Full wwPDB EM Validation Report ⓘ

Apr 24, 2025 – 12:37 PM EDT

PDB ID	:	9BMO / pdb_00009bmo
EMDB ID	:	EMD-44705
Title	:	State-6 of motor domain from full-length human dynein-1 in 5mM AMPPNP
Authors	:	Chai, P.; Zhang, K.
Deposited on	:	2024-05-02
Resolution	:	3.60 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:

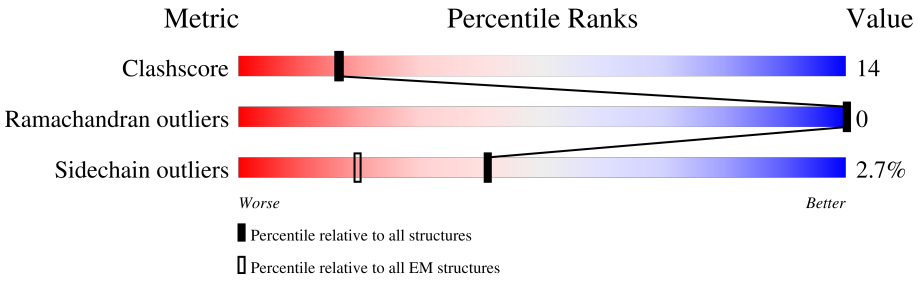
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

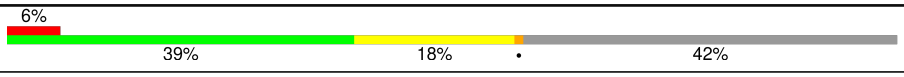
The reported resolution of this entry is 3.60 Å.

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	

2 Entry composition

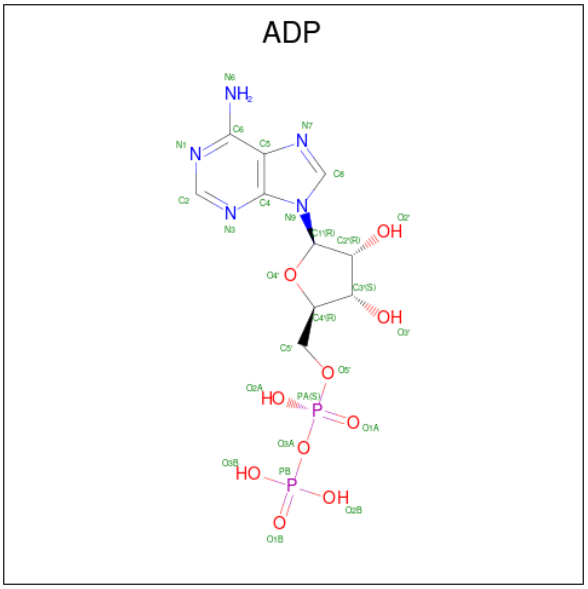
There are 3 unique types of molecules in this entry. The entry contains 21867 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

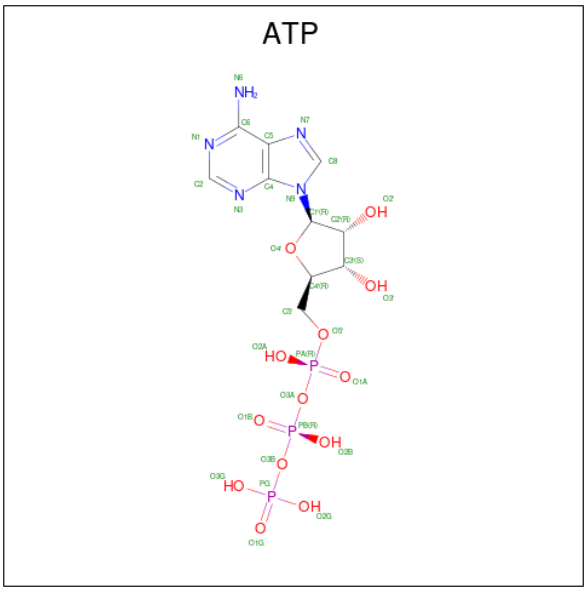
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2711	21755	13852	3757	4035	111	0	0

- 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).



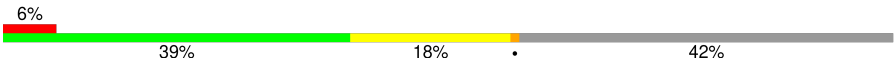
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

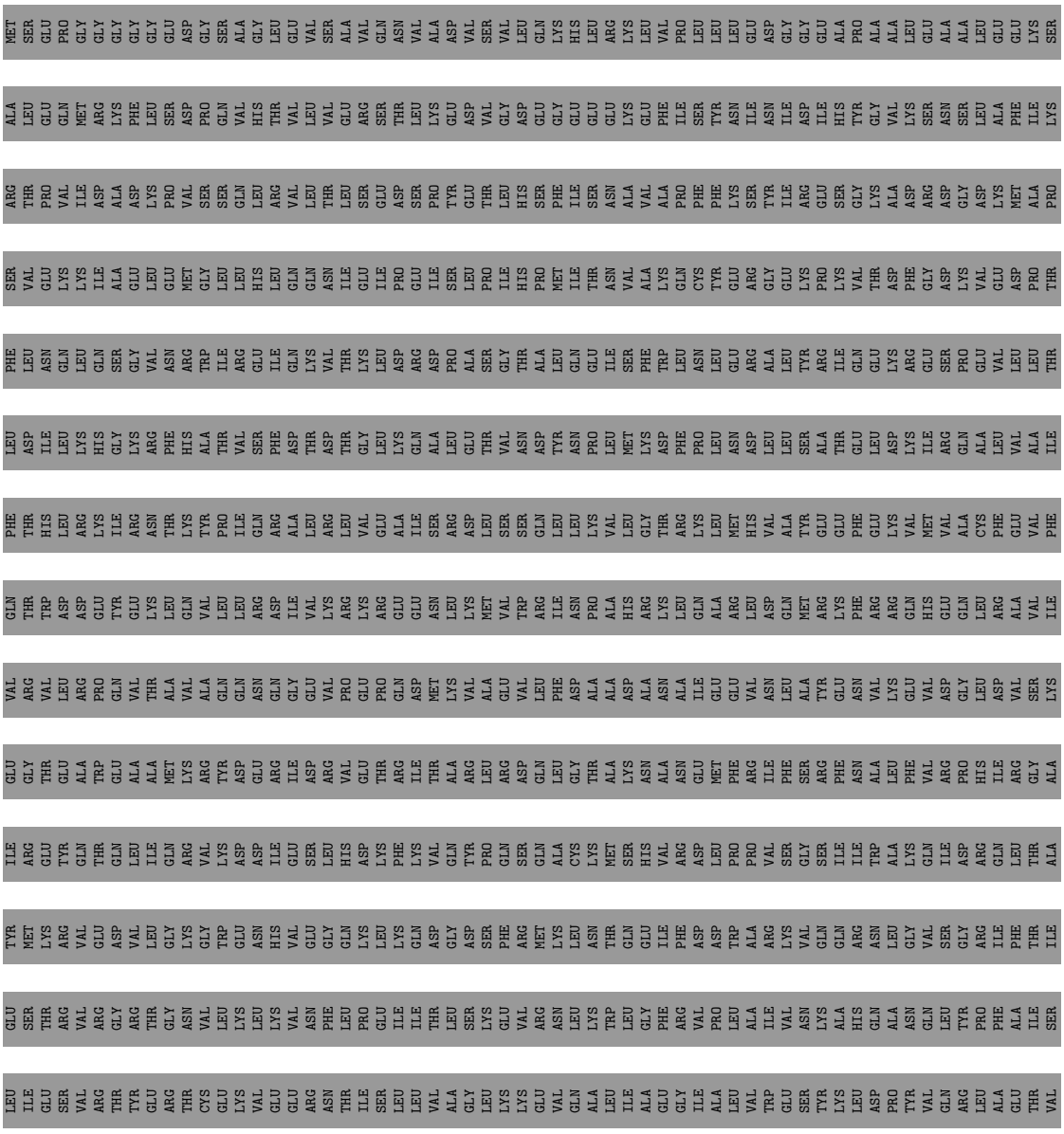
3 Residue-property plots (i)

