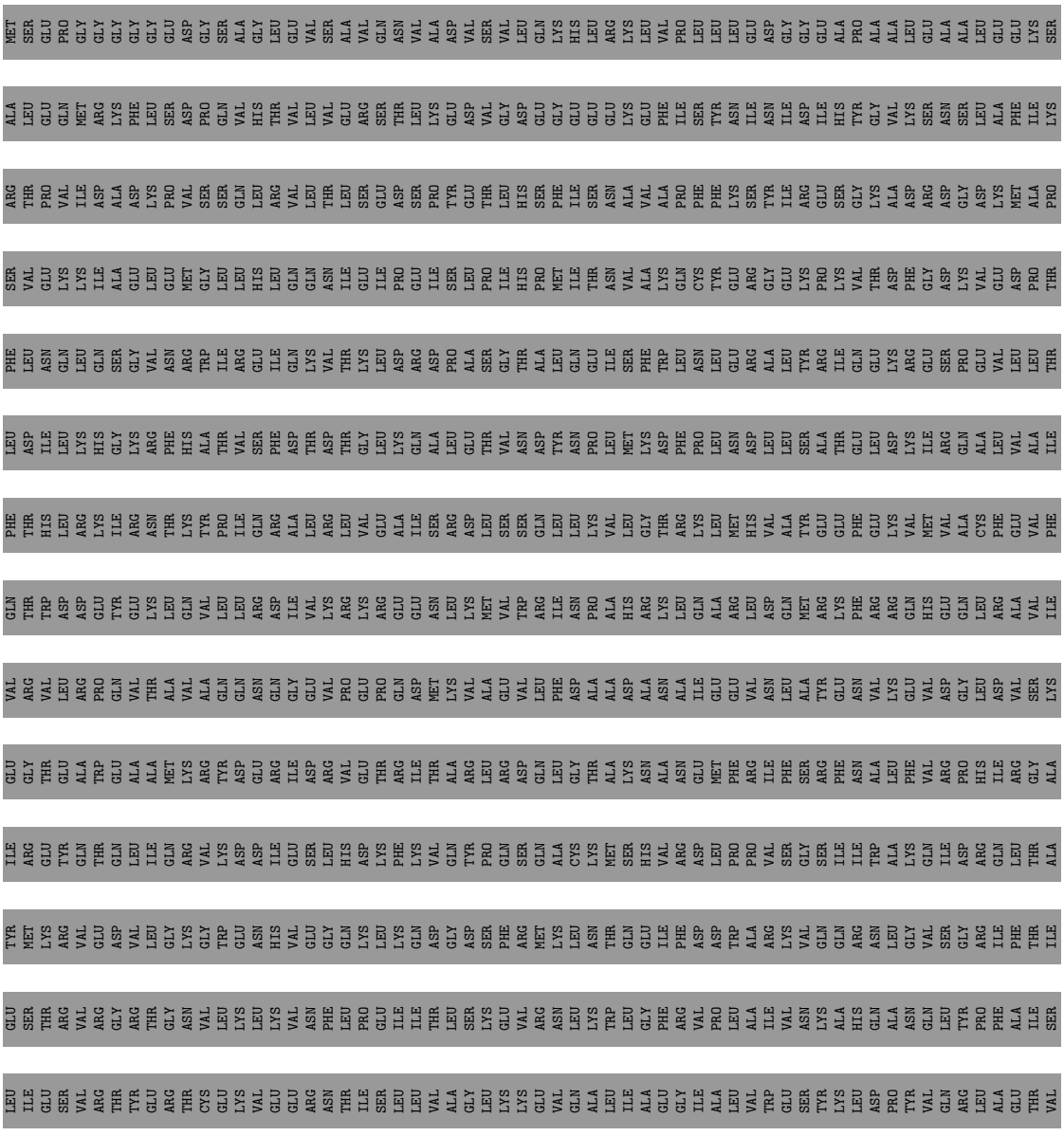
3 Residue-property plots (i)

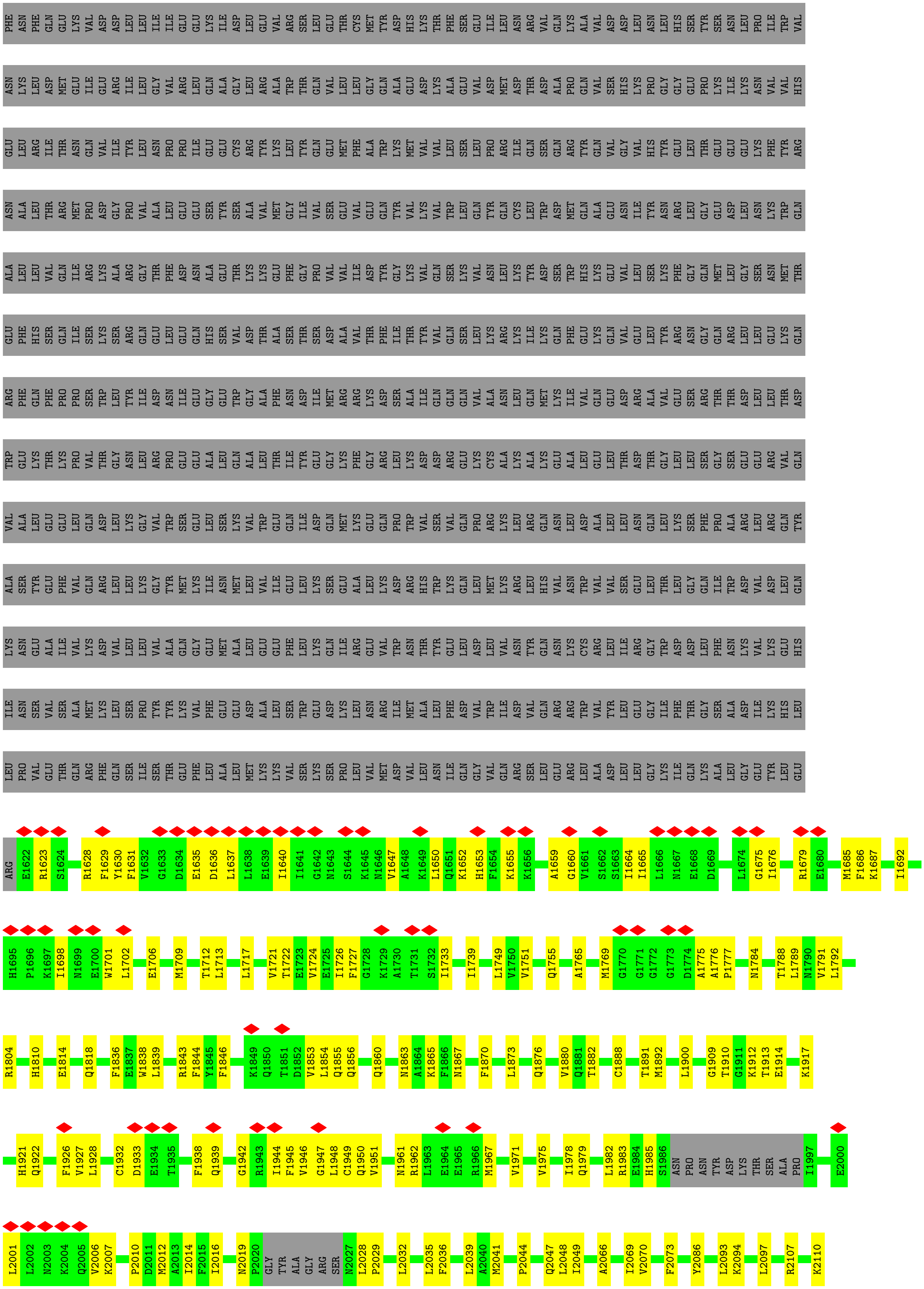
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

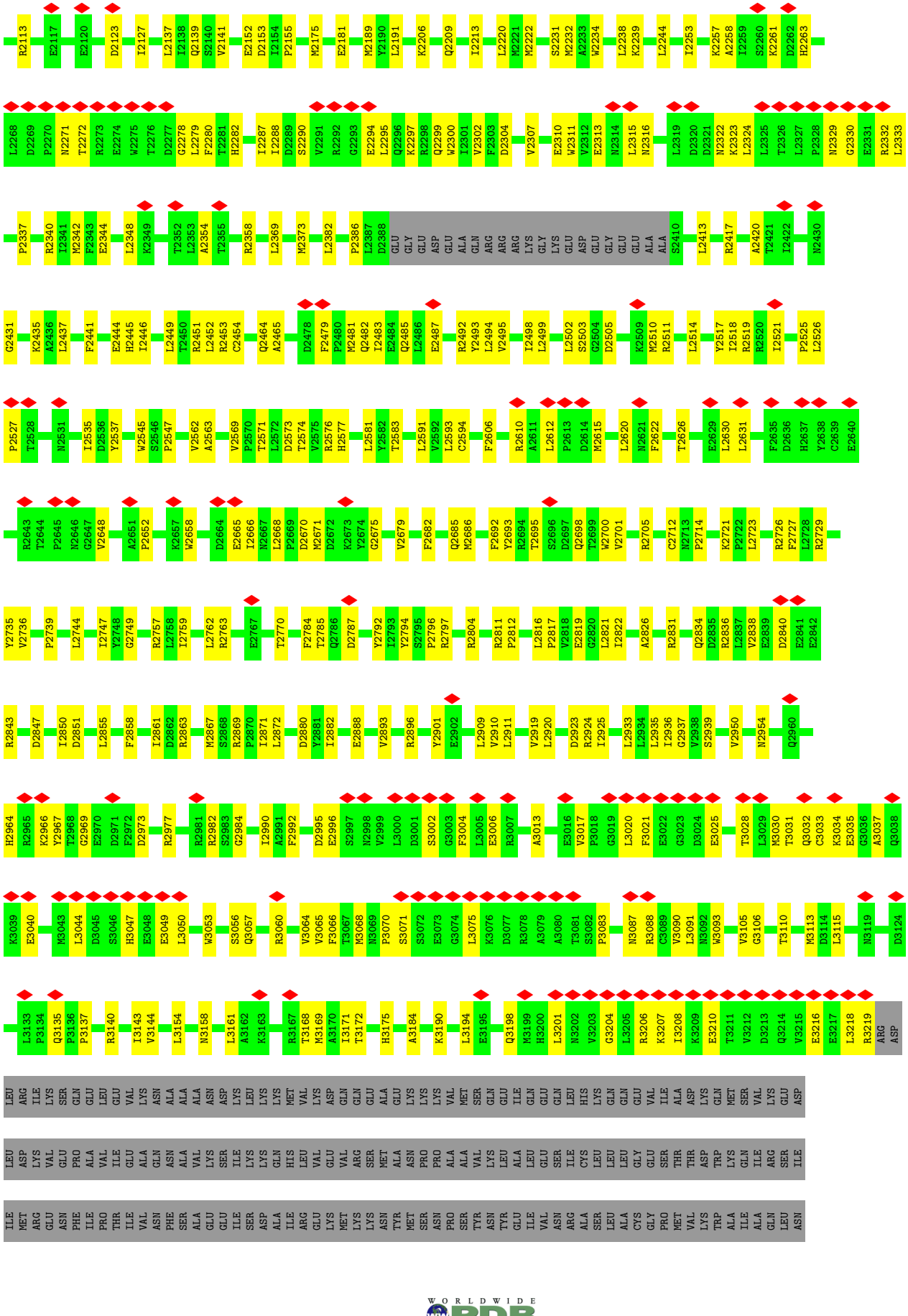
- Molecule 1: Cytoplasmic dynein 1 heavy chain 1

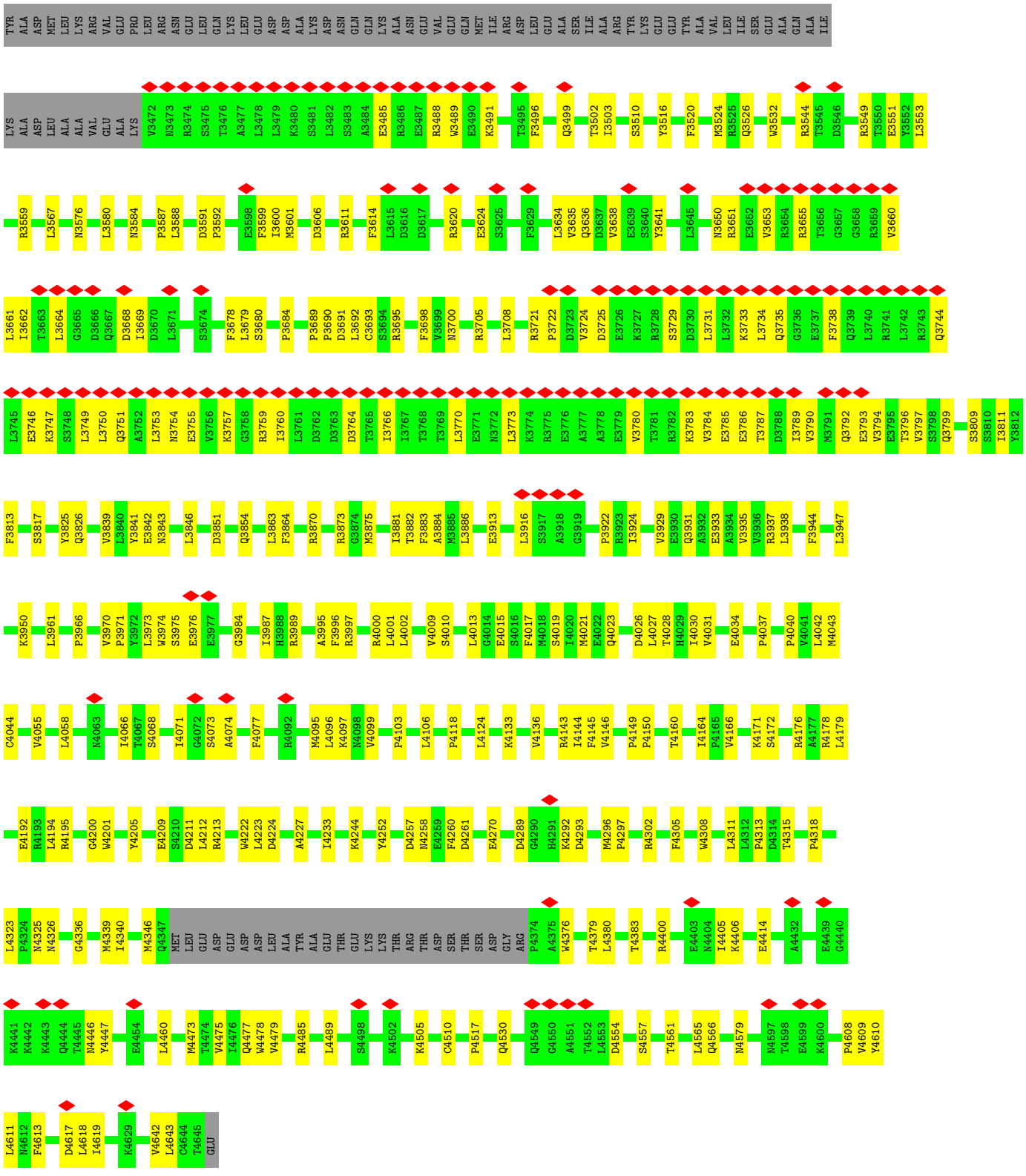
Chain A:








R2113 E2117 E2120 D2123 I2127 L2137 I2138 Q2139 S2140 V2141 E2152 D2153 I2154 P2155 M2175 E2181 M2189 Y2190 L2191 K2206 Q2209 I2213 L2220 M2221 M2222 S2231 M2232 A2233 W2234 L2238 K2239 L2244 I2253 K2257 A2258 I2259 S2260 K2261 D2262 H2263
L2268 D2269 P2270 N2271 T2272 R2273 E2274 W2275 T2276 D2277 G2278 L2279 F2280 T2281 H2282 I2287 I2288 D2289 S2290 V2291 R2292 G2293 E2294 L2295 Q2296 K2297 R2298 Q2299 W2300 I2301 V2302 F2303 D2304 V2307 E2310 W2311 V2312 E2313 N2314 L2315 N2316 L2319 D2320 D2321 N2322 K2323 L2324 L2325 T2326 L2327 P2328 N2329 G2330 E2331 R2332 L2333
P2337 R2340 I2341 M2342 F2343 E2344 L2348 K2349 T2352 L2353 A2354 T2355 R2358 L2369 M2373 L2382 P2386 L2387 D2388 GLU GLY GLU ASP GLU ALA GLN ARG ARG LYS GLY LYS GLU ASP GLU GLY GLU GLU ALA ALA S2410 L2413 R2417 A2420 T2421 I2422 N2430
G2431 K2435 A2436 L2437 F2441 E2444 H2445 I2446 L2449 T2450 R2451 L2452 R2453 C2454 Q2464 A2465 D2478 F2479 P2480 M2481 Q2482 I2483 E2484 Q2485 L2486 E2487 R2492 Y2493 L2494 V2495 I2498 L2499 L2502 S2503 G2504 D2505 K2509 M2510 R2511 L2514 Y2517 I2518 R2519 R2520 I2521 P2525 L2526
P2527 T2528 N2531 I2535 D2536 Y2537 W2545 S2546 P2547 V2562 A2563 V2569 P2570 T2571 L2572 D2573 T2574 V2575 R2576 H2577 L2581 Y2582 T2583 L2591 V2592 L2593 C2594 F2606 R2610 A2611 L2612 P2613 D2614 M2615 L2620 N2621 F2622 T2626 E2629 L2630 L2631 F2635 D2636 H2637 Y2638 C2639 E2640
R2643 T2644 P2645 N2646 G2647 V2648 A2651 P2652 K2657 W2658 D2664 E2665 I2666 N2667 L2668 P2669 D2670 M2671 D2672 K2673 Y2674 G2675 V2679 F2682 Q2685 M2686 F2692 Y2693 R2694 T2695 S2696 D2697 Q2698 T2699 W2700 V2701 R2705 C2712 N2713 P2714 K2721 P2722 L2723 R2726 F2727 L2728 R2729
Y2735 V2736 P2739 L2744 I2747 Y2748 G2749 R2757 L2758 I2759 L2762 R2763 E2767 T2770 F2784 T2785 Q2786 D2787 Y2792 I2793 Y2794 S2795 P2796 R2797 R2804 R2811 P2812 L2816 P2817 V2818 E2819 G2820 L2821 I2822 A2826 R2831 Q2834 D2835 R2836 I2837 V2838 E2839 D2840 E2841 E2842
R2843 D2847 I2850 D2851 L2855 F2858 I2861 D2862 R2863 M2867 S2868 R2869 P2870 I2871 L2872 D2880 Y2881 I2882 E2888 V2893 R2896 Y2901 E2902 L2909 V2910 L2911 V2919 L2920 D2923 R2924 I2925 L2933 L2934 L2935 I2936 G2937 V2938 S2939 V2950 N2954 Q2960
H2964 R2965 K2966 Y2967 T2968 G2969 E2970 D2971 F2972 D2973 R2977 R2981 R2982 S2983 G2984 I2990 A2991 F2992 D2995 E2996 S2997 N2998 V2999 L3000 D3001 S3002 G3003 F3004 L3005 E3006 R3007 A3013 E3016 V3017 P3018 G3019 L3020 F3021 E3022 G3023 D3024 E3025 T3028 L3029 M3030 T3031 Q3032 C3033 K3034 E3035 G3036 A3037 Q3038
K3039 E3040 M3043 L3044 D3045 S3046 H3047 E3048 E3049 L3050 W3053 S3056 Q3057 R3060 V3064 V3065 F3066 T3067 M3068 N3069 P3070 S3071 S3072 E3073 G3074 L3075 K3076 D3077 R3078 A3079 A3080 T3081 S3082 P3083 N3087 R3088 C3089 V3090 L3091 N3092 W3093 V3105 G3106 T3110 M3113 D3114 L3115 N3119 D3124
L3133 P3134 Q3135 P3136 P3137 R3140 I3143 V3144 L3154 N3158 L3161 A3162 K3163 R3167 T3168 M3169 A3170 I3171 T3172 H3175 A3184 K3190 L3194 E3195 Q3198 M3199 H3200 L3201 N3202 V3203 G3204 L3205 R3206 K3207 I3208 K3209 E3210 T3211 V3212 D3213 Q3214 V3215 E3216 E3217 L3218 R3219 ARG ASP
LEU ARG ILE LYS SER GLN GLU LEU GLU VAL LYS ASN 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 ALA VAL LYS SER ILE LYS LYS GLN HIS LEU VAL GLU GLU VAL MET ALA ASN PRO PRO ALA ALA VAL LYS LEU ALA LEU GLU SER ILE CYS LEU LEU LEU ALA GLY GLU SER THR THR ASP TRP LYS GLN ILE ARG SER ILE
ILE MET ARG GLU ASN PHE SER ALA GLU GLU ILE SER ASP ALA ILE ARG GLU LYS MET LYS LYS MET TYR GLU ILE VAL ASN ARG ALA SER LEU 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 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 T3495 F3496 Q3499 T3502 I3503 S3510 Y3516 F3520 M3524 R3525 Q3526 W3532 R3544 T3545 D3546 R3549 T3550 E3551 Y3552 L3553
R3559 L3567 N3576 L3580 N3584 P3587 L3588 D3591 P3592 E3598 F3599 I3600 M3601 D3606 R3611 F3614 L3615 D3616 D3617 R3620 E3624 S3625 F3629 L3634 V3635 Q3636 D3637 V3638 E3639 S3640 Y3641 L3645 M3650 R3651 E3652 V3653 R3654 R3655 T3656 G3657 G3658 R3659 V3660
L3661 I3662 T3663 L3664 G3665 D3666 Q3667 D3668 I3669 D3670 L3671 S3674 F3678 L3679 S3680 P3684 P3689 P3690 D3691 L3692 C3693 S3694 R3695 F3698 V3699 N3700 R3705 L3708 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 M3791 Q3792 E3793 V3794 E3795 T3796 V3797 S3798 Q3799 S3809 S3810 I3811 Y3812
F3813 S3817 Y3825 Q3826 V3839 L3840 Y3841 E3842 N3843 L3846 D3851 Q3854 L3863 F3864 R3870 R3873 G3874 M3875 I3881 T3882 F3883 A3884 M3885 L3886 E3913 L3916 S3917 A3918 G3919 P3922 R3923 I3924 V3929 E3930 Q3931 A3932 E3933 A3934 V3935 V3936 R3937 L3938 F3944 L3947
K3950 L3961 P3966 V3970 P3971 Y3972 L3973 W3974 S3975 E3976 E3977 G3984 I3987 H3988 R3989 A3995 F3996 R3997 R4000 L4001 L4002 V4009 S4010 L4013 G4014 E4015 S4016 F4017 M4018 S4019 I4020 M4021 E4022 Q4023 D4026 L4027 T4028 H4029 I4030 V4031 E4034 P4037 P4040 V4041 L4042 M4043
C4044 V4055 L4058 N4063 I4066 T4067 S4068 I4071 G4072 S4073 A4074 F4077 R4092 M4095 L4096 K4097 N4098 V4099 P4103 L4106 P4118 L4124 K4133 V4136 R4143 I4144 F4145 V4146 P4149 P4150 T4160 I4164 P4165 V4166 K4171 S4172 R4176 A4177 R4178 L4179
E4192 R4193 L4194 R4195 G4200 W4201 Y4205 E4209 S4210 D4211 L4212 R4213 W4222 L4223 D4224 A4227 I4233 K4244 Y4252 D4257 N4258 E4259 F4260 D4261 E4270 D4289 G4290 H4291 K4292 D4293 M4296 P4297 R4302 F4305 W4308 L4311 L4312 P4313 D4314 T4315 P4318
L4323 P4324 N4325 N4326 G4336 M4339 I4340 M4346 Q4347 MET LEU GLU ASP GLU ASP ASP LEU ALA TYR ALA GLU THR GLU LYS LYS THR ARG THR ASP SER THR SER ASP GLY ARG P4374 A4375 W4376 T4379 L4380 T4383 R4400 E4403 N4404 I4405 K4406 E4414 A4432 E4439 G4440
K4441 K4442 K4443 Q4444 T4445 M4446 Y4447 E4454 L4460 M4473 T4474 V4475 T4476 Q4477 W4478 V4479 R4485 L4489 S4498 K4502 K4505 C4510 P4517 Q4530 Q4549 G4550 A4551 T4552 L4553 D4554 S4557 T4561 L4565 Q4566 N4579 N4597 T4598 E4599 K4600 P4608 V4609 Y4610
L4611 N4612 F4613 D4617 L4618 I4619 K4629 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	116933	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	1.338	Depositor
Minimum map value	-0.874	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1573, 1.1573, 1.1573	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.18	0/22200	0.35	0/30095

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	21735	0	21770	494	0
2	A	81	0	36	8	0
3	A	31	0	12	0	0
All	All	21847	0	21818	495	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 11.