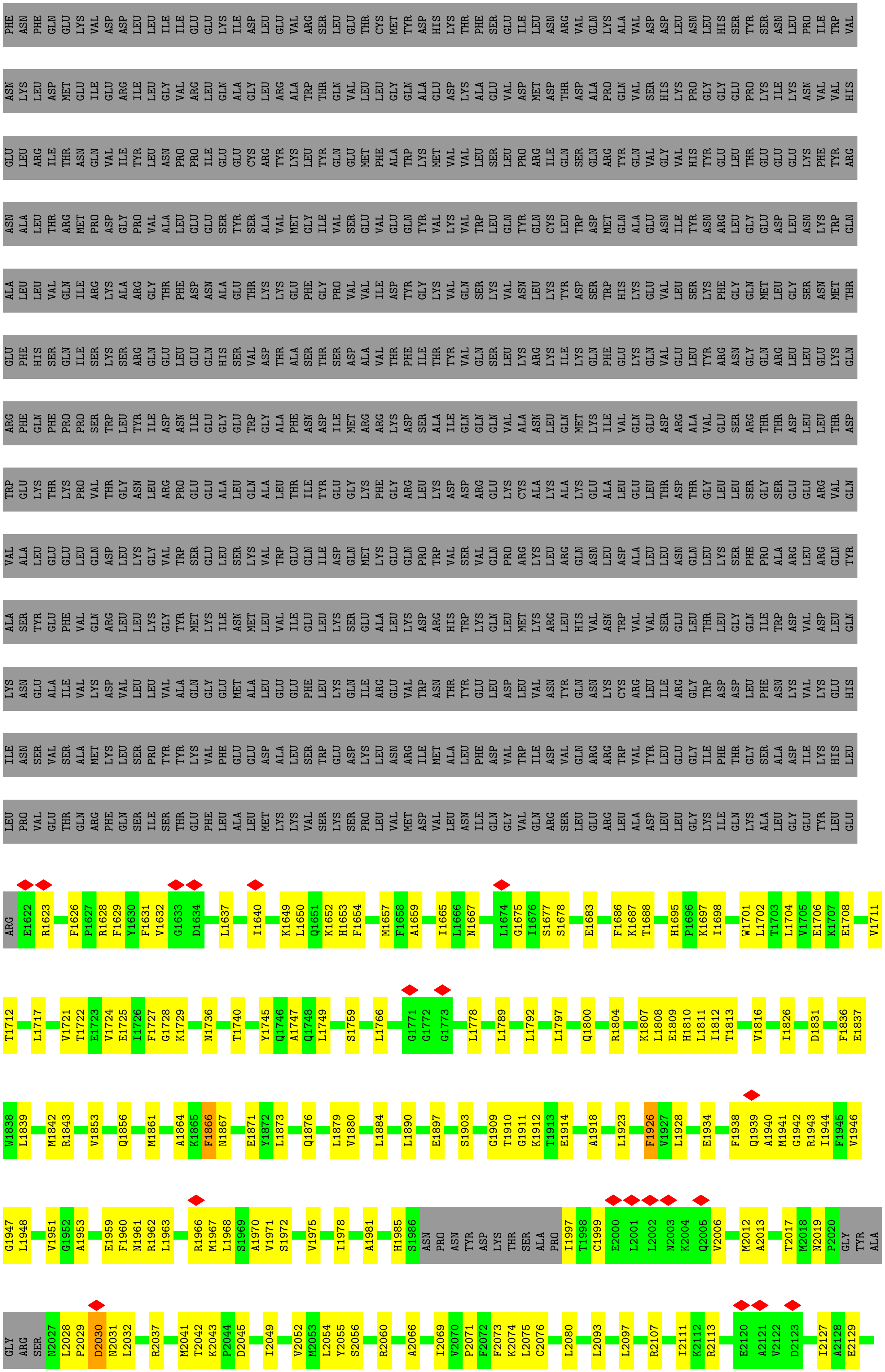
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

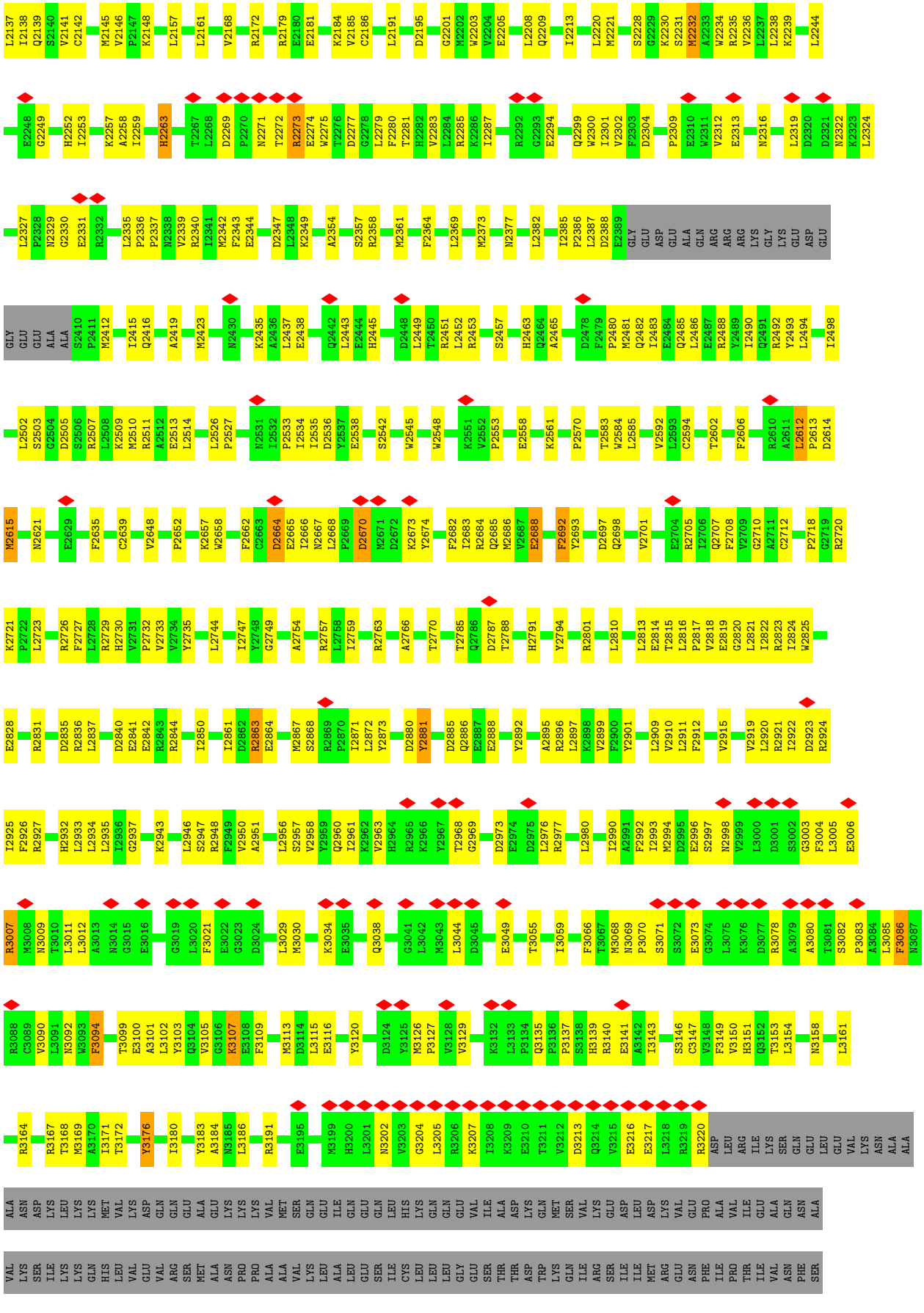
- Molecule 1: Cytoplasmic dynein 1 heavy chain 1

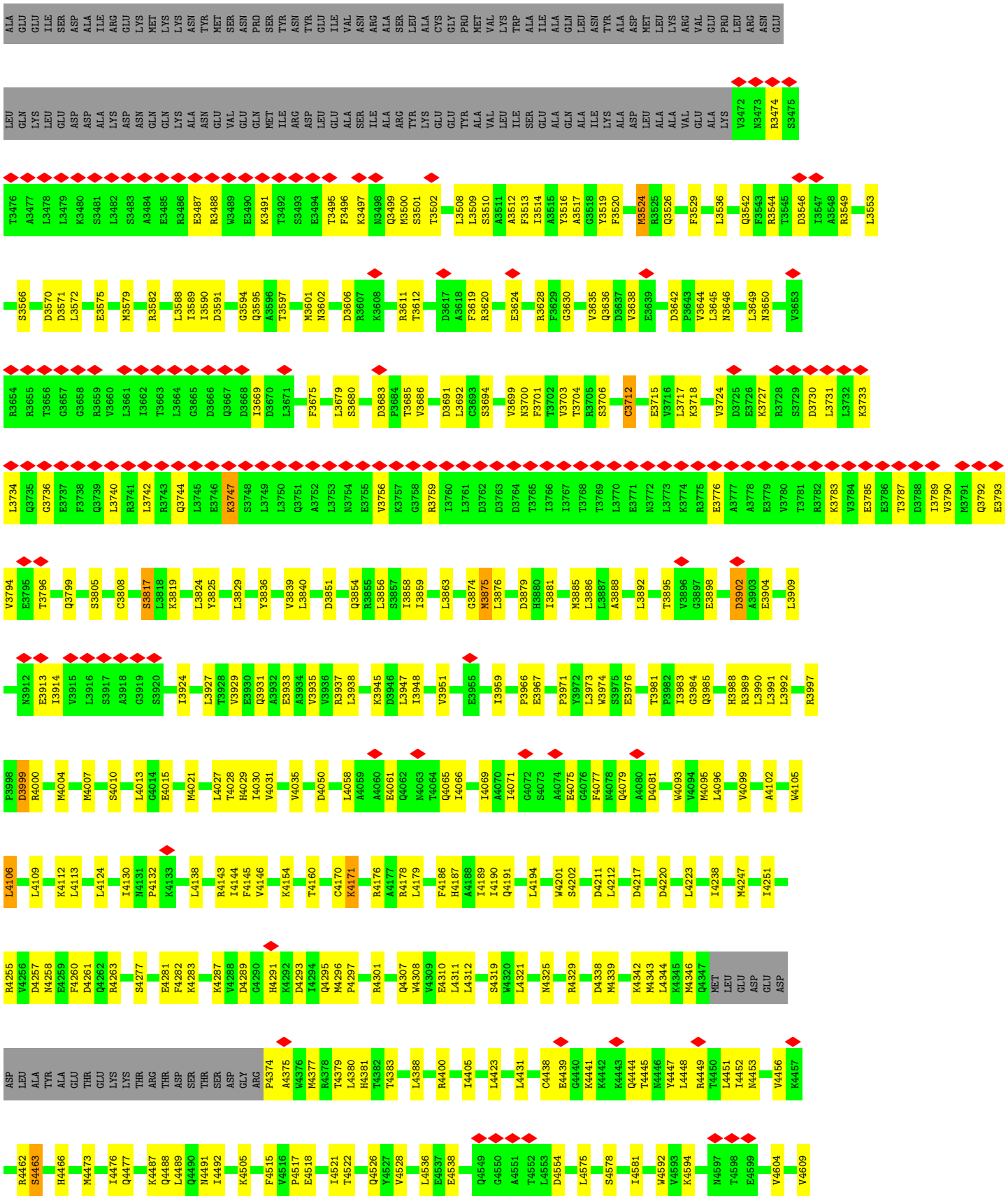
Chain A:








L2137 I2138 Q2139 S2140 V2141 C2142 M2145 V2146 P2147 K2148 L2157 L2161 V2168 R2172 R2179 E2180 E2181 K2184 V2185 C2186 L2191 D2195 G2201 M2202 W2203 V2204 E2205 L2208 Q2209 I2213 L2220 M2221 S2228 G2229 K2230 S2231 M2232 A2233 W2234 R2235 V2236 L2237 L2238 K2239 L2244
E2248 G2249 H2252 I2253 K2257 A2258 I2259 H2263 T2267 L2268 D2269 P2270 N2271 T2272 R2273 E2274 W2275 T2276 D2277 G2278 L2279 F2280 T2281 H2282 V2283 L2284 R2285 K2286 I2287 R2292 G2293 E2294 Q2299 W2300 I2301 V2302 F2303 D2304 P2309 E2310 W2311 V2312 E2313 N2316 L2319 D2320 D2321 N2322 K2323 L2324
L2327 P2328 N2329 G2330 E2331 R2332 L2335 P2336 P2337 N2338 V2339 R2340 I2341 M2342 F2343 E2344 D2347 L2348 K2349 A2354 S2357 R2358 M2361 F2364 L2369 M2373 N2377 L2382 I2385 P2386 L2387 D2388 E2389 GLY GLU ASP GLU ALA GLN ARG ARG LYS GLY LYS GLU ASP GLU
GLY GLU GLU ALA ALA S2410 P2411 M2412 I2415 Q2416 A2419 M2423 N2430 K2435 A2436 L2437 E2438 Q2442 L2443 E2444 H2445 D2448 L2449 T2450 R2451 L2452 R2453 S2457 H2463 Q2464 A2465 D2478 F2479 P2480 M2481 Q2482 I2483 E2484 Q2485 L2486 E2487 R2488 Y2489 T2490 Q2491 R2492 Y2493 L2494 I2498
L2502 S2503 G2504 D2505 S2506 R2507 L2508 K2509 M2510 R2511 A2512 E2513 L2514 L2526 P2527 N2531 I2532 P2533 I2534 I2535 D2536 Y2537 E2538 S2542 W2545 W2548 K2551 V2552 P2553 E2558 K2561 P2570 T2583 W2584 L2585 V2592 L2593 C2594 T2602 F2606 R2610 A2611 L2612 P2613 D2614
M2615 N2621 E2629 F2635 C2639 V2648 P2652 K2657 W2658 F2662 C2663 D2664 E2665 I2666 N2667 L2668 P2669 D2670 M2671 D2672 K2673 Y2674 F2682 I2683 R2684 Q2685 M2686 V2687 E2688 F2692 Y2693 D2697 Q2698 V2701 E2704 R2705 I2706 Q2707 F2708 V2709 G2710 A2711 C2712 P2718 G2719 R2720
K2721 P2722 L2723 R2726 F2727 L2728 R2729 H2730 V2731 P2732 V2733 V2734 Y2735 L2744 I2747 Y2748 G2749 A2754 R2757 L2758 I2759 R2763 A2766 T2770 T2785 Q2786 D2787 T2788 H2791 Y2794 R2801 L2810 L2813 E2814 T2815 L2816 P2817 V2818 E2819 G2820 L2821 I2822 R2823 I2824 W2825
E2828 R2831 D2835 R2836 L2837 D2840 E2841 E2842 R2843 R2844 I2850 I2861 D2862 R2863 E2864 M2867 S2868 R2869 P2870 I2871 L2872 Y2873 D2880 Y2881 D2885 Q2886 E2887 E2888 Y2892 A2895 R2896 L2897 K2898 V2899 F2900 Y2901 L2909 V2910 L2911 F2912 V2915 V2919 L2920 R2921 I2922 D2923 R2924
I2925 F2926 R2927 H2932 L2933 L2934 L2935 I2936 G2937 K2943 L2946 S2947 R2948 F2949 V2950 A2951 L2956 S2957 V2958 Y2959 Q2960 I2961 K2962 V2963 H2964 R2965 K2966 Y2967 T2968 G2969 D2973 E2974 D2975 L2976 R2977 L2980 I2990 A2991 F2992 I2993 M2994 D2995 E2996 S2997 N2998 V2999 L3000 D3001 S3002 G3003 F3004 L3005 E3006
R3007 M3008 N3009 T3010 L3011 L3012 A3013 N3014 G3015 E3016 G3019 L3020 F3021 E3022 G3023 D3024 L3029 M3030 K3034 E3035 Q3038 G3041 L3042 M3043 L3044 D3045 E3049 T3055 I3059 F3066 T3067 M3068 N3069 P3070 S3071 S3072 E3073 G3074 L3075 K3076 D3077 R3078 A3079 A3080 T3081 S3082 P3083 A3084 L3085 F3086 N3087
R3088 C3089 V3090 L3091 N3092 W3093 F3094 T3099 E3100 A3101 L3102 Y3103 Q3104 V3105 G3106 K3107 E3108 F3109 M3113 D3114 L3115 E3116 Y3120 D3124 Y3125 M3126 P3127 V3128 V3129 K3132 L3133 P3134 Q3135 P3136 P3137 S3138 H3139 R3140 E3141 A3142 I3143 S3146 C3147 V3148 F3149 V3150 H3151 Q3152 T3153 L3154 N3158 L3161
R3164 R3167 T3168 M3169 A3170 I3171 T3172 Y3176 I3180 Y3183 A3184 N3185 L3186 R3191 E3195 M3199 H3200 L3201 N3202 V3203 G3204 L3205 R3206 K3207 T3208 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 GLU 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 GLU ASN PRO PRO ALA ALA VAL LYS LEU ALA LEU GLU 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 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 M3500 S3501 T3502 L3508 L3509 S3510 A3511 A3512 F3513 I3514 A3515 Y3516 A3517 G3518 Y3519 F3520 M3524 R3525 Q3526 F3529 L3536 Q3542 F3543 R3544 T3545 D3546 I3547 A3548 R3549 L3553
S3566 D3570 D3571 L3572 E3575 M3579 R3582 L3588 I3589 I3590 D3591 G3594 Q3595 A3596 T3597 M3601 N3602 D3606 R3607 K3608 R3611 T3612 D3617 A3618 F3619 R3620 E3624 R3628 F3629 G3630 V3635 Q3636 D3637 V3638 E3639 D3642 P3643 V3644 L3645 N3646 L3649 N3650 V3653
R3654 R3655 T3656 G3657 G3658 R3659 V3660 L3661 I3662 T3663 L3664 G3665 D3666 Q3667 D3668 I3669 D3670 L3671 F3675 L3679 S3680 D3683 P3684 T3685 V3686 D3691 L3692 C3693 S3694 V3699 N3700 F3701 T3702 V3703 T3704 R3705 S3706 C3712 E3715 V3716 L3717 K3718 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 Q3799 S3805 C3808 S3817 L3818 K3819 L3824 Y3825 L3829 Y3836 V3839 L3840 D3851 Q3854 R3855 L3856 S3857 I3858 I3859 L3863 G3874 M3875 L3876 D3879 H3880 I3881 M3885 L3886 L3887 A3888 L3892 T3895 V3896 G3897 E3898 D3902 A3903 E3904 L3909
N3912 E3913 I3914 V3915 L3916 S3917 A3918 G3919 S3920 I3924 L3927 T3928 V3929 E3930 Q3931 A3932 E3933 A3934 V3935 V3936 R3937 L3938 K3945 D3946 L3947 I3948 V3951 E3955 I3959 P3966 E3967 P3971 Y3972 L3973 W3974 S3975 E3976 T3981 P3982 I3983 G3984 Q3985 H3988 R3989 L3990 L3991 L3992 R3997
P3998 D3999 R4000 M4004 M4007 S4010 L4013 G4014 E4015 M4021 L4027 T4028 H4029 I4030 V4031 V4035 D4050 L4058 A4059 A4060 E4061 Q4062 N4063 T4064 Q4065 I4066 I4069 A4070 I4071 G4072 S4073 A4074 E4075 G4076 F4077 N4078 Q4079 A4080 D4081 W4093 Y4094 M4095 L4096 V4099 A4102 W4105
L4106 L4109 K4112 L4113 L4124 I4130 N4131 P4132 K4133 L4138 R4143 I4144 F4145 V4146 K4164 T4160 C4170 K4171 R4176 A4177 R4178 L4179 F4186 H4187 A4188 I4189 I4190 Q4191 L4194 W4201 S4202 D4211 L4212 D4217 D4220 L4223 I4238 M4247 I4251
R4255 V4256 D4257 N4258 E4259 F4260 D4261 Q4262 R4263 S4277 E4281 F4282 K4283 K4287 V4288 D4289 G4290 H4291 K4292 D4293 I4294 Q4295 M4296 P4297 R4301 Q4307 W4308 V4309 E4310 L4311 L4312 S4319 W4320 L4321 N4325 R4329 D4338 M4339 K4342 M4343 L4344 K4345 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 M4377 R4378 T4379 L4380 H4381 T4382 T4383 L4388 R4400 I4405 L4423 L4431 C4438 E4439 G4440 K4441 K4442 K4443 Q4444 T4445 N4446 Y4447 L4448 R4449 T4450 L4451 I4452 N4453 V4456 K4457
R4462 S4463 H4466 M4473 I4476 Q4477 K4487 Q4488 L4489 Q4490 N4491 I4492 K4505 F4515 V4516 P4517 E4518 I4521 T4522 Q4526 Y4527 V4528 L4536 E4537 E4538 Q4549 G4550 A4551 T4552 L4553 D4554 L4575 S4578 I4581 W4592 V4593 K4594 N4597 T4598 E4599 V4604 V4609


Y4610
L4611
N4612
F4613
T4614
D4617
L4618
I4619
E4625
T4628
K4629
F4635
R4638
V4642
T4645
GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82309	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	1.305	Depositor
Minimum map value	-0.690	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.038	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: 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	0.26	0/22220	0.52	3/30121 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4132	PRO	CA-N-CD	-12.08	94.59	111.50
1	A	4132	PRO	N-CD-CG	-6.11	94.04	103.20
1	A	2494	LEU	CA-CB-CG	5.62	128.24	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	606	0
2	A	81	0	36	8	0
3	A	31	0	12	7	0
All	All	21867	0	21837	606	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 14.