All (495) 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:3790:VAL:HG13	1:A:3794:VAL:HB	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2220:LEU:HB2	1:A:2342:MET:HG2	1.63	0.80
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.64	0.79
1:A:3499:GLN:HA	1:A:3502:THR:HG22	1.64	0.78
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.65	0.77
1:A:1950:GLN:HG2	1:A:2006:VAL:HG13	1.67	0.77
1:A:2569:VAL:HB	1:A:2747:ILE:HG13	1.66	0.77
1:A:4227:ALA:HB2	1:A:4233:ILE:HD12	1.69	0.74
1:A:3154:LEU:HB3	1:A:3171:ILE:HD13	1.68	0.74
1:A:3485:GLU:OE2	1:A:3489:TRP:NE1	2.19	0.74
1:A:3175:HIS:HB3	1:A:3516:TYR:HE1	1.55	0.72
1:A:2444:GLU:HG2	1:A:2510:MET:HE2	1.71	0.71
1:A:2855:LEU:HD11	1:A:2863:ARG:HE	1.55	0.71
1:A:2872:LEU:HD12	1:A:2920:LEU:HD12	1.72	0.71
1:A:3689:PRO:HG2	1:A:3692:LEU:HD23	1.72	0.71
1:A:1698:ILE:HD12	1:A:1701:TRP:HE1	1.55	0.70
1:A:3817:SER:HB2	1:A:4346:MET:HE1	1.72	0.70
1:A:2615:MET:HG3	1:A:2658:TRP:HB2	1.72	0.70
1:A:2670:ASP:HA	1:A:2721:LYS:HE3	1.74	0.70
1:A:4192:GLU:OE1	1:A:4195:ARG:NH1	2.25	0.69
1:A:1647:VAL:HA	1:A:1650:LEU:HD13	1.74	0.69
1:A:4027:LEU:HB3	1:A:4058:LEU:HD22	1.74	0.69
1:A:1628:ARG:NH1	1:A:1706:GLU:OE2	2.25	0.68
1:A:2304:ASP:OD1	1:A:2726:ARG:NH2	2.25	0.68
1:A:2851:ASP:HA	1:A:2867:MET:HE1	1.75	0.68
1:A:1961:ASN:ND2	1:A:2019:ASN:O	2.26	0.68
1:A:3113:MET:HE1	1:A:3184:ALA:HA	1.76	0.68
1:A:1913:THR:OG1	2:A:4701:ADP:O1A	2.11	0.68
1:A:1628:ARG:HA	1:A:1951:VAL:HG22	1.76	0.68
1:A:2739:PRO:HD2	1:A:2796:PRO:HG2	1.76	0.67
1:A:1706:GLU:HG3	1:A:1709:MET:HE2	1.76	0.67
1:A:3588:LEU:HD23	1:A:3698:PHE:HE1	1.59	0.65
1:A:1888:CYS:HB2	1:A:2041:MET:HE1	1.78	0.65
1:A:3661:LEU:HD11	1:A:3668:ASP:HB3	1.79	0.65
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	1.78	0.65
1:A:1686:PHE:HA	1:A:1712:THR:HG21	1.77	0.64
1:A:3721:ARG:O	1:A:3725:ASP:N	2.27	0.64
1:A:4406:LYS:HG2	1:A:4530:GLN:HE22	1.62	0.64
1:A:3551:GLU:OE1	1:A:3559:ARG:NH1	2.31	0.64
1:A:3721:ARG:HB3	1:A:3724:VAL:HB	1.79	0.64
1:A:2494:LEU:O	1:A:2498:ILE:HD12	1.98	0.63
1:A:4313:PRO:HB2	1:A:4315:THR:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3935:VAL:HG22	1:A:3996:PHE:HE1	1.63	0.63
1:A:4565:LEU:HD13	1:A:4642:VAL:HG22	1.80	0.63
1:A:4400:ARG:NH1	1:A:4414:GLU:OE2	2.32	0.63
1:A:2258:ALA:HB1	1:A:2682:PHE:HD1	1.64	0.63
1:A:2562:VAL:O	1:A:2804:ARG:NH1	2.32	0.63
1:A:1664:ILE:HG22	1:A:1676:ILE:HG22	1.80	0.62
1:A:2287:ILE:HA	1:A:2294:GLU:HG3	1.81	0.62
1:A:2324:LEU:HD12	1:A:2332:ARG:HD2	1.82	0.62
1:A:2757:ARG:HA	1:A:2763:ARG:HH21	1.64	0.61
1:A:2840:ASP:OD1	1:A:2843:ARG:NH2	2.33	0.61
1:A:2935:LEU:N	1:A:3066:PHE:O	2.32	0.61
1:A:3938:LEU:HD13	1:A:3995:ALA:HB2	1.82	0.61
1:A:4171:LYS:HG3	1:A:4172:SER:H	1.66	0.61
1:A:4176:ARG:NH2	1:A:4224:ASP:OD1	2.30	0.61
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.82	0.61
1:A:2073:PHE:HE2	1:A:2093:LEU:HA	1.65	0.60
1:A:1655:LYS:NZ	1:A:2330:GLY:O	2.33	0.60
1:A:4209:GLU:OE1	1:A:4213:ARG:NH2	2.35	0.60
1:A:2492:ARG:HH22	1:A:2525:PRO:HB2	1.66	0.60
1:A:3031:THR:O	1:A:3035:GLU:HG2	2.01	0.60
1:A:2263:HIS:CG	1:A:2695:THR:HB	2.36	0.60
1:A:2819:GLU:HA	1:A:2861:ILE:HD11	1.82	0.60
1:A:4178:ARG:HD2	1:A:4296:MET:HE1	1.84	0.60
1:A:3115:LEU:HD23	1:A:3143:ILE:HG13	1.84	0.60
1:A:4068:SER:HB2	1:A:4097:LYS:HE2	1.84	0.59
1:A:2923:ASP:OD1	1:A:2954:ASN:ND2	2.33	0.59
1:A:3974:TRP:NE1	1:A:3976:GLU:OE2	2.36	0.59
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.35	0.59
1:A:1755:GLN:HG2	1:A:1814:GLU:OE2	2.01	0.59
1:A:2271:ASN:OD1	1:A:2272:THR:N	2.34	0.59
1:A:1844:PHE:HZ	1:A:1922:GLN:HE21	1.49	0.59
1:A:3971:PRO:HG2	1:A:3973:LEU:HD11	1.83	0.59
1:A:2593:LEU:HD23	1:A:2736:VAL:HG21	1.82	0.59
1:A:2901:TYR:OH	1:A:2909:LEU:N	2.36	0.59
1:A:3071:SER:O	1:A:3075:LEU:N	2.31	0.59
1:A:3886:LEU:HD11	1:A:4346:MET:HG3	1.84	0.59
1:A:4019:SER:O	1:A:4023:GLN:NE2	2.26	0.59
1:A:3207:LYS:HE2	1:A:3753:LEU:HG	1.84	0.58
1:A:4194:LEU:HD23	1:A:4201:TRP:CD1	2.39	0.58
1:A:2253:ILE:O	1:A:2693:TYR:OH	2.20	0.58
1:A:1913:THR:O	1:A:1917:LYS:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2191:LEU:HD11	1:A:2232:MET:HE2	1.85	0.58
1:A:4178:ARG:HH11	1:A:4296:MET:HE1	1.69	0.58
1:A:1687:LYS:HG2	1:A:1712:THR:HG22	1.84	0.58
1:A:4260:PHE:HE2	1:A:4618:LEU:HD11	1.69	0.58
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.36	0.58
1:A:2483:ILE:O	1:A:2487:GLU:HG3	2.04	0.57
1:A:2499:LEU:HD21	1:A:2518:ILE:HG21	1.85	0.57
1:A:4030:ILE:HG21	1:A:4145:PHE:CZ	2.37	0.57
1:A:1982:LEU:HD21	1:A:2012:MET:HB3	1.85	0.57
1:A:2910:VAL:HG11	1:A:3105:VAL:HG22	1.86	0.57
1:A:3638:VAL:HG11	1:A:3679:LEU:HB3	1.85	0.57
1:A:3843:ASN:HB3	1:A:3846:LEU:HD12	1.87	0.57
1:A:1650:LEU:HD21	1:A:1698:ILE:HD11	1.85	0.57
1:A:2453:ARG:NH1	1:A:2505:ASP:OD2	2.38	0.57
1:A:3135:GLN:O	1:A:3137:PRO:HD3	2.05	0.57
1:A:2834:GLN:NE2	1:A:2843:ARG:HD2	2.20	0.56
1:A:1946:VAL:HG12	1:A:2001:LEU:HD13	1.87	0.56
1:A:2086:TYR:OH	1:A:2153:ASP:OD2	2.11	0.56
1:A:2231:SER:OG	1:A:2344:GLU:OE2	2.22	0.56
1:A:3216:GLU:OE1	1:A:3219:ARG:NH2	2.38	0.56
1:A:2581:LEU:HD13	1:A:2591:LEU:HD11	1.88	0.56
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.39	0.56
1:A:3882:THR:HG22	1:A:4339:MET:HG3	1.86	0.56
1:A:2626:THR:HG22	1:A:2679:VAL:HG11	1.87	0.56
1:A:3751:GLN:HA	1:A:3754:ASN:HD22	1.71	0.56
1:A:4040:PRO:HB3	1:A:4124:LEU:HD23	1.88	0.56
1:A:2322:ASN:OD1	1:A:2323:LYS:N	2.39	0.56
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.69	0.56
1:A:3588:LEU:HD23	1:A:3698:PHE:CE1	2.39	0.55
1:A:1909:GLY:N	2:A:4701:ADP:O2B	2.39	0.55
1:A:3746:GLU:HG2	1:A:3773:LEU:HD11	1.88	0.55
1:A:3913:GLU:N	1:A:3913:GLU:OE1	2.39	0.55
1:A:3161:LEU:HD11	1:A:3524:MET:HE2	1.89	0.55
1:A:1967:MET:HA	1:A:1967:MET:HE2	1.89	0.55
1:A:3017:VAL:HB	1:A:3020:LEU:HD23	1.88	0.55
1:A:2666:ILE:HG22	1:A:2712:CYS:HB3	1.87	0.55
1:A:2992:PHE:HB3	1:A:3064:VAL:HA	1.89	0.55
1:A:3691:ASP:O	1:A:3695:ARG:HG2	2.07	0.55
1:A:3759:ARG:HG3	1:A:3760:ILE:HG12	1.88	0.55
1:A:4205:TYR:OH	1:A:4261:ASP:OD2	2.16	0.55
1:A:3851:ASP:HB3	1:A:3854:GLN:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2762:LEU:HD21	1:A:2821:LEU:HD22	1.89	0.55
1:A:4297:PRO:HG3	1:A:4308:TRP:CG	2.42	0.55
1:A:1917:LYS:HG2	1:A:1927:VAL:HG21	1.89	0.55
1:A:2222:MET:HE1	1:A:2234:TRP:CD1	2.41	0.54
1:A:1623:ARG:HE	1:A:1637:LEU:HD22	1.72	0.54
1:A:3584:ASN:O	1:A:3651:ARG:NH2	2.37	0.54
1:A:4257:ASP:OD1	1:A:4258:ASN:N	2.39	0.54
1:A:1631:PHE:HA	1:A:1947:GLY:HA3	1.89	0.54
1:A:3729:SER:O	1:A:3733:LYS:HG2	2.07	0.54
1:A:1939:GLN:H	1:A:1939:GLN:CD	2.15	0.54
1:A:3875:MET:HE1	1:A:3883:PHE:HB2	1.89	0.54
1:A:4031:VAL:HG21	1:A:4058:LEU:HD21	1.90	0.54
1:A:2982:ARG:HB3	1:A:2990:ILE:HD11	1.89	0.54
1:A:1652:LYS:NZ	1:A:2329:ASN:O	2.37	0.54
1:A:4460:LEU:HD21	1:A:4478:TRP:CD1	2.42	0.54
1:A:2278:GLY:O	1:A:2282:HIS:N	2.31	0.53
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.42	0.53
1:A:1950:GLN:NE2	1:A:2007:LYS:H	2.05	0.53
1:A:2933:LEU:HB2	1:A:3065:VAL:HG23	1.91	0.53
1:A:1698:ILE:HD12	1:A:1701:TRP:NE1	2.23	0.53
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.89	0.53
1:A:2571:THR:H	1:A:2574:THR:HB	1.74	0.53
1:A:1814:GLU:OE2	1:A:1818:GLN:NE2	2.37	0.53
1:A:2499:LEU:O	1:A:2503:SER:OG	2.21	0.53
1:A:3873:ARG:HD3	1:A:4021:MET:HE1	1.91	0.52
1:A:3722:PRO:HA	1:A:3725:ASP:HB3	1.91	0.52
1:A:1713:LEU:HD22	1:A:1749:LEU:HD21	1.91	0.52
1:A:2261:LYS:HG2	1:A:2310:GLU:OE1	2.09	0.52
1:A:2313:GLU:OE1	1:A:2316:ASN:ND2	2.42	0.52
1:A:2354:ALA:HB1	1:A:2358:ARG:HH21	1.73	0.52
1:A:3194:LEU:HD21	1:A:3499:GLN:HG2	1.91	0.52
1:A:1685:MET:HE2	1:A:1685:MET:HA	1.91	0.52
1:A:3113:MET:HG3	1:A:3115:LEU:HD13	1.92	0.52
1:A:1985:HIS:NE2	1:A:2010:PRO:HB3	2.24	0.52
1:A:3520:PHE:HB3	1:A:3524:MET:HB2	1.91	0.52
1:A:2685:GLN:HE22	1:A:2692:PHE:HA	1.74	0.52
1:A:3870:ARG:NH2	1:A:4034:GLU:OE1	2.43	0.52
1:A:2498:ILE:HG23	1:A:2502:LEU:HD22	1.92	0.51
1:A:3204:GLY:O	1:A:3208:ILE:HG12	2.10	0.51
1:A:2354:ALA:HB1	1:A:2358:ARG:HE	1.75	0.51
1:A:2831:ARG:HB3	1:A:2924:ARG:NH2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1979:GLN:O	1:A:1983:ARG:HG3	2.10	0.51
1:A:2936:ILE:HG23	1:A:3068:MET:HG3	1.92	0.51
1:A:4166:VAL:HB	1:A:4302:ARG:HH22	1.75	0.51
1:A:2658:TRP:CE3	1:A:2705:ARG:HA	2.46	0.51
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.93	0.51
1:A:3764:ASP:OD1	1:A:3764:ASP:N	2.44	0.51
1:A:3169:MET:HG2	1:A:3698:PHE:CE2	2.46	0.51
1:A:3207:LYS:HZ2	1:A:3754:ASN:CG	2.18	0.51
1:A:3935:VAL:HG13	1:A:3947:LEU:HD23	1.92	0.51
1:A:1912:LYS:NZ	2:A:4701:ADP:O2B	2.43	0.51
1:A:3028:THR:HG22	1:A:3032:GLN:HE21	1.76	0.51
1:A:3786:GLU:O	1:A:3790:VAL:HG23	2.10	0.51
1:A:3690:PRO:HA	1:A:3693:CYS:SG	2.51	0.51
2:A:4703:ADP:N3	2:A:4703:ADP:H2'	2.25	0.51
1:A:1888:CYS:O	1:A:1892:MET:HG2	2.10	0.51
1:A:3158:ASN:OD1	1:A:3168:THR:HB	2.10	0.50
1:A:3650:ASN:OD1	1:A:3695:ARG:NH1	2.44	0.50
1:A:2797:ARG:NH1	1:A:3087:ASN:OD1	2.43	0.50
1:A:3567:LEU:HB2	1:A:3599:PHE:CE1	2.46	0.50
1:A:3734:LEU:HD12	1:A:3735:GLN:HG3	1.93	0.50
1:A:1623:ARG:HB3	1:A:1630:TYR:CD2	2.47	0.50
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.45	0.50
1:A:1722:THR:O	1:A:1726:ILE:HG12	2.12	0.50
1:A:3796:THR:HA	1:A:3799:GLN:HG3	1.93	0.50
1:A:2693:TYR:HE1	1:A:2700:TRP:HE3	1.58	0.50
1:A:3526:GLN:OE1	1:A:3549:ARG:NH2	2.38	0.50
1:A:3785:GLU:O	1:A:3789:ILE:HG13	2.11	0.50
1:A:3929:VAL:O	1:A:3933:GLU:HG3	2.11	0.50
1:A:2189:MET:HE3	1:A:2239:LYS:HG3	1.94	0.50
1:A:2337:PRO:O	1:A:2340:ARG:NH1	2.45	0.50
1:A:3194:LEU:HD11	1:A:3499:GLN:HE21	1.76	0.50
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	1.94	0.50
1:A:2234:TRP:CZ2	1:A:2302:VAL:HG21	2.47	0.50
1:A:3783:LYS:O	1:A:3787:THR:HG23	2.12	0.50
1:A:1880:VAL:HG21	1:A:2049:ILE:HG12	1.92	0.50
1:A:2029:PRO:HG2	1:A:2032:LEU:HD12	1.94	0.50
1:A:2449:LEU:HD11	1:A:2454:CYS:SG	2.52	0.50
1:A:2969:GLY:HA2	1:A:3004:PHE:HE1	1.76	0.50
1:A:3488:ARG:HG2	1:A:3491:LYS:HE3	1.94	0.50
1:A:3499:GLN:HB3	1:A:3544:ARG:HH22	1.77	0.50
1:A:1652:LYS:HA	1:A:1655:LYS:HE3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2816:LEU:HD23	1:A:2817:PRO:O	2.12	0.49
1:A:4037:PRO:HB2	1:A:4118:PRO:HG2	1.93	0.49
1:A:4066:ILE:HD11	1:A:4095:MET:HE3	1.93	0.49
1:A:2612:LEU:HB3	1:A:2615:MET:HE2	1.94	0.49
1:A:3793:GLU:OE2	1:A:3794:VAL:HG23	2.12	0.49
1:A:1914:GLU:HG2	2:A:4701:ADP:O1A	2.12	0.49
1:A:4068:SER:HA	1:A:4095:MET:HB3	1.93	0.49
1:A:1882:THR:HG22	1:A:2048:LEU:HD22	1.94	0.49
1:A:2759:ILE:HG13	1:A:2759:ILE:O	2.12	0.49
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.95	0.49
1:A:1630:TYR:HE1	1:A:1946:VAL:HG23	1.76	0.49
1:A:1769:MET:HE1	1:A:1775:ALA:O	2.12	0.49
1:A:2527:PRO:HG3	1:A:2545:TRP:CG	2.46	0.49
1:A:4475:VAL:O	1:A:4479:VAL:HG23	2.13	0.49
1:A:3755:GLU:HB3	1:A:3757:LYS:HG3	1.95	0.49
1:A:2836:ARG:HD3	1:A:3091:LEU:HD21	1.94	0.49
1:A:4178:ARG:NH1	1:A:4296:MET:HE1	2.27	0.49
1:A:1631:PHE:CZ	1:A:1944:ILE:HD11	2.48	0.49
1:A:2152:GLU:O	1:A:2155:PRO:HD2	2.12	0.48
1:A:2671:MET:HE2	1:A:2675:GLY:HA2	1.95	0.48
1:A:3198:GLN:NE2	1:A:3496:PHE:HB3	2.29	0.48
1:A:2686:MET:HG2	1:A:2692:PHE:HB3	1.96	0.48
1:A:1880:VAL:CG2	1:A:2049:ILE:HG12	2.44	0.48
1:A:3044:LEU:HB3	1:A:3049:GLU:HG3	1.95	0.48
1:A:3169:MET:HG2	1:A:3698:PHE:HE2	1.78	0.48
1:A:1640:ILE:HG13	1:A:1650:LEU:HG	1.96	0.48
1:A:3787:THR:O	1:A:3790:VAL:HB	2.12	0.48
1:A:3485:GLU:HG2	1:A:3770:LEU:HD21	1.96	0.48
1:A:4311:LEU:O	1:A:4311:LEU:HD23	2.13	0.48
1:A:1628:ARG:HG3	1:A:1706:GLU:OE1	2.13	0.48
1:A:2652:PRO:HD2	1:A:2705:ARG:CZ	2.43	0.48
1:A:2910:VAL:HG12	2:A:4704:ADP:N1	2.29	0.48
1:A:3201:LEU:HD22	1:A:3496:PHE:HD2	1.78	0.48
1:A:3780:VAL:O	1:A:3784:VAL:HG23	2.14	0.48
1:A:4613:PHE:HA	1:A:4643:LEU:HD13	1.96	0.48
1:A:1810:HIS:NE2	1:A:1876:GLN:O	2.47	0.48
1:A:2386:PRO:HG3	1:A:2413:LEU:HD13	1.95	0.47
1:A:3884:ALA:HB1	1:A:4009:VAL:HG11	1.95	0.47
1:A:3916:LEU:HD21	1:A:3937:ARG:HG2	1.96	0.47
1:A:1660:GLY:HA2	1:A:1679:ARG:NH2	2.29	0.47
1:A:3734:LEU:HA	1:A:3738:PHE:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3034:LYS:HG3	1:A:3050:LEU:HD11	1.95	0.47