All (606) 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:2452:LEU:HD23	1:A:2729:ARG:HD2	1.57	0.84
1:A:3570:ASP:OD1	1:A:3571:ASP:N	2.20	0.74
1:A:4388:LEU:HD21	1:A:4431:LEU:HB3	1.70	0.74
1:A:2935:LEU:HD13	1:A:2943:LYS:HB3	1.70	0.73
1:A:3736:GLY:O	1:A:3740:LEU:N	2.22	0.73
1:A:3107:LYS:HZ2	1:A:3141:GLU:HG2	1.53	0.73
1:A:4448:LEU:O	1:A:4452:ILE:HG12	1.90	0.71
1:A:2228:SER:OG	1:A:2230:LYS:NZ	2.24	0.70
1:A:4176:ARG:NH1	1:A:4220:ASP:OD1	2.25	0.70
1:A:4473:MET:HG3	1:A:4477:GLN:HG3	1.73	0.70
1:A:2749:GLY:HA2	1:A:2770:THR:HG21	1.72	0.70
1:A:2412:MET:HA	1:A:2415:ILE:HG22	1.73	0.70
1:A:2028:LEU:HD12	1:A:2029:PRO:HD2	1.74	0.69
1:A:2880:ASP:OD2	1:A:2881:TYR:N	2.26	0.69
1:A:2996:GLU:OE2	1:A:3069:ASN:ND2	2.25	0.69
1:A:4081:ASP:OD1	1:A:4112:LYS:NZ	2.24	0.69
1:A:1938:PHE:CE2	1:A:1967:MET:HG2	2.26	0.69
1:A:3967:GLU:OE1	1:A:3967:GLU:N	2.21	0.69
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.73	0.69
1:A:3102:LEU:HB3	1:A:3176:TYR:HE2	1.58	0.69
1:A:3886:LEU:HD11	1:A:4346:MET:HG3	1.75	0.69
1:A:3006:GLU:HA	1:A:3009:ASN:ND2	2.07	0.68
1:A:4010:SER:HB2	1:A:4015:GLU:HA	1.75	0.67
1:A:2054:LEU:HG	1:A:2097:LEU:HD22	1.77	0.67
1:A:3990:LEU:HD13	1:A:4004:MET:HG3	1.76	0.67
1:A:2585:LEU:HD12	1:A:2707:GLN:HE21	1.60	0.67
1:A:2688:GLU:HB2	1:A:2730:HIS:HE1	1.59	0.67
1:A:3914:ILE:HB	1:A:3937:ARG:HD3	1.77	0.67
1:A:1711:VAL:HG22	1:A:1853:VAL:HG21	1.78	0.66
1:A:1836:PHE:HA	1:A:1839:LEU:HB2	1.77	0.66
1:A:4113:LEU:HD11	1:A:4124:LEU:HD13	1.78	0.66
1:A:1631:PHE:HA	1:A:1944:ILE:HG22	1.77	0.66
1:A:1951:VAL:HG13	1:A:1953:ALA:H	1.61	0.66
1:A:1880:VAL:HG21	1:A:2049:ILE:HG12	1.78	0.66
1:A:4400:ARG:HH21	1:A:4405:ILE:HG12	1.61	0.65
1:A:2231:SER:OG	1:A:2344:GLU:OE2	2.13	0.65
1:A:2961:ILE:O	1:A:2998:ASN:ND2	2.26	0.65
1:A:3566:SER:OG	1:A:3602:ASN:ND2	2.29	0.65
1:A:3158:ASN:ND2	1:A:3169:MET:O	2.25	0.65
1:A:2747:ILE:HD11	2:A:4703:ADP:C6	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3135:GLN:O	1:A:3137:PRO:HD3	1.97	0.65
1:A:2269:ASP:HB2	1:A:2274:GLU:HG2	1.79	0.65
1:A:4463:SER:O	1:A:4466:HIS:NE2	2.27	0.65
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.79	0.64
1:A:3513:PHE:HZ	1:A:3575:GLU:HB3	1.61	0.64
1:A:3981:THR:HG23	1:A:3984:GLY:H	1.62	0.64
1:A:1778:LEU:HB3	1:A:1826:ILE:HD11	1.79	0.64
1:A:3727:LYS:O	1:A:3731:LEU:N	2.31	0.64
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.78	0.64
1:A:1812:ILE:HD13	1:A:2056:SER:HA	1.79	0.64
1:A:2688:GLU:HB2	1:A:2730:HIS:CE1	2.32	0.64
1:A:2271:ASN:ND2	1:A:2272:THR:HG23	2.13	0.64
1:A:2527:PRO:HD2	1:A:2534:ILE:HD12	1.78	0.64
1:A:3885:MET:HB3	1:A:4343:MET:HE1	1.80	0.64
1:A:2963:VAL:HG11	1:A:2998:ASN:HA	1.80	0.64
1:A:4099:VAL:HG12	1:A:4106:LEU:HD21	1.80	0.63
1:A:3620:ARG:NH2	1:A:3642:ASP:OD2	2.31	0.63
1:A:2269:ASP:OD2	1:A:2272:THR:OG1	2.16	0.63
1:A:2910:VAL:HG21	1:A:3105:VAL:HG22	1.81	0.63
1:A:1912:LYS:HE2	1:A:2017:THR:HB	1.81	0.63
1:A:3519:TYR:O	1:A:3700:ASN:ND2	2.32	0.63
1:A:3099:THR:HA	1:A:3102:LEU:HD12	1.81	0.62
1:A:2794:TYR:HE1	1:A:2836:ARG:HD2	1.65	0.62
1:A:3734:LEU:HD13	1:A:3783:LYS:HB3	1.82	0.62
1:A:2934:LEU:HD13	1:A:3066:PHE:CZ	2.35	0.62
1:A:2919:VAL:HG23	1:A:2950:VAL:HG22	1.81	0.62
1:A:2684:ARG:NH1	1:A:2688:GLU:OE2	2.30	0.61
1:A:2957:SER:HB2	1:A:2990:ILE:HD12	1.81	0.61
1:A:3851:ASP:HB3	1:A:3854:GLN:HB3	1.80	0.61
1:A:2452:LEU:HB3	1:A:2729:ARG:HG3	1.83	0.61
1:A:1628:ARG:NH1	1:A:1871:GLU:OE2	2.34	0.61
1:A:4187:HIS:ND1	1:A:4212:LEU:HD22	2.15	0.61
1:A:2925:ILE:HG21	1:A:2933:LEU:HB2	1.81	0.61
1:A:2485:GLN:OE1	1:A:2488:ARG:NH1	2.34	0.61
1:A:3172:THR:HG21	1:A:3694:SER:HB2	1.81	0.60
1:A:3500:MET:HA	1:A:3500:MET:HE2	1.81	0.60
1:A:3147:CYS:O	1:A:3150:VAL:HG12	2.01	0.60
1:A:4260:PHE:CE2	1:A:4618:LEU:HD11	2.37	0.60
1:A:2925:ILE:HG13	1:A:3090:VAL:HG21	1.83	0.60
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.84	0.60
1:A:1842:MET:HA	1:A:1861:MET:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2863:ARG:O	1:A:2863:ARG:NH1	2.34	0.59
1:A:4445:THR:O	1:A:4449:ARG:N	2.30	0.59
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	1.84	0.59
1:A:2232:MET:HA	1:A:2235:ARG:HB2	1.84	0.59
1:A:2666:ILE:HG22	1:A:2712:CYS:HB3	1.85	0.59
1:A:1912:LYS:N	2:A:4701:ADP:O3B	2.35	0.59