1:A:1724:VAL:HA	1:A:1727:PHE:HD2	1.79	0.47
1:A:3158:ASN:ND2	1:A:3169:MET:O	2.47	0.47
1:A:2445:HIS:CD2	1:A:2449:LEU:HD22	2.49	0.47
1:A:2648:VAL:HG13	1:A:2701:VAL:HG22	1.96	0.47
1:A:4446:ASN:OD1	1:A:4447:TYR:N	2.44	0.47
1:A:1727:PHE:CD1	1:A:1733:ILE:HD11	2.50	0.47
1:A:1863:ASN:HD22	1:A:4222:TRP:HE1	1.61	0.47
1:A:2785:THR:HG23	1:A:2787:ASP:H	1.80	0.47
1:A:3620:ARG:O	1:A:3624:GLU:HG3	2.15	0.47
1:A:3950:LYS:NZ	1:A:3973:LEU:O	2.47	0.47
1:A:3749:LEU:HG	1:A:3766:ILE:HD11	1.97	0.47
1:A:1928:LEU:HD23	1:A:1948:LEU:HD21	1.96	0.47
1:A:3154:LEU:HD21	1:A:3532:TRP:HZ2	1.80	0.47
1:A:3664:LEU:HD13	1:A:3669:ILE:HD12	1.96	0.47
1:A:4071:ILE:HG23	1:A:4077:PHE:HE1	1.79	0.47
1:A:1623:ARG:HB3	1:A:1630:TYR:HD2	1.80	0.47
1:A:1788:THR:HA	1:A:1791:VAL:HG12	1.97	0.47
1:A:3870:ARG:HD3	1:A:4143:ARG:HH12	1.80	0.47
1:A:2620:LEU:HD22	1:A:2630:LEU:HD21	1.96	0.46
1:A:1949:CYS:SG	1:A:1978:ILE:HD13	2.55	0.46
1:A:2606:PHE:O	1:A:2610:ARG:HG2	2.14	0.46
1:A:3825:TYR:CZ	1:A:3875:MET:HG3	2.50	0.46
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	1.97	0.46
1:A:1932:CYS:C	1:A:1962:ARG:HH21	2.23	0.46
1:A:3738:PHE:HE2	1:A:3783:LYS:HE2	1.81	0.46
1:A:3950:LYS:HZ2	1:A:3975:SER:HB3	1.79	0.46
1:A:1724:VAL:HA	1:A:1727:PHE:CD2	2.51	0.46
1:A:1769:MET:CE	1:A:1777:PRO:HD2	2.46	0.46
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.97	0.46
1:A:2446:ILE:HD11	1:A:2714:PRO:HB3	1.97	0.46
1:A:2452:LEU:HD23	1:A:2452:LEU:HA	1.72	0.46
1:A:2723:LEU:HD13	1:A:2727:PHE:CD2	2.51	0.46
1:A:2964:HIS:H	1:A:2967:TYR:HB2	1.79	0.46
1:A:3744:GLN:O	1:A:3747:LYS:HG3	2.15	0.46
1:A:3793:GLU:O	1:A:3797:VAL:HG23	2.15	0.46
1:A:3811:ILE:HD11	1:A:3864:PHE:CE1	2.51	0.46
1:A:4610:TYR:HB2	1:A:4643:LEU:HD22	1.98	0.46
1:A:2110:LYS:HA	1:A:2113:ARG:NH1	2.31	0.46
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.98	0.46
1:A:1727:PHE:HD1	1:A:1733:ILE:HD11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2577:HIS:O	1:A:2581:LEU:HD23	2.16	0.46
1:A:2811:ARG:HB3	1:A:2812:PRO:HD3	1.98	0.46
1:A:4554:ASP:N	1:A:4557:SER:OG	2.49	0.46
1:A:3576:ASN:ND2	1:A:3700:ASN:O	2.45	0.46
1:A:3746:GLU:O	1:A:3750:LEU:HG	2.16	0.46
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.98	0.46
1:A:4473:MET:HG3	1:A:4477:GLN:HB2	1.97	0.46
1:A:2297:LYS:HB2	1:A:2299:GLN:NE2	2.31	0.45
1:A:2445:HIS:ND1	1:A:2505:ASP:OD1	2.43	0.45
1:A:3601:MET:HE1	1:A:3611:ARG:HB2	1.98	0.45
1:A:1659:ALA:HB2	1:A:1926:PHE:HB2	1.98	0.45
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.99	0.45
1:A:3488:ARG:O	1:A:3491:LYS:HG3	2.15	0.45
1:A:3489:TRP:CZ2	1:A:3750:LEU:HD22	2.50	0.45
1:A:4179:LEU:HD12	1:A:4223:LEU:HD11	1.97	0.45
1:A:4289:ASP:OD1	1:A:4292:LYS:HB3	2.16	0.45
1:A:2413:LEU:HG	1:A:2417:ARG:HE	1.82	0.45
1:A:2784:PHE:HB3	1:A:2792:TYR:CD2	2.51	0.45
1:A:3881:ILE:HG21	1:A:4002:LEU:HD11	1.97	0.45
1:A:4042:LEU:O	1:A:4145:PHE:N	2.45	0.45
1:A:2973:ASP:O	1:A:2977:ARG:HD3	2.17	0.45
1:A:2261:LYS:HG3	1:A:2311:TRP:HB3	1.98	0.45
1:A:2511:ARG:HB3	1:A:2535:ILE:CD1	2.47	0.45
1:A:2537:TYR:CD1	1:A:2547:PRO:HA	2.52	0.45
1:A:2749:GLY:N	1:A:2770:THR:HG21	2.32	0.45
1:A:3013:ALA:HA	1:A:3088:ARG:NH1	2.31	0.45
1:A:3792:GLN:O	1:A:3796:THR:OG1	2.32	0.45
1:A:1945:PHE:HA	1:A:1948:LEU:HD12	1.97	0.45
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.52	0.45
1:A:1751:VAL:O	1:A:1755:GLN:HG3	2.17	0.45
1:A:1863:ASN:HD22	1:A:4222:TRP:NE1	2.15	0.45
1:A:2369:LEU:HA	1:A:2373:MET:SD	2.57	0.45
1:A:3653:VAL:HG12	1:A:3662:ILE:HD11	1.97	0.45
1:A:4013:LEU:HD23	1:A:4017:PHE:CZ	2.51	0.45
1:A:4517:PRO:HG2	1:A:4619:ILE:HD12	1.99	0.45
1:A:4400:ARG:NE	1:A:4405:ILE:HD11	2.31	0.45
1:A:4566:GLN:NE2	1:A:4643:LEU:HD12	2.32	0.45
1:A:2481:MET:HG3	1:A:2485:GLN:NE2	2.32	0.45
1:A:2518:ILE:HA	1:A:2521:ILE:HG12	1.98	0.45
1:A:3030:MET:HE1	1:A:3050:LEU:HB2	1.99	0.44
1:A:4013:LEU:HD23	1:A:4017:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2784:PHE:HB2	1:A:2794:TYR:HE2	1.82	0.44
1:A:2880:ASP:HB2	1:A:2882:ILE:HG23	1.99	0.44
1:A:3037:ALA:HA	1:A:3040:GLU:HG2	1.97	0.44
1:A:2097:LEU:HD13	1:A:2097:LEU:HA	1.78	0.44
1:A:1853:VAL:HA	1:A:1856:GLN:HG3	1.99	0.44
1:A:3606:ASP:N	1:A:3606:ASP:OD1	2.48	0.44
1:A:1628:ARG:HD2	1:A:1951:VAL:HG22	1.99	0.44
1:A:1687:LYS:H	1:A:1712:THR:HG22	1.83	0.44
1:A:2290:SER:HB2	1:A:2295:LEU:HG	2.00	0.44
1:A:2499:LEU:HD12	1:A:2535:ILE:HD11	1.99	0.44
1:A:3033:CYS:HB2	1:A:3053:TRP:HZ3	1.82	0.44
1:A:3705:ARG:CZ	1:A:3813:PHE:HD2	2.30	0.44
1:A:3944:PHE:CE1	1:A:3974:TRP:HB3	2.52	0.44
1:A:1836:PHE:HA	1:A:1839:LEU:HB2	2.00	0.44
1:A:3826:GLN:NE2	1:A:4136:VAL:HG23	2.32	0.44
1:A:1717:LEU:O	1:A:1721:VAL:HG23	2.18	0.44
1:A:2563:ALA:HB3	1:A:2804:ARG:HD2	1.99	0.44
1:A:3206:ARG:O	1:A:3210:GLU:HG2	2.17	0.44
1:A:3614:PHE:CE2	1:A:3641:TYR:HA	2.53	0.44
1:A:2822:ILE:HD11	1:A:2858:PHE:CE2	2.53	0.44
1:A:1765:ALA:O	1:A:1769:MET:HG2	2.18	0.44
1:A:4260:PHE:CE2	1:A:4608:PRO:HB3	2.53	0.44
1:A:2123:ASP:O	1:A:2127:ILE:HG13	2.18	0.43
1:A:2693:TYR:CE1	1:A:2700:TRP:HE3	2.36	0.43
1:A:3113:MET:HE2	1:A:3113:MET:HB3	1.72	0.43
1:A:2209:GLN:O	1:A:2213:ILE:HG12	2.19	0.43
1:A:2492:ARG:HG2	1:A:2545:TRP:NE1	2.33	0.43
1:A:2920:LEU:HD23	1:A:2920:LEU:HA	1.78	0.43
1:A:3021:PHE:HD1	1:A:3025:GLU:HG3	1.83	0.43
1:A:1784:ASN:O	1:A:1788:THR:HG22	2.18	0.43
1:A:2517:TYR:CE2	1:A:2521:ILE:HD13	2.53	0.43
1:A:1647:VAL:HG11	1:A:1692:ILE:HD13	2.00	0.43
1:A:2937:GLY:C	1:A:3070:PRO:HD3	2.43	0.43
1:A:3738:PHE:CE2	1:A:3783:LYS:HE2	2.53	0.43
1:A:3922:PRO:HG2	1:A:3924:ILE:HD11	1.99	0.43
1:A:1675:GLY:HA3	1:A:1685:MET:HE2	2.01	0.43
1:A:3636:GLN:HA	1:A:3680:SER:HB3	2.01	0.43
1:A:4010:SER:HB3	1:A:4015:GLU:HA	2.00	0.43
1:A:4510:CYS:HG	1:A:4561:THR:HG1	1.61	0.43
1:A:2238:LEU:HB2	1:A:2300:TRP:CZ3	2.53	0.43
1:A:4095:MET:HE3	1:A:4095:MET:HB2	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2382:LEU:HD23	1:A:2420:ALA:HB2	1.99	0.43
1:A:1713:LEU:HD23	1:A:1713:LEU:HA	1.91	0.43
1:A:2665:GLU:HB3	1:A:2668:LEU:HB2	1.99	0.43
1:A:2826:ALA:HA	1:A:2850:ILE:HD11	2.01	0.43
1:A:2847:ASP:O	1:A:2850:ILE:HG22	2.18	0.43
1:A:3655:ARG:NE	1:A:3660:VAL:HG22	2.34	0.43
1:A:4095:MET:O	1:A:4096:LEU:HD23	2.19	0.43
1:A:4178:ARG:HE	1:A:4305:PHE:HZ	1.66	0.43
1:A:2028:LEU:HD21	1:A:2036:PHE:HB2	2.01	0.43
1:A:2838:VAL:HG22	1:A:3093:TRP:CE2	2.54	0.43
1:A:2919:VAL:HG23	1:A:2950:VAL:HG22	2.01	0.43
1:A:3931:GLN:O	1:A:3935:VAL:HG23	2.19	0.43
1:A:3950:LYS:NZ	1:A:3975:SER:HB3	2.33	0.43
1:A:1788:THR:O	1:A:1792:LEU:HD23	2.19	0.42
1:A:1961:ASN:HD21	1:A:2019:ASN:HB3	1.84	0.42
1:A:3218:LEU:HD21	1:A:3760:ILE:O	2.19	0.42
1:A:2465:ALA:HB2	1:A:2493:TYR:CE1	2.54	0.42
1:A:4044:CYS:O	1:A:4146:VAL:HA	2.18	0.42
1:A:2984:GLY:HA2	1:A:3057:GLN:HB3	2.00	0.42
1:A:3002:SER:O	1:A:3006:GLU:HG2	2.18	0.42
1:A:3106:GLY:HA3	1:A:3144:VAL:HG13	2.01	0.42
1:A:4001:LEU:HD21	1:A:4340:ILE:HD11	2.02	0.42
1:A:2449:LEU:HA	1:A:2449:LEU:HD12	1.74	0.42
1:A:2939:SER:O	1:A:3172:THR:HB	2.20	0.42
1:A:3734:LEU:HD22	1:A:3783:LYS:HB3	2.02	0.42
1:A:1873:LEU:O	1:A:1876:GLN:NE2	2.47	0.42
1:A:1900:LEU:HB2	1:A:2035:LEU:O	2.18	0.42
1:A:1910:THR:HG22	1:A:2044:PRO:HD3	2.00	0.42
1:A:2431:GLY:O	1:A:2435:LYS:HE2	2.20	0.42
1:A:3496:PHE:HA	1:A:3499:GLN:CD	2.44	0.42
1:A:2234:TRP:CE2	1:A:2302:VAL:HG21	2.54	0.42
1:A:2279:LEU:N	1:A:2698:GLN:HG2	2.35	0.42
1:A:3731:LEU:O	1:A:3734:LEU:HG	2.19	0.42
1:A:1838:TRP:CZ2	1:A:1843:ARG:HG2	2.54	0.42
1:A:2280:PHE:CE2	1:A:2315:LEU:HD21	2.55	0.42
1:A:4485:ARG:O	1:A:4489:LEU:HD23	2.18	0.42
1:A:1769:MET:HE1	1:A:1776:ALA:HA	2.02	0.42
1:A:2622:PHE:O	1:A:2668:LEU:HD23	2.20	0.42
1:A:4043:MET:HE1	1:A:4055:VAL:HB	2.01	0.42
1:A:4103:PRO:HB3	1:A:4133:LYS:O	2.19	0.42
1:A:1846:PHE:HE1	1:A:1856:GLN:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1933:ASP:N	1:A:1933:ASP:OD1	2.49	0.42
1:A:1938:PHE:O	1:A:1942:GLY:N	2.40	0.42
1:A:2175:MET:SD	1:A:2175:MET:N	2.93	0.42
1:A:2348:LEU:HD23	1:A:2348:LEU:HA	1.86	0.42
1:A:3870:ARG:HD3	1:A:4143:ARG:NH1	2.34	0.42
1:A:3961:LEU:O	1:A:3997:ARG:NH1	2.49	0.42
1:A:4211:ASP:HB3	1:A:4252:TYR:CE1	2.55	0.42
1:A:2519:ARG:HG2	1:A:2526:LEU:HD13	2.02	0.41
1:A:2307:VAL:HG23	1:A:2311:TRP:CZ2	2.55	0.41
1:A:2452:LEU:HD13	1:A:2729:ARG:HE	1.83	0.41
1:A:2869:ARG:O	1:A:2871:ILE:HD12	2.20	0.41
1:A:2594:CYS:O	1:A:2735:TYR:HA	2.20	0.41
1:A:4042:LEU:HB2	1:A:4144:ILE:HA	2.02	0.41
1:A:2449:LEU:HA	1:A:2453:ARG:HH21	1.86	0.41
1:A:2503:SER:HB3	1:A:2514:LEU:HD22	2.03	0.41
1:A:2834:GLN:HE21	1:A:2843:ARG:HD2	1.85	0.41
1:A:3175:HIS:HB3	1:A:3516:TYR:CE1	2.44	0.41
1:A:3984:GLY:O	1:A:3987:ILE:HG22	2.20	0.41
1:A:4380:LEU:HA	1:A:4383:THR:HG22	2.02	0.41
1:A:1860:GLN:HG2	1:A:1865:LYS:HG2	2.03	0.41
1:A:2631:LEU:HD12	1:A:2682:PHE:HD2	1.84	0.41
1:A:2723:LEU:HD13	1:A:2727:PHE:HD2	1.86	0.41
1:A:2797:ARG:NH2	2:A:4703:ADP:O2A	2.53	0.41
1:A:2896:ARG:HA	1:A:2896:ARG:HD2	1.69	0.41
1:A:3030:MET:HG3	1:A:3047:HIS:CD2	2.55	0.41
1:A:3056:SER:O	1:A:3060:ARG:HG2	2.21	0.41
1:A:3190:LYS:HB3	1:A:3503:ILE:HD11	2.03	0.41
1:A:3841:TYR:O	1:A:3842:GLU:HG2	2.20	0.41
1:A:1702:LEU:HD23	1:A:1702:LEU:HA	1.92	0.41
1:A:1985:HIS:CD2	1:A:2010:PRO:HB3	2.56	0.41
1:A:2288:ILE:CD1	1:A:2333:LEU:HB3	2.50	0.41
1:A:2744:LEU:HA	1:A:2747:ILE:HG22	2.02	0.41
1:A:4376:TRP:HA	1:A:4379:THR:HG22	2.01	0.41
1:A:1739:ILE:HG23	1:A:1804:ARG:HD3	2.02	0.41
1:A:1891:THR:HG21	1:A:2039:LEU:HB2	2.02	0.41
1:A:2964:HIS:NE2	1:A:2966:LYS:HB2	2.35	0.41
1:A:4026:ASP:OD1	1:A:4028:THR:OG1	2.28	0.41
1:A:4293:ASP:N	1:A:4293:ASP:OD1	2.53	0.41
1:A:2257:LYS:HA	1:A:2257:LYS:HD2	1.81	0.41
1:A:2464:GLN:HB2	1:A:2583:THR:HG23	2.03	0.41
1:A:1636:ASP:HB3	1:A:1653:HIS:ND1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1665:ILE:N	1:A:1675:GLY:O	2.48	0.41
1:A:1945:PHE:HE2	1:A:1978:ILE:HD12	1.86	0.41
1:A:1967:MET:O	1:A:1971:VAL:HG22	2.21	0.41
1:A:2441:PHE:HA	1:A:2449:LEU:HD23	2.03	0.41
1:A:2479:PHE:HE1	1:A:2482:GLN:HG2	1.85	0.41
1:A:2888:GLU:OE1	1:A:2888:GLU:N	2.52	0.41
1:A:2925:ILE:HD12	1:A:3090:VAL:HG11	2.02	0.41
1:A:3083:PRO:O	1:A:3087:ASN:N	2.54	0.41
1:A:3591:ASP:OD1	1:A:3591:ASP:N	2.48	0.41
1:A:3592:PRO:HG3	1:A:3684:PRO:HB3	2.02	0.41
1:A:3789:ILE:O	1:A:3793:GLU:N	2.46	0.41
1:A:3924:ILE:H	1:A:3924:ILE:HD12	1.86	0.41
1:A:3970:VAL:O	1:A:3989:ARG:NH1	2.53	0.41
1:A:4073:SER:OG	1:A:4074:ALA:N	2.54	0.41
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	2.02	0.41
1:A:4336:GLY:O	1:A:4340:ILE:HG12	2.20	0.41
1:A:1623:ARG:HA	1:A:1629:PHE:CZ	2.56	0.41
1:A:1945:PHE:CZ	1:A:1975:VAL:HG12	2.56	0.41
1:A:2863:ARG:H	1:A:2863:ARG:HD2	1.85	0.41
1:A:3587:PRO:HG2	1:A:3678:PHE:CE1	2.56	0.41
1:A:4289:ASP:OD1	1:A:4289:ASP:N	2.53	0.41
1:A:4610:TYR:HA	1:A:4617:ASP:O	2.21	0.41
1:A:1789:LEU:HD12	1:A:1789:LEU:HA	1.88	0.40
1:A:1855:GLN:HG2	1:A:1867:ASN:ND2	2.36	0.40
1:A:2014:ILE:HG22	1:A:2016:ILE:HD11	2.03	0.40
1:A:3110:THR:O	1:A:3140:ARG:NH1	2.54	0.40
1:A:1917:LYS:O	1:A:1921:HIS:CD2	2.74	0.40
1:A:2137:LEU:O	1:A:2141:VAL:HG23	2.21	0.40
1:A:3600:ILE:HD13	1:A:3600:ILE:HA	1.89	0.40
1:A:4244:LYS:HE3	1:A:4270:GLU:HA	2.03	0.40
1:A:1635:GLU:H	1:A:1635:GLU:CD	2.28	0.40
1:A:3634:LEU:HD23	1:A:3635:VAL:N	2.37	0.40
1:A:4027:LEU:O	1:A:4031:VAL:HG22	2.22	0.40
1:A:4160:THR:O	1:A:4164:ILE:HG13	2.21	0.40
1:A:4200:GLY:HA2	1:A:4323:LEU:HD21	2.04	0.40
1:A:2206:LYS:HD3	1:A:2206:LYS:HA	1.78	0.40
1:A:2893:VAL:HG13	1:A:2911:LEU:HD13	2.03	0.40
1:A:2969:GLY:HA2	1:A:3004:PHE:CE1	2.57	0.40
1:A:2995:ASP:OD1	1:A:2996:GLU:N	2.54	0.40
1:A:4149:PRO:HA	1:A:4150:PRO:HD3	1.96	0.40
1:A:1854:LEU:HA	1:A:1870:PHE:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2094:LYS:NZ	2:A:4701:ADP:H8	2.20	0.40
1:A:2495:VAL:HG13	1:A:2518:ILE:HD13	2.03	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	2697/4646 (58%)	2623 (97%)	74 (3%)	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	2405/4125 (58%)	2405 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1790	ASN
1	A	1863	ASN

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Mol	Chain	Res	Type
1	A	1894	GLN
1	A	1922	GLN
1	A	1976	GLN
1	A	2005	GLN
1	A	2130	ASN
1	A	2169	GLN
1	A	2171	HIS
1	A	2482	GLN
1	A	2531	ASN
1	A	2707	GLN
1	A	2781	GLN
1	A	2789	GLN
1	A	2827	HIS
1	A	3047	HIS
1	A	3069	ASN
1	A	3181	ASN
1	A	3188	HIS
1	A	3198	GLN
1	A	3522	GLN
1	A	3535	HIS
1	A	3584	ASN
1	A	3622	ASN
1	A	3772	ASN
1	A	3845	ASN
1	A	4397	HIS
1	A	4526	GLN
1	A	4530	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	4704	-	24,29,29	0.85	0	29,45,45	1.22	2 (6%)
3	ATP	A	4702	-	28,33,33	0.87	1 (3%)	34,52,52	0.62	1 (2%)
2	ADP	A	4703	-	24,29,29	0.89	1 (4%)	29,45,45	1.23	2 (6%)
2	ADP	A	4701	-	24,29,29	0.84	0	29,45,45	1.57	4 (13%)

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	4704	-	-	1/12/32/32	0/3/3/3
3	ATP	A	4702	-	-	5/18/38/38	0/3/3/3
2	ADP	A	4703	-	-	0/12/32/32	0/3/3/3
2	ADP	A	4701	-	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4702	ATP	PA-O3A	-2.43	1.56	1.59
2	A	4703	ADP	O4'-C1'	2.01	1.43	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4701	ADP	C4'-O4'-C1'	-4.43	105.87	109.92
2	A	4701	ADP	O4'-C1'-N9	3.81	113.79	108.75
2	A	4703	ADP	N3-C2-N1	-3.73	123.60	128.67
2	A	4704	ADP	N3-C2-N1	-3.65	123.72	128.67
2	A	4701	ADP	N3-C2-N1	-3.44	124.00	128.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4704	ADP	C4-C5-N7	-2.58	106.61	109.34
3	A	4702	ATP	C5-C6-N6	2.29	123.80	120.31
2	A	4703	ADP	C4-C5-N7	-2.20	107.01	109.34
2	A	4701	ADP	C4-C5-N7	-2.10	107.12	109.34

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

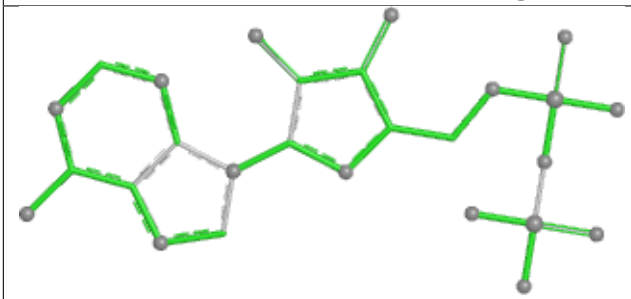
There are no ring outliers.

3 monomers are involved in 8 short contacts:

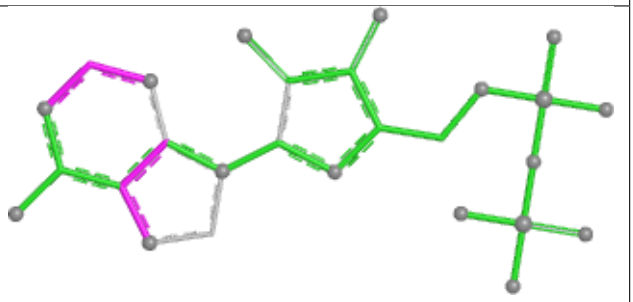
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4704	ADP	1	0
2	A	4703	ADP	2	0
2	A	4701	ADP	5	0

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.