1:A:2277:ASP:O	1:A:2698:GLN:NE2	2.34	0.59
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.68	0.59
1:A:3909:LEU:HD21	1:A:4343:MET:HG2	1.82	0.59
1:A:1686:PHE:HA	1:A:1712:THR:HG21	1.85	0.59
1:A:3588:LEU:HD12	1:A:3679:LEU:HB2	1.84	0.59
1:A:2813:LEU:HD21	1:A:2816:LEU:HB2	1.84	0.59
1:A:3825:TYR:CZ	1:A:3875:MET:HG3	2.38	0.59
1:A:1975:VAL:HA	1:A:1978:ILE:HG22	1.85	0.59
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.83	0.58
1:A:1934:GLU:OE2	1:A:1934:GLU:N	2.33	0.58
1:A:2309:PRO:HA	1:A:2312:VAL:HG12	1.85	0.58
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	1.85	0.58
1:A:2179:ARG:NH2	1:A:2195:ASP:OD2	2.36	0.58
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.37	0.58
1:A:4260:PHE:HE2	1:A:4618:LEU:HD11	1.69	0.58
1:A:1808:LEU:O	1:A:1812:ILE:HG22	2.04	0.58
1:A:2179:ARG:HD3	1:A:2208:LEU:HD11	1.86	0.58
1:A:3021:PHE:CD2	1:A:3029:LEU:HD22	2.39	0.58
1:A:2419:ALA:O	1:A:2423:MET:HG2	2.04	0.57
1:A:1649:LYS:HD2	1:A:2273:ARG:HH12	1.70	0.57
1:A:1880:VAL:HG22	2:A:4701:ADP:N1	2.19	0.57
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.85	0.57
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.86	0.57
1:A:3974:TRP:HZ2	1:A:3985:GLN:HG2	1.69	0.57
1:A:4186:PHE:O	1:A:4189:ILE:HG22	2.04	0.57
1:A:1623:ARG:NH2	1:A:1637:LEU:HD22	2.19	0.57
1:A:3902:ASP:OD1	1:A:3902:ASP:N	2.34	0.57
1:A:2819:GLU:OE1	1:A:2819:GLU:N	2.25	0.57
1:A:4295:GLN:OE1	1:A:4296:MET:N	2.38	0.57
1:A:1766:LEU:HD22	1:A:1778:LEU:HD11	1.86	0.57
1:A:2526:LEU:HD13	1:A:2534:ILE:HG13	1.85	0.57
1:A:2585:LEU:HD12	1:A:2707:GLN:NE2	2.20	0.56
1:A:4178:ARG:HD2	1:A:4296:MET:HE3	1.86	0.56
1:A:2316:ASN:OD1	1:A:2358:ARG:NH1	2.38	0.56
1:A:1879:LEU:HD23	1:A:1918:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1853:VAL:HA	1:A:1856:GLN:HG3	1.86	0.56
1:A:3624:GLU:O	1:A:3628:ARG:HG2	2.05	0.56
1:A:1967:MET:O	1:A:1971:VAL:HG22	2.06	0.56
1:A:2670:ASP:HA	1:A:2721:LYS:HE3	1.88	0.56
1:A:2901:TYR:OH	1:A:2909:LEU:N	2.38	0.56
1:A:3881:ILE:HG13	1:A:4339:MET:HE1	1.88	0.56
1:A:4487:LYS:O	1:A:4491:ASN:ND2	2.38	0.56
1:A:1909:GLY:N	2:A:4701:ADP:O2B	2.36	0.55
1:A:3217:GLU:HB3	1:A:3220:ARG:HH21	1.71	0.55
1:A:1873:LEU:O	1:A:1876:GLN:NE2	2.38	0.55
1:A:4066:ILE:HD12	1:A:4095:MET:HG3	1.86	0.55
1:A:4518:GLU:OE2	1:A:4518:GLU:N	2.30	0.55
1:A:1961:ASN:HD21	1:A:2019:ASN:HB3	1.72	0.55
1:A:2148:LYS:HG2	1:A:2361:MET:HB3	1.87	0.55
1:A:3909:LEU:HB3	1:A:4344:LEU:HD13	1.88	0.55
1:A:1632:VAL:O	1:A:1943:ARG:NH1	2.26	0.55
1:A:2354:ALA:HB1	1:A:2358:ARG:HH22	1.71	0.55
1:A:2785:THR:HG22	1:A:2787:ASP:H	1.71	0.55
1:A:2279:LEU:O	1:A:2283:VAL:HG23	2.06	0.55
1:A:2505:ASP:OD1	1:A:2505:ASP:N	2.40	0.55
1:A:3030:MET:N	1:A:3030:MET:SD	2.79	0.55
1:A:1687:LYS:HG2	1:A:1712:THR:HG22	1.88	0.55
1:A:2337:PRO:O	1:A:2340:ARG:NH1	2.39	0.55
1:A:2801:ARG:NH1	1:A:2801:ARG:O	2.40	0.55
1:A:3999:ASP:OD1	1:A:4329:ARG:NH1	2.40	0.55
1:A:4066:ILE:HG22	1:A:4093:TRP:HB2	1.89	0.55
1:A:4423:LEU:HD13	1:A:4466:HIS:CE1	2.41	0.55
1:A:4476:ILE:HD12	1:A:4476:ILE:H	1.72	0.55
1:A:1653:HIS:HB3	1:A:1657:MET:HE3	1.89	0.54
1:A:3874:GLY:HA3	1:A:4144:ILE:HG13	1.88	0.54
1:A:4452:ILE:O	1:A:4456:VAL:HG22	2.07	0.54
1:A:4628:THR:O	1:A:4629:LYS:HG2	2.08	0.54
1:A:4027:LEU:O	1:A:4031:VAL:HG12	2.07	0.54
1:A:2452:LEU:HD21	3:A:4702:ATP:H4'	1.88	0.54
1:A:2766:ALA:O	1:A:2770:THR:HG23	2.06	0.54
1:A:3071:SER:HB3	1:A:3078:ARG:HH22	1.72	0.54
1:A:2141:VAL:O	1:A:2145:MET:HB2	2.08	0.54
1:A:2602:THR:HG23	1:A:2662:PHE:HE1	1.72	0.54
1:A:2612:LEU:HB3	1:A:2615:MET:SD	2.47	0.54
1:A:3929:VAL:O	1:A:3933:GLU:HG2	2.08	0.54
1:A:1903:SER:O	1:A:1903:SER:OG	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3526:GLN:OE1	1:A:3549:ARG:NH2	2.33	0.54
1:A:1963:LEU:HD23	1:A:1967:MET:HB3	1.90	0.54
1:A:2980:LEU:HD21	1:A:3011:LEU:HD11	1.88	0.54
1:A:3572:LEU:HD21	1:A:3701:PHE:HA	1.89	0.54
1:A:4374:PRO:HG2	1:A:4377:MET:HB2	1.89	0.54
1:A:1866:PHE:HD2	1:A:1923:LEU:HD11	1.73	0.54
1:A:2485:GLN:NE2	1:A:2542:SER:O	2.38	0.54
1:A:4170:CYS:SG	1:A:4301:ARG:NH2	2.80	0.54
1:A:1879:LEU:HD12	2:A:4701:ADP:C6	2.43	0.53
1:A:2819:GLU:HA	1:A:2861:ILE:HD11	1.90	0.53
1:A:3646:ASN:OD1	1:A:3650:ASN:ND2	2.41	0.53
1:A:1654:PHE:CE1	1:A:1702:LEU:HD11	2.44	0.53
1:A:1912:LYS:HG2	1:A:2041:MET:HG3	1.90	0.53