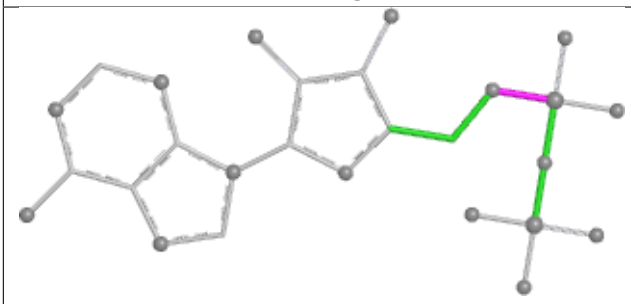
Ligand ADP A 4704



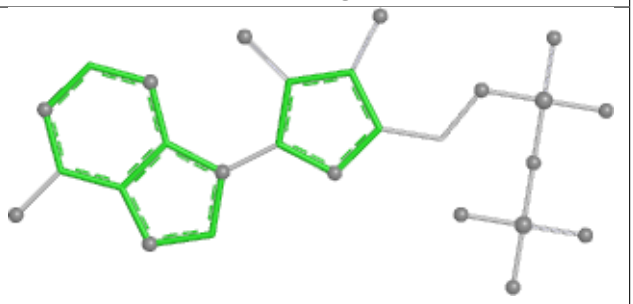
Bond lengths



Bond angles

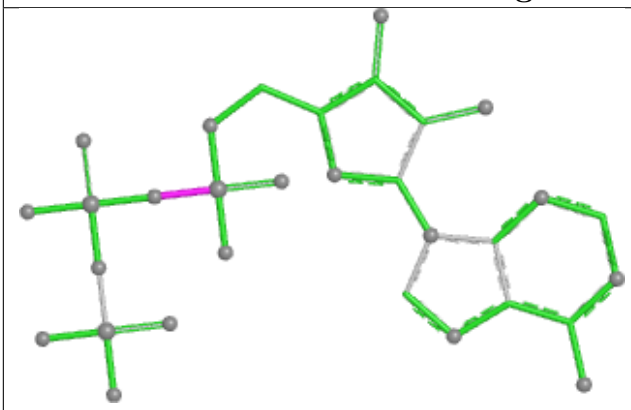


Torsions

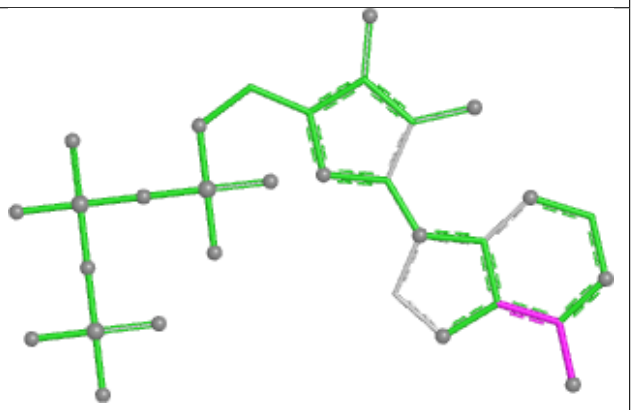


Rings

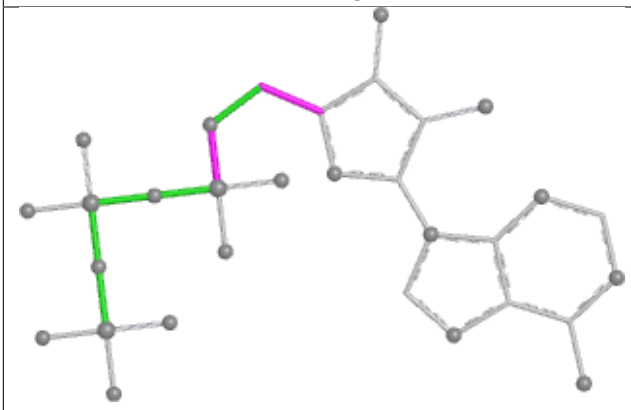
Ligand ATP A 4702



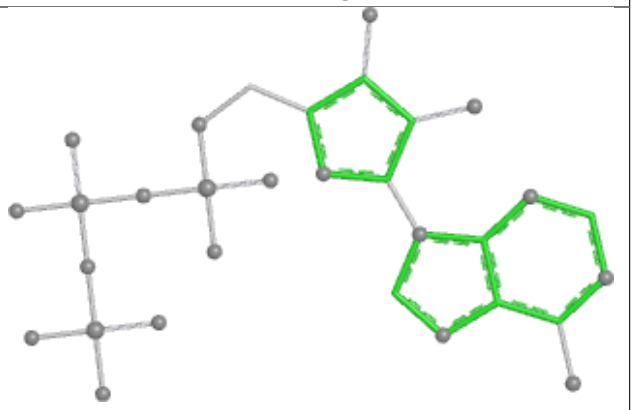
Bond lengths



Bond angles

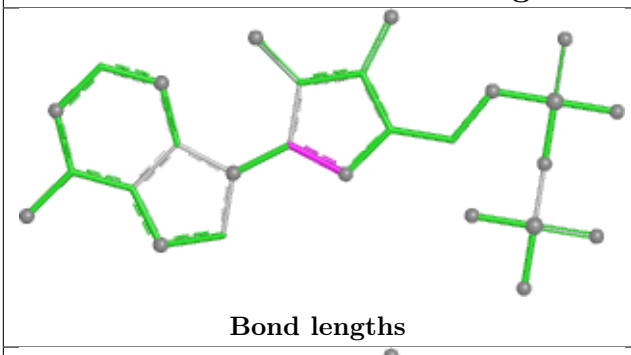


Torsions

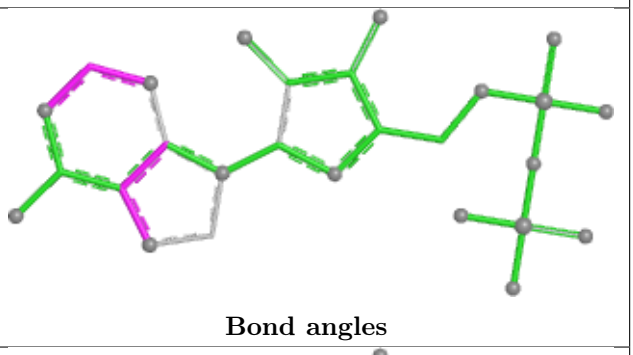


Rings

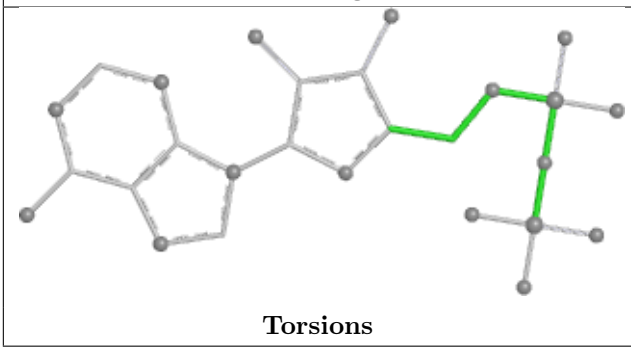
Ligand ADP A 4703



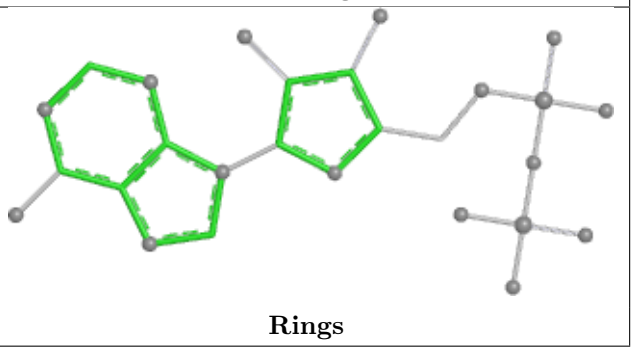
Bond lengths



Bond angles

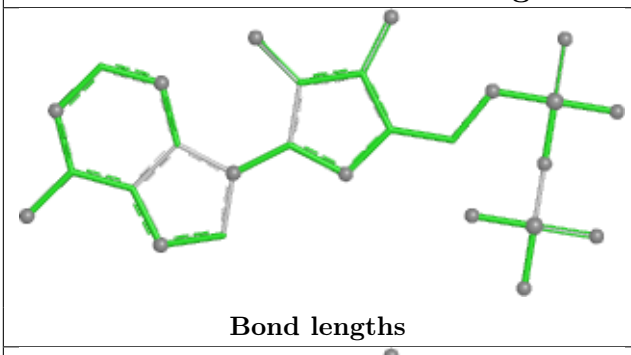


Torsions

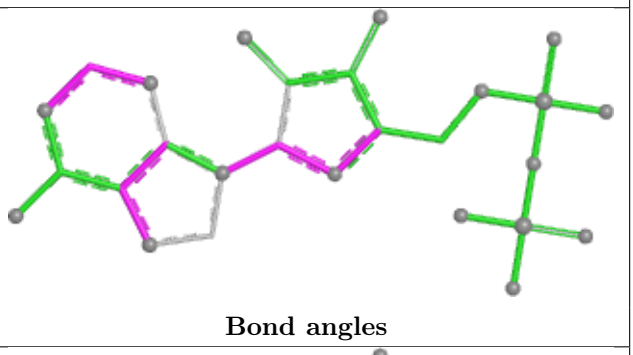


Rings

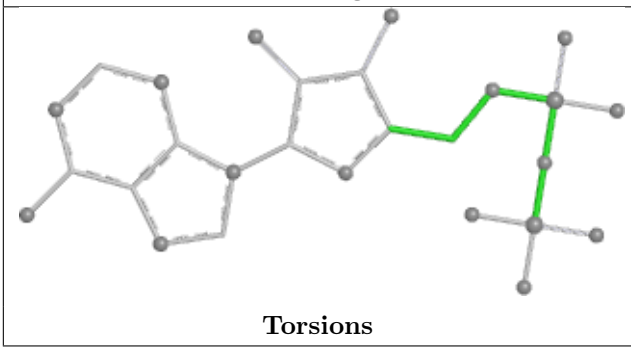
Ligand ADP A 4701



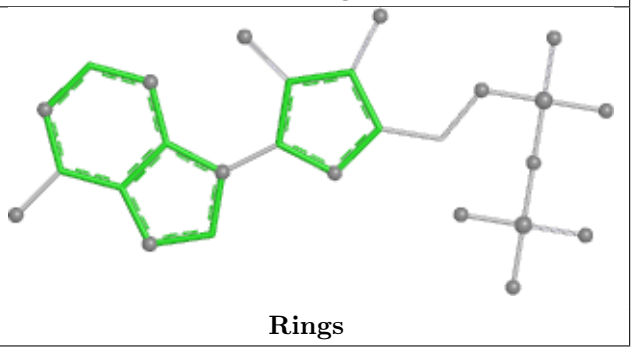
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

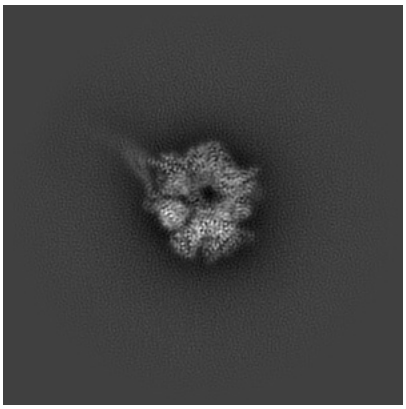
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-46859. These allow visual inspection of the internal detail of the map and identification of artifacts.

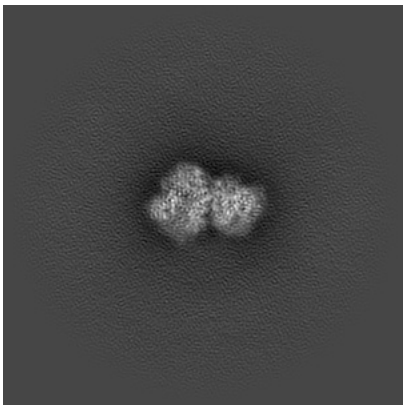
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

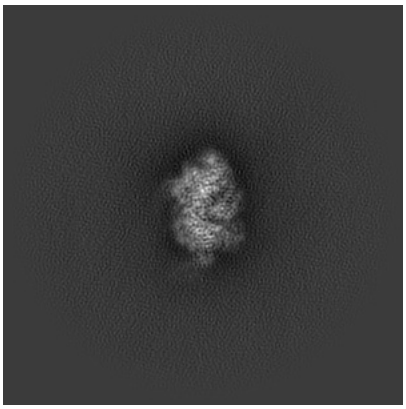
6.1.1 Primary map



X

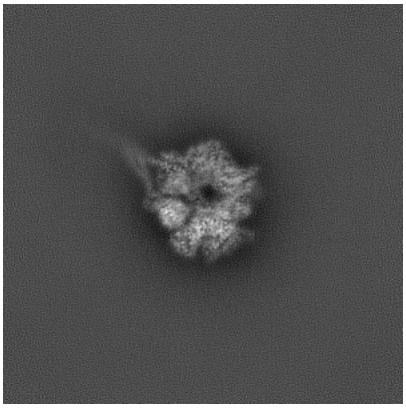


Y

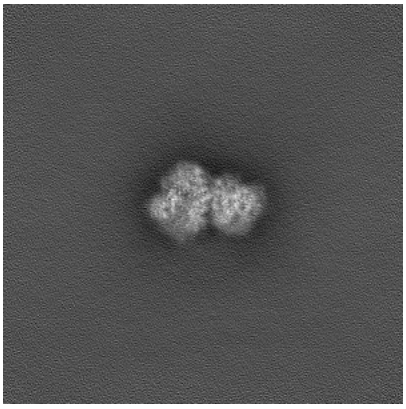


Z

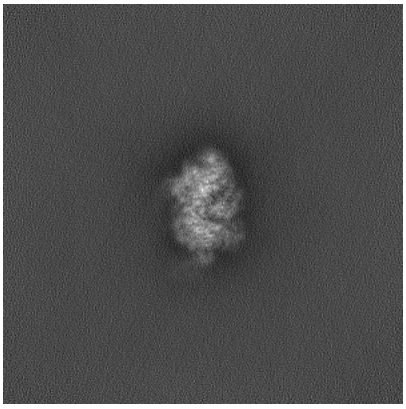
6.1.2 Raw map



X



Y

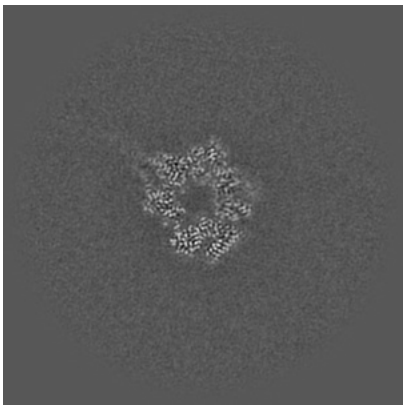


Z

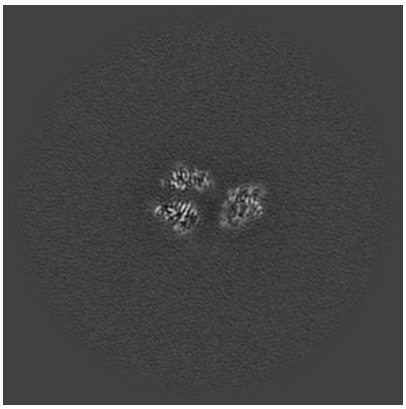
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

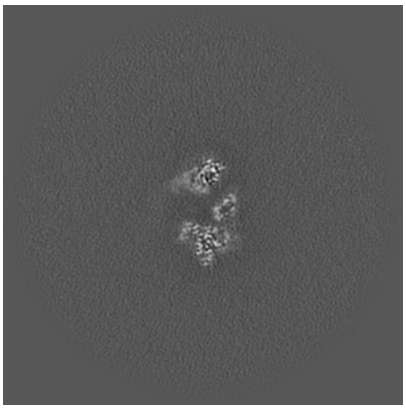
6.2.1 Primary map



X Index: 192

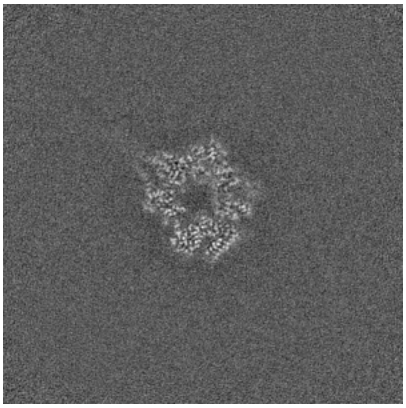


Y Index: 192

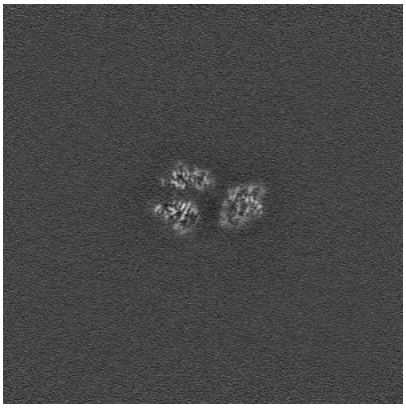


Z Index: 192

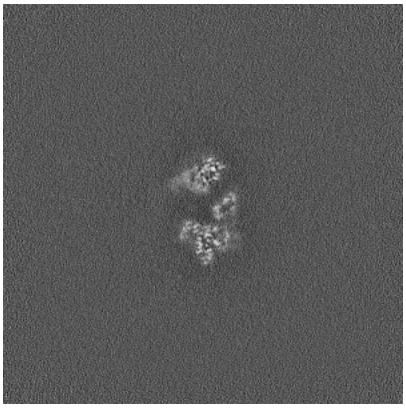
6.2.2 Raw map



X Index: 192



Y Index: 192

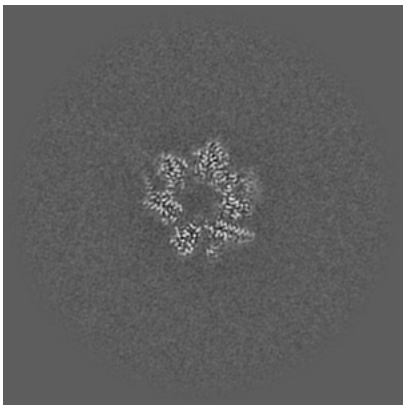


Z Index: 192

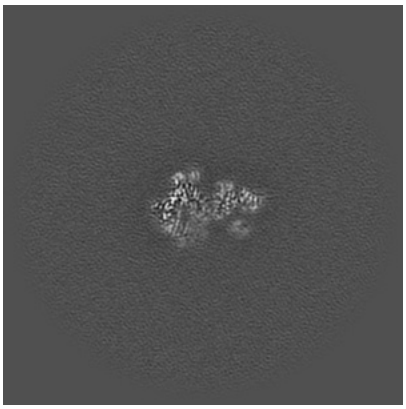
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

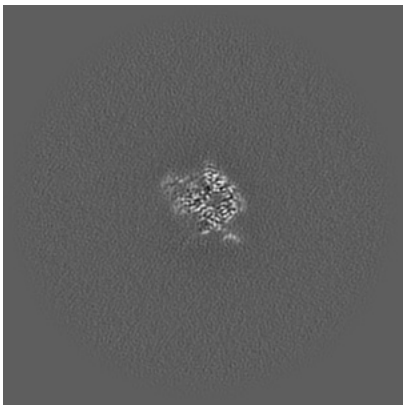
6.3.1 Primary map



X Index: 196

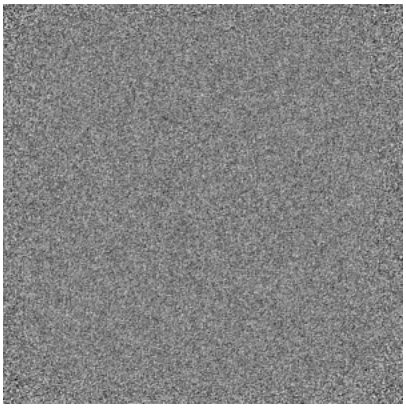


Y Index: 209

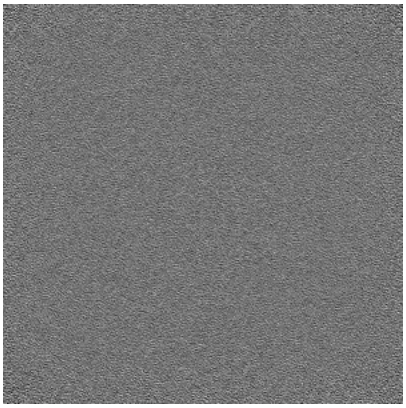


Z Index: 169

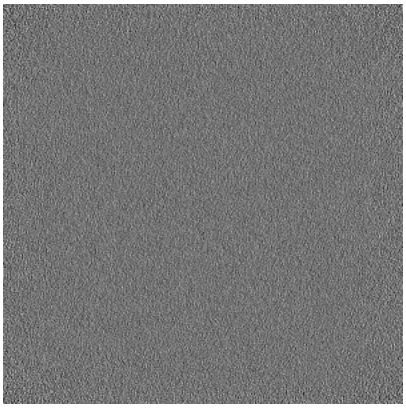
6.3.2 Raw map



X Index: 0



Y Index: 0

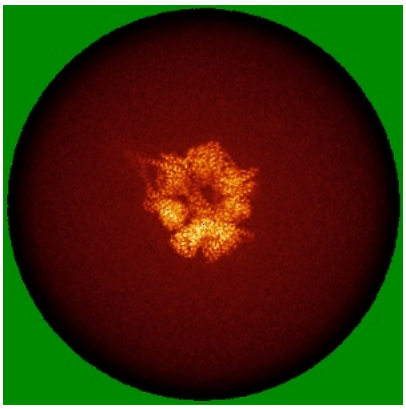


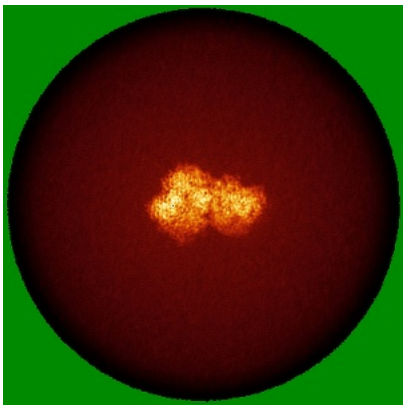
Z Index: 0

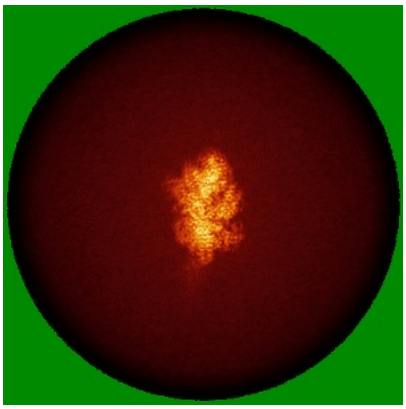
The images above show the largest variance slices of the map in three orthogonal directions.