1:A:1940:ALA:O	1:A:1944:ILE:HG23	2.08	0.53
1:A:2071:PRO:O	1:A:2075:LEU:HG	2.08	0.53
1:A:4488:GLN:O	1:A:4492:ILE:HG12	2.08	0.53
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	1.90	0.53
1:A:2498:ILE:HG23	1:A:2502:LEU:HD22	1.91	0.53
1:A:2621:ASN:HA	1:A:2664:ASP:HB2	1.90	0.53
1:A:1812:ILE:HD11	1:A:2055:TYR:HD1	1.73	0.53
1:A:2277:ASP:OD1	1:A:2277:ASP:N	2.38	0.53
1:A:4211:ASP:OD1	1:A:4255:ARG:NH1	2.42	0.53
1:A:2505:ASP:HA	1:A:2735:TYR:HB2	1.89	0.53
1:A:1626:PHE:HE1	1:A:1706:GLU:HG3	1.73	0.53
1:A:2744:LEU:HA	1:A:2747:ILE:HG22	1.91	0.53
1:A:3005:LEU:HD21	1:A:3082:SER:HB3	1.91	0.53
1:A:3730:ASP:O	1:A:3734:LEU:HG	2.09	0.53
1:A:3924:ILE:HD12	1:A:3924:ILE:H	1.74	0.53
1:A:3999:ASP:OD1	1:A:4329:ARG:HG3	2.08	0.52
1:A:1938:PHE:CZ	1:A:1967:MET:HG2	2.43	0.52
1:A:1623:ARG:HA	1:A:1629:PHE:HE2	1.75	0.52
1:A:3888:ALA:HA	1:A:4013:LEU:HD11	1.91	0.52
1:A:2747:ILE:HD11	2:A:4703:ADP:C5	2.45	0.52
1:A:3817:SER:OG	1:A:4346:MET:SD	2.67	0.52
1:A:1816:VAL:HG11	1:A:2052:VAL:HG22	1.92	0.52
1:A:2673:LYS:NZ	1:A:2674:TYR:OH	2.43	0.52
1:A:2814:GLU:HG2	1:A:2815:THR:HG23	1.91	0.52
1:A:3879:ASP:OD1	1:A:4342:LYS:NZ	2.34	0.52
1:A:4247:MET:HA	1:A:4251:ILE:HG13	1.91	0.52
1:A:2445:HIS:CD2	1:A:2449:LEU:HD13	2.45	0.52
1:A:2720:ARG:HH21	1:A:3083:PRO:HB3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2821:LEU:O	1:A:2824:ILE:HG22	2.10	0.52
1:A:3785:GLU:O	1:A:3789:ILE:HG13	2.10	0.52
1:A:2012:MET:SD	1:A:2013:ALA:N	2.83	0.51
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.92	0.51
1:A:3742:LEU:HD12	1:A:3776:GLU:HB3	1.92	0.51
1:A:2635:PHE:O	1:A:2639:CYS:N	2.37	0.51
1:A:2129:GLU:N	1:A:2129:GLU:OE1	2.43	0.51
1:A:3947:LEU:O	1:A:3951:VAL:HG23	2.11	0.51
1:A:1812:ILE:HD11	1:A:2055:TYR:CD1	2.45	0.51
1:A:3006:GLU:HA	1:A:3009:ASN:HD21	1.72	0.51
1:A:3514:ILE:HD11	1:A:3553:LEU:HD13	1.91	0.51
1:A:3744:GLN:O	1:A:3747:LYS:HG3	2.11	0.51
1:A:2682:PHE:O	1:A:2686:MET:HG3	2.10	0.51
1:A:2667:ASN:HB3	1:A:2723:LEU:HD11	1.93	0.51
1:A:4439:GLU:HB3	1:A:4441:LYS:HE3	1.92	0.51
1:A:3109:PHE:HB3	1:A:3180:ILE:HG21	1.93	0.51
1:A:1946:VAL:HG23	1:A:2006:VAL:HG21	1.93	0.50
1:A:2872:LEU:HD12	1:A:2920:LEU:HD12	1.92	0.50
1:A:4521:ILE:HG13	1:A:4522:THR:N	2.26	0.50
1:A:2031:ASN:OD1	1:A:2031:ASN:N	2.45	0.50
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.92	0.50
1:A:3730:ASP:O	1:A:3734:LEU:N	2.42	0.50
1:A:2283:VAL:O	1:A:2287:ILE:HG13	2.12	0.50
1:A:3103:TYR:OH	1:A:3107:LYS:NZ	2.42	0.50
1:A:4260:PHE:HD1	1:A:4263:ARG:NH2	2.10	0.50
1:A:2483:ILE:HD12	1:A:2486:LEU:HD22	1.93	0.50
1:A:3099:THR:OG1	1:A:3100:GLU:OE2	2.29	0.50
1:A:3909:LEU:HD11	1:A:4343:MET:HG2	1.93	0.50
1:A:4065:GLN:OE1	1:A:4065:GLN:N	2.33	0.50
1:A:4575:LEU:HB3	1:A:4635:PHE:CZ	2.46	0.50
1:A:3989:ARG:HA	1:A:3992:LEU:HD12	1.94	0.50
1:A:4617:ASP:N	1:A:4617:ASP:OD2	2.43	0.50
1:A:1800:GLN:OE1	1:A:1804:ARG:NH1	2.45	0.49
1:A:2201:GLY:O	1:A:2205:GLU:HG2	2.12	0.49
1:A:2235:ARG:HH12	1:A:2253:ILE:HD11	1.76	0.49
1:A:2923:ASP:OD2	1:A:2927:ARG:NH2	2.42	0.49
1:A:2503:SER:HB3	1:A:2514:LEU:HD22	1.93	0.49
1:A:3115:LEU:HD23	1:A:3143:ILE:HD13	1.94	0.49
1:A:4202:SER:OG	1:A:4261:ASP:OD2	2.29	0.49
1:A:4380:LEU:HA	1:A:4383:THR:HG22	1.93	0.49
1:A:1810:HIS:NE2	1:A:1876:GLN:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2191:LEU:HD12	3:A:4702:ATP:C6	2.47	0.49
1:A:3612:THR:O	1:A:3635:VAL:HA	2.12	0.49
1:A:1914:GLU:OE2	2:A:4701:ADP:H3'	2.13	0.49
1:A:2369:LEU:HD23	1:A:2373:MET:SD	2.52	0.49
1:A:3790:VAL:HG22	1:A:3794:VAL:HG21	1.94	0.49
1:A:2042:THR:HG23	1:A:2043:LYS:HG2	1.94	0.49
1:A:3501:SER:HB2	1:A:3542:GLN:HB2	1.94	0.49
1:A:3566:SER:HG	1:A:3602:ASN:HD22	1.60	0.49
1:A:3924:ILE:HB	1:A:3927:LEU:HD12	1.94	0.49
1:A:1864:ALA:HB2	1:A:1897:GLU:HB2	1.93	0.49
1:A:3601:MET:HE2	1:A:3601:MET:N	2.27	0.49
1:A:3999:ASP:OD2	1:A:4000:ARG:N	2.46	0.49
1:A:2480:PRO:HG2	1:A:2482:GLN:HE22	1.77	0.49
1:A:2369:LEU:HD21	3:A:4702:ATP:C4	2.48	0.49
1:A:2509:LYS:O	1:A:2513:GLU:HG3	2.13	0.49
1:A:3636:GLN:HA	1:A:3680:SER:HB3	1.95	0.49
1:A:3840:LEU:HA	1:A:3859:ILE:HD11	1.94	0.49
1:A:4004:MET:O	1:A:4007:MET:HG3	2.13	0.49
1:A:4194:LEU:HD23	1:A:4201:TRP:CD1	2.47	0.49
1:A:4375:ALA:O	1:A:4379:THR:HG23	2.13	0.49