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

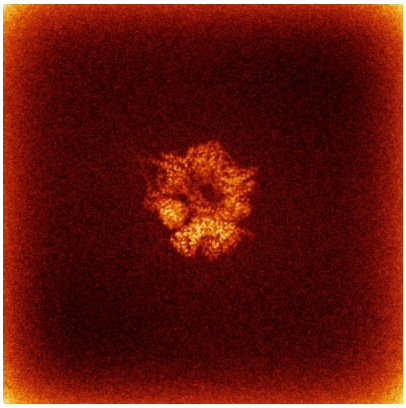
6.4.1 Primary map

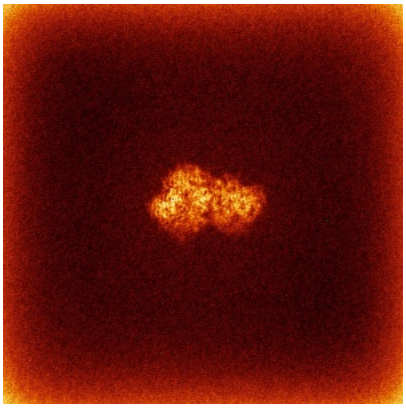

X

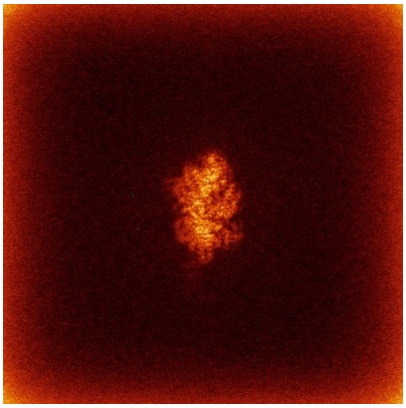

Y


Z

6.4.2 Raw map


X

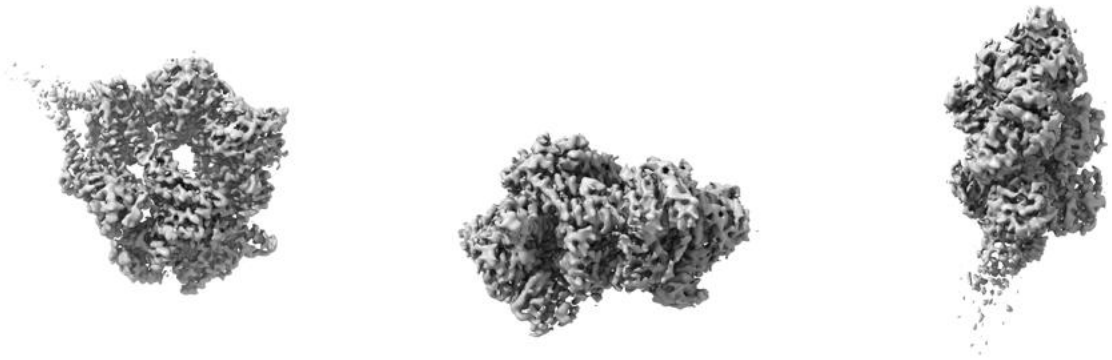

Y


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.

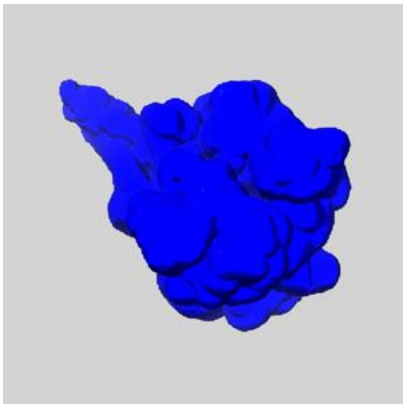
6.6 Mask visualisation (i)

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

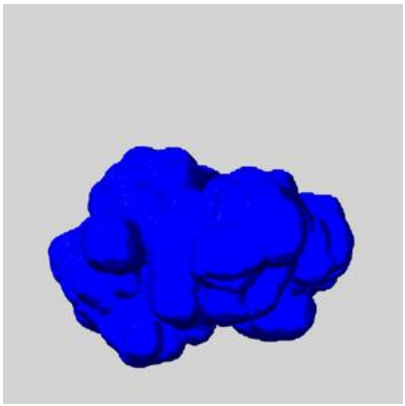
A mask typically either:

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

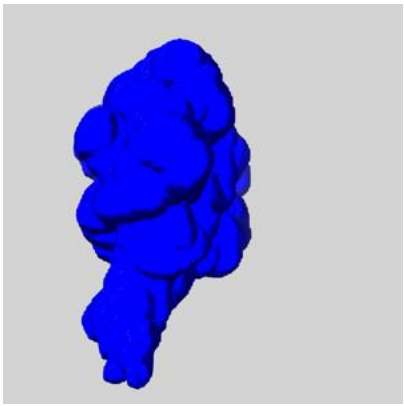
6.6.1 emd_46859_msk_1.map (i)



X



Y

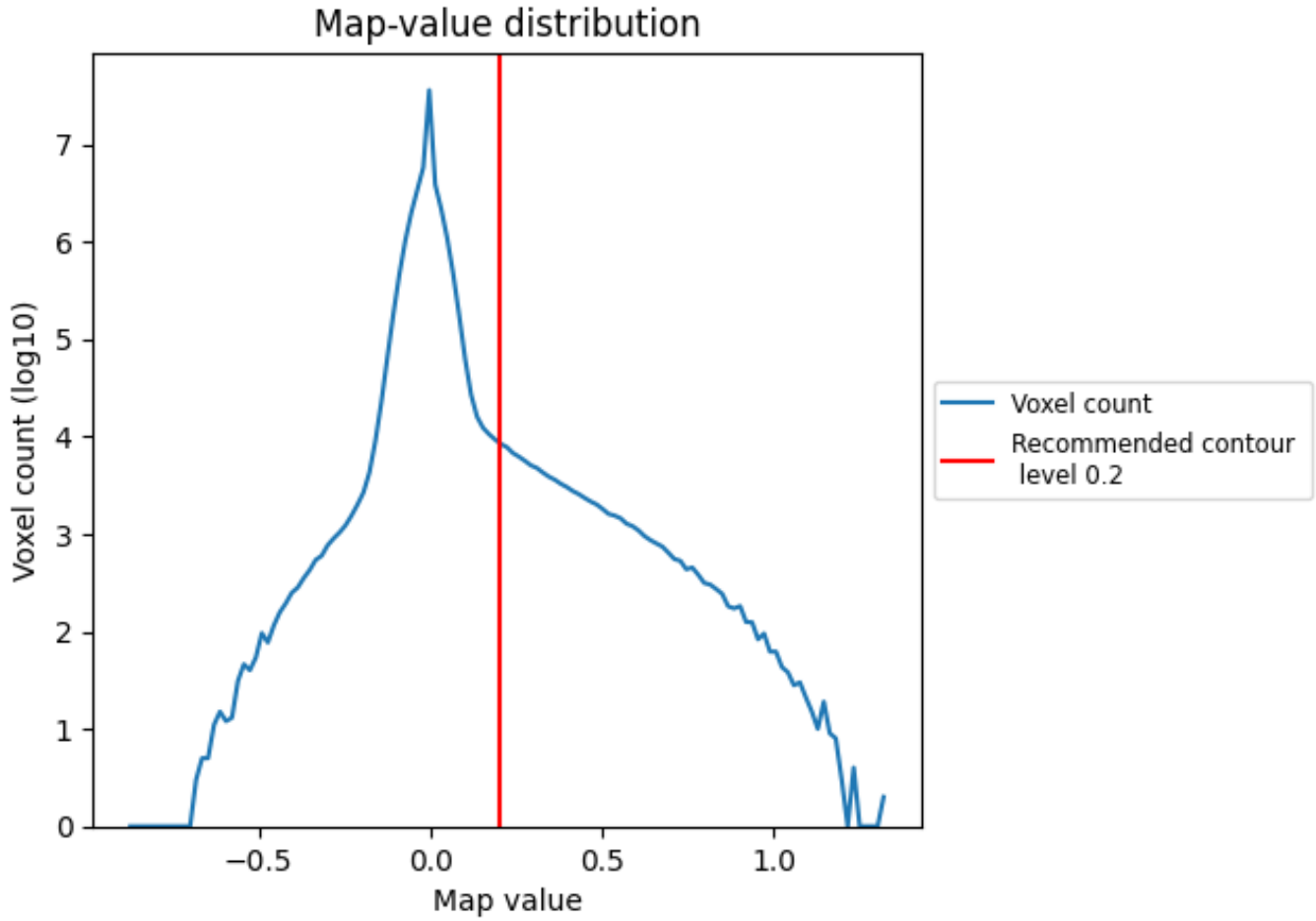


Z

7 Map analysis

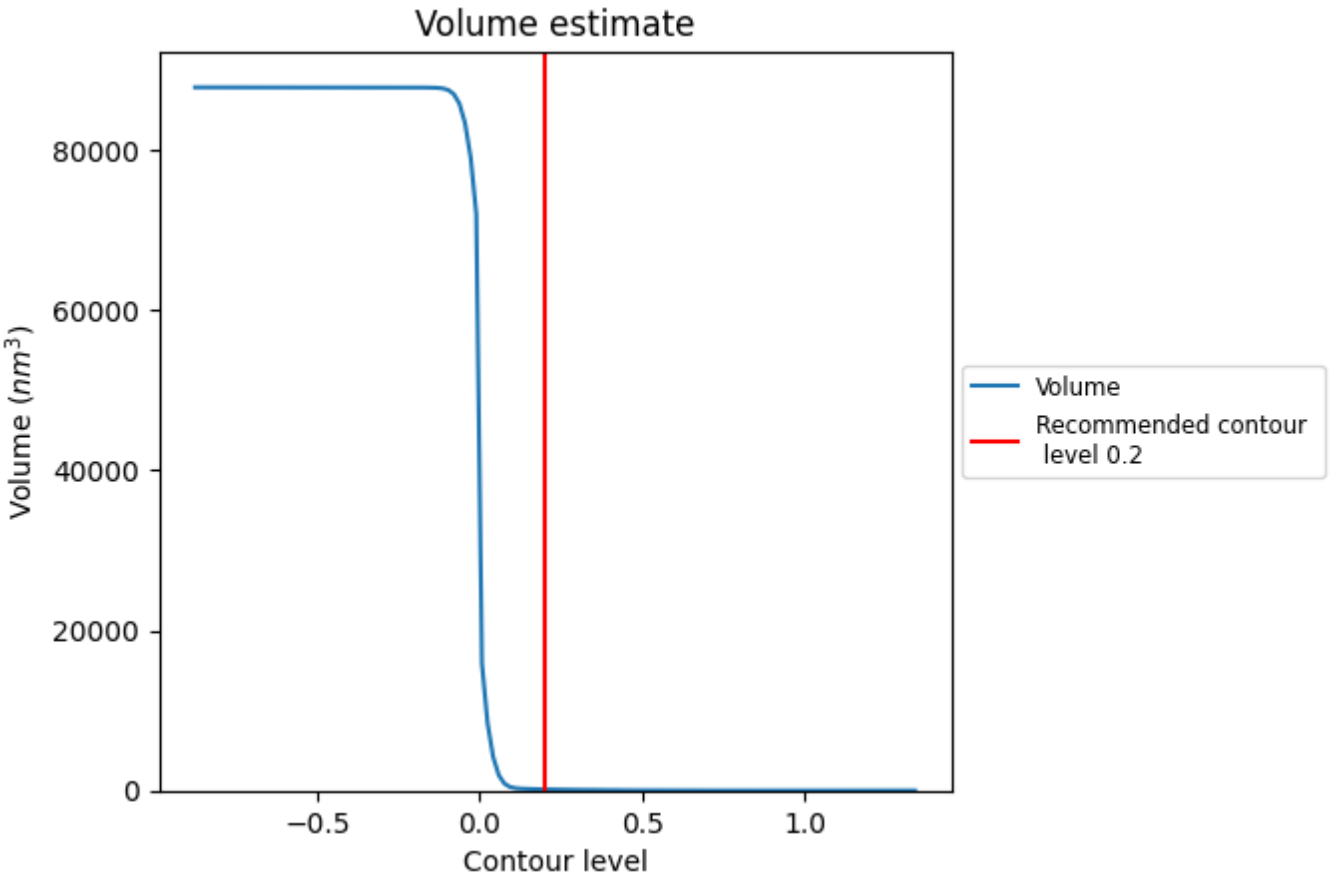
This section contains the results of statistical analysis of the map.

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.

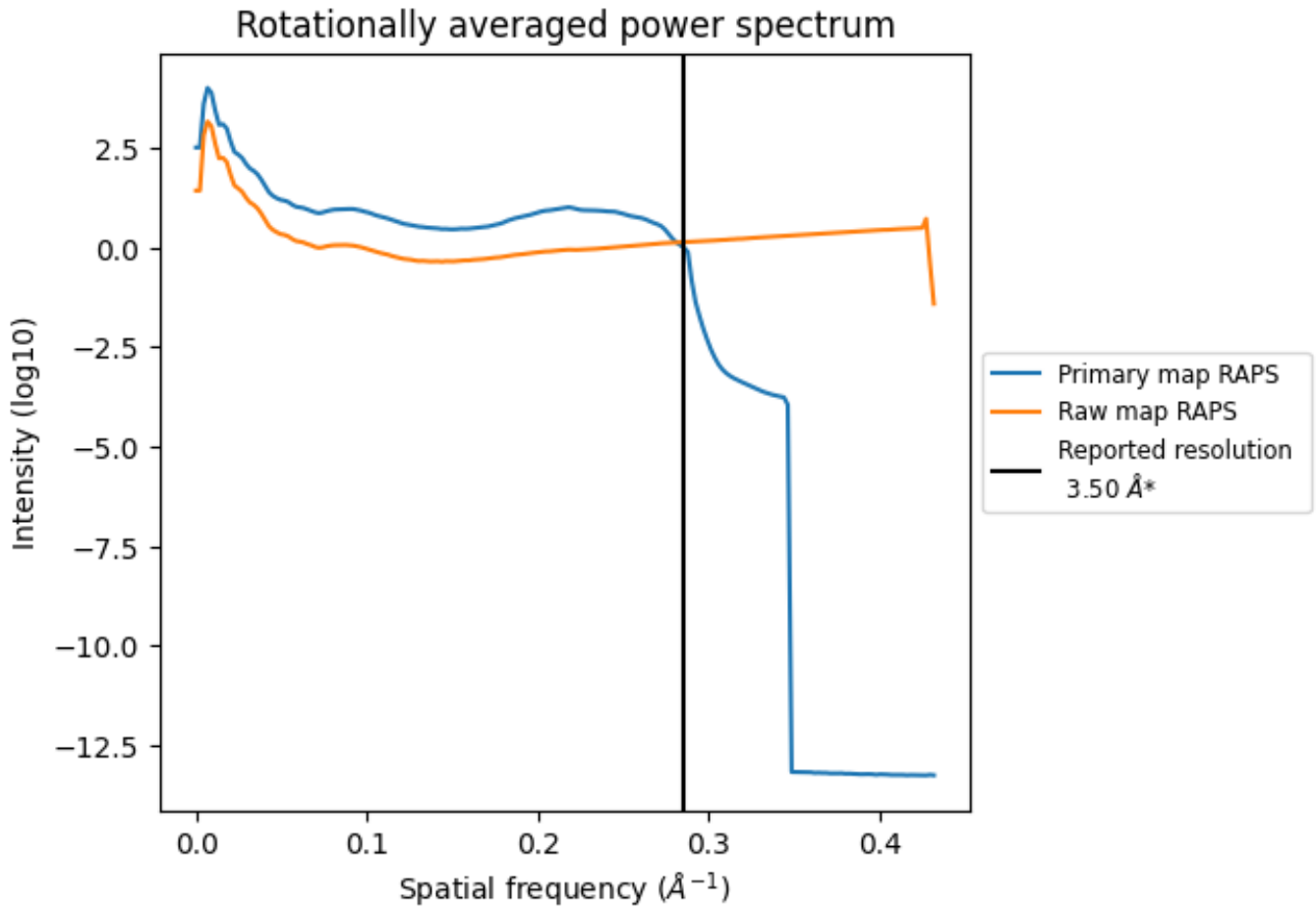
7.2 Volume estimate



The volume at the recommended contour level is 149 nm^3; this corresponds to an approximate mass of 135 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)

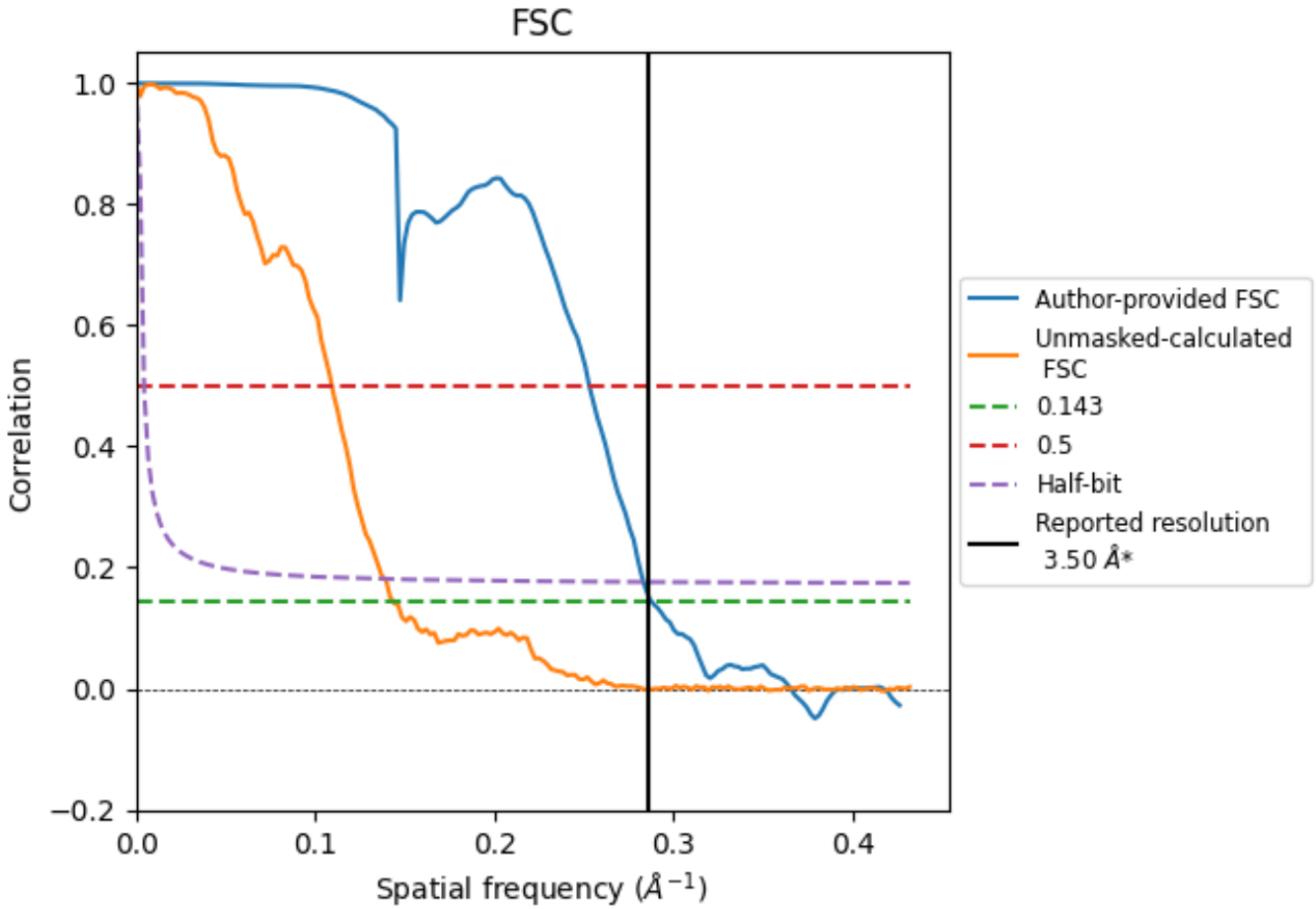


*Reported resolution corresponds to spatial frequency of 0.286 $Å^{-1}$

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 0.286 Å^{-1}

8.2 Resolution estimates (i)

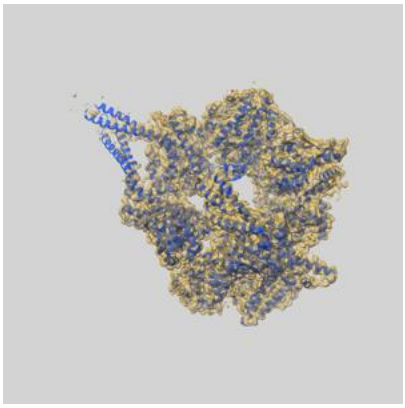
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.47	3.95	3.53
Unmasked-calculated*	6.96	9.15	7.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.96 differs from the reported value 3.5 by more than 10 %

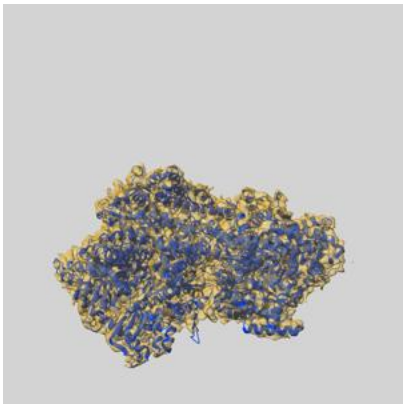
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-46859 and PDB model 9DH8. Per-residue inclusion information can be found in section 3 on page 5.

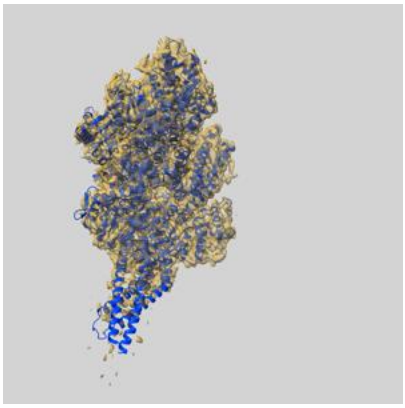
9.1 Map-model overlay



X



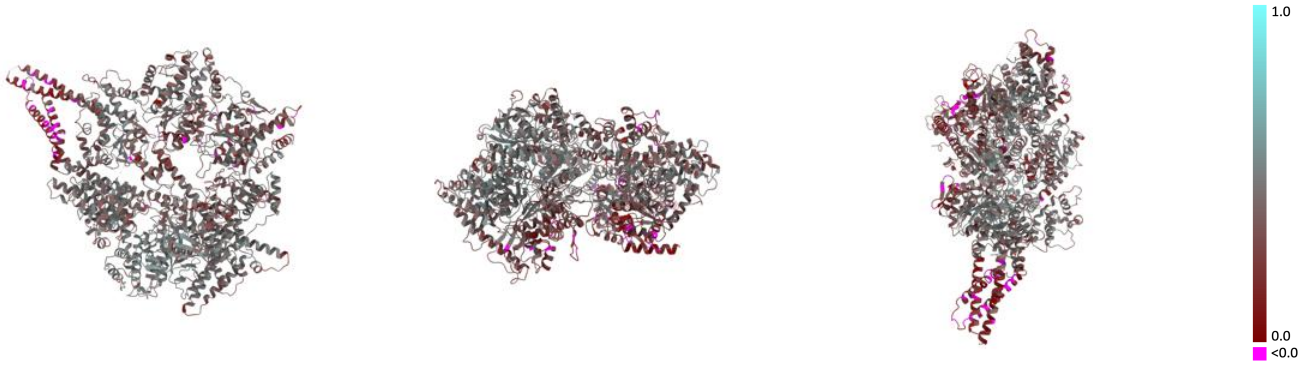
Y



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.

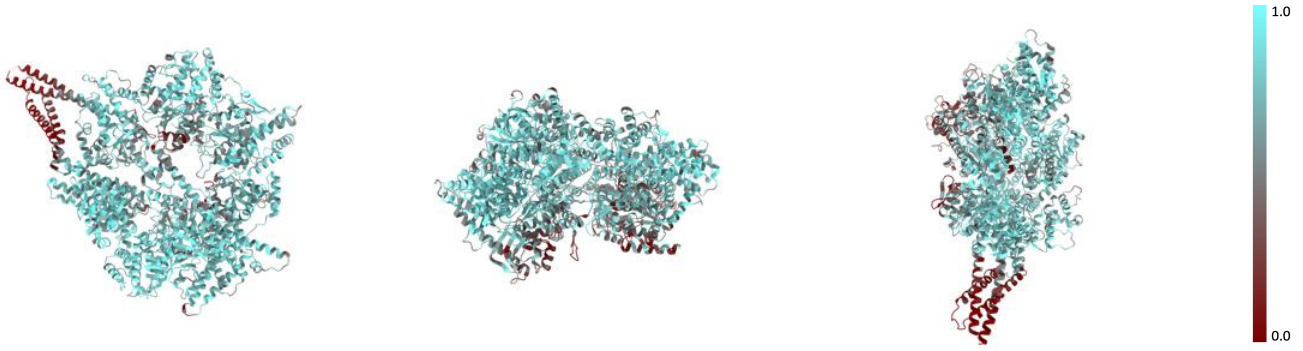
9.2 Q-score mapped to coordinate model (i)



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.

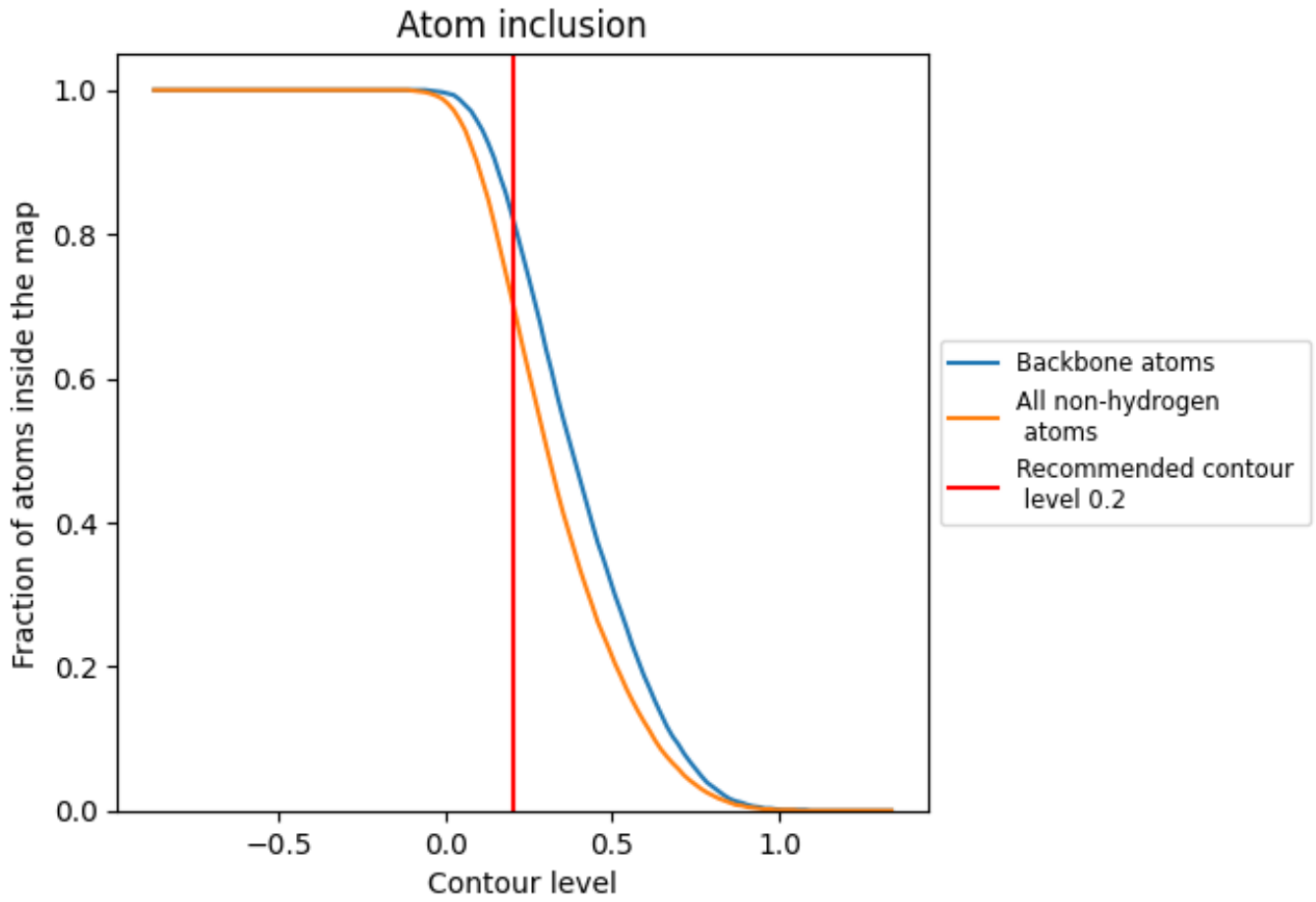
9.3 Atom inclusion mapped to coordinate model (i)



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, 82% of all backbone atoms, 71% 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	0.7090	0.3840
A	0.7090	0.3840