1:A:2943:LYS:HG2	1:A:3094:PHE:CD2	2.48	0.48
1:A:2349:LYS:HE2	1:A:2349:LYS:HB2	1.67	0.48
1:A:2825:TRP:HZ3	1:A:2850:ILE:HG23	1.78	0.48
1:A:2492:ARG:HG2	1:A:2545:TRP:NE1	2.27	0.48
1:A:2533:PRO:HB2	1:A:2535:ILE:HG22	1.94	0.48
1:A:3756:VAL:O	1:A:3759:ARG:HG2	2.14	0.48
1:A:1747:ALA:HB2	1:A:1807:LYS:HG2	1.94	0.48
1:A:2686:MET:HG2	1:A:2692:PHE:HB3	1.95	0.48
1:A:2946:LEU:O	1:A:2950:VAL:HG23	2.14	0.48
1:A:2837:LEU:HD13	1:A:2842:GLU:HB3	1.96	0.48
1:A:3590:ILE:O	1:A:3701:PHE:N	2.36	0.48
1:A:3645:LEU:HB3	1:A:3649:LEU:HD13	1.95	0.48
1:A:2960:GLN:HB3	1:A:2993:ILE:HB	1.94	0.48
1:A:2835:ASP:OD1	1:A:3092:ASN:HA	2.13	0.48
1:A:3044:LEU:HB3	1:A:3049:GLU:HG3	1.94	0.48
1:A:4154:LYS:HB2	1:A:4312:LEU:HD12	1.95	0.48
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.94	0.48
1:A:3071:SER:OG	1:A:3073:GLU:OE1	2.30	0.48
1:A:2932:HIS:HD2	1:A:3012:LEU:HB2	1.79	0.48
1:A:1938:PHE:O	1:A:1942:GLY:N	2.34	0.47
1:A:1966:ARG:HH21	1:A:1970:ALA:N	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2075:LEU:HD11	1:A:4536:LEU:HD12	1.96	0.47
1:A:2220:LEU:HB2	1:A:2342:MET:HG3	1.95	0.47
1:A:3204:GLY:O	1:A:3207:LYS:HG2	2.14	0.47
1:A:3624:GLU:HG3	1:A:3669:ILE:HD13	1.95	0.47
1:A:4257:ASP:OD1	1:A:4258:ASN:N	2.47	0.47
1:A:2465:ALA:HB2	1:A:2493:TYR:CE1	2.49	0.47
1:A:3730:ASP:HA	1:A:3733:LYS:HB2	1.95	0.47
1:A:1985:HIS:HA	1:A:1997:ILE:HG13	1.94	0.47
1:A:2073:PHE:CD2	1:A:2093:LEU:HD13	2.49	0.47
1:A:2280:PHE:HE1	1:A:2301:ILE:HG21	1.78	0.47
1:A:2864:GLU:OE1	1:A:2864:GLU:N	2.41	0.47
1:A:3611:ARG:HD3	1:A:3612:THR:N	2.30	0.47
1:A:1861:MET:HE1	1:A:1890:LEU:HA	1.96	0.47
1:A:2280:PHE:CE1	1:A:2301:ILE:HG21	2.49	0.47
1:A:2335:LEU:HD23	1:A:2336:PRO:O	2.14	0.47
1:A:2787:ASP:OD1	1:A:2788:THR:N	2.47	0.47
1:A:2840:ASP:OD1	1:A:2841:GLU:N	2.48	0.47
1:A:2263:HIS:ND1	1:A:2263:HIS:N	2.62	0.47
1:A:2754:ALA:HA	1:A:2757:ARG:HH12	1.80	0.47
1:A:2897:LEU:HD11	1:A:2911:LEU:HD11	1.96	0.47
1:A:3150:VAL:HA	1:A:3153:THR:HG22	1.96	0.47
1:A:3789:ILE:O	1:A:3793:GLU:HG3	2.15	0.47
1:A:4075:GLU:O	1:A:4079:GLN:HG2	2.15	0.47
1:A:1701:TRP:HA	1:A:1704:LEU:HD12	1.95	0.47
1:A:3575:GLU:O	1:A:3579:MET:HG3	2.14	0.47
1:A:2186:CYS:O	1:A:2191:LEU:N	2.47	0.47
1:A:2205:GLU:O	1:A:2209:GLN:HG3	2.13	0.47
1:A:2382:LEU:O	1:A:2416:GLN:NE2	2.45	0.47
1:A:4283:LYS:NZ	1:A:4293:ASP:OD2	2.40	0.47
1:A:1831:ASP:OD1	1:A:1831:ASP:N	2.45	0.47
1:A:3924:ILE:HG12	1:A:3948:ILE:HD11	1.97	0.47
1:A:2932:HIS:CD2	1:A:3012:LEU:HB2	2.50	0.47
1:A:3638:VAL:HG21	1:A:3679:LEU:HB3	1.97	0.47
1:A:1926:PHE:O	1:A:1953:ALA:HB1	2.15	0.46
1:A:2994:MET:HE3	1:A:2998:ASN:HB3	1.97	0.46
1:A:3591:ASP:OD1	1:A:3591:ASP:N	2.46	0.46
1:A:3683:ASP:OD2	1:A:3685:THR:OG1	2.27	0.46
1:A:1637:LEU:O	1:A:1640:ILE:HG22	2.15	0.46
1:A:3004:PHE:N	1:A:3004:PHE:CD1	2.83	0.46
1:A:3101:ALA:O	1:A:3105:VAL:HG23	2.16	0.46
1:A:3796:THR:HA	1:A:3799:GLN:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4154:LYS:NZ	1:A:4310:GLU:O	2.48	0.46
1:A:1687:LYS:H	1:A:1712:THR:CG2	2.28	0.46
1:A:2592:VAL:HG23	1:A:2733:VAL:HG22	1.95	0.46
1:A:3529:PHE:CE2	1:A:3549:ARG:HD3	2.50	0.46
1:A:2238:LEU:HD21	1:A:2249:GLY:HA3	1.96	0.46
1:A:3078:ARG:O	1:A:3082:SER:OG	2.23	0.46
1:A:2234:TRP:CZ2	1:A:2302:VAL:HG21	2.51	0.46
1:A:2668:LEU:O	1:A:2721:LYS:NZ	2.35	0.46
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.48	0.46
1:A:3724:VAL:HG23	1:A:3794:VAL:HG22	1.97	0.46
1:A:3824:LEU:HD22	1:A:4130:ILE:HG12	1.98	0.46
1:A:4307:GLN:O	1:A:4311:LEU:HG	2.16	0.46
1:A:2615:MET:SD	1:A:2615:MET:N	2.89	0.46
1:A:2937:GLY:O	1:A:3070:PRO:HD3	2.16	0.46
1:A:2968:THR:OG1	1:A:2969:GLY:N	2.48	0.46
1:A:3116:GLU:HG3	1:A:3140:ARG:HH21	1.81	0.46
1:A:3154:LEU:HD22	1:A:3516:TYR:HB3	1.98	0.46
1:A:4223:LEU:HD12	1:A:4223:LEU:HA	1.75	0.46
1:A:4526:GLN:HG2	1:A:4536:LEU:HD11	1.98	0.46
1:A:2864:GLU:O	1:A:2868:SER:OG	2.25	0.46
1:A:2973:ASP:OD1	1:A:3007:ARG:NH1	2.46	0.46
1:A:3783:LYS:HD3	1:A:3783:LYS:HA	1.70	0.46
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.40	0.46
1:A:2228:SER:HB2	1:A:2364:PHE:HB3	1.98	0.46
1:A:3792:GLN:O	1:A:3796:THR:OG1	2.33	0.46
1:A:3895:THR:HB	1:A:3898:GLU:OE1	2.15	0.46
1:A:4223:LEU:HD11	1:A:4238:ILE:HD12	1.98	0.46
1:A:4538:GLU:OE1	1:A:4594:LYS:NZ	2.40	0.46
1:A:1677:SER:HA	1:A:1683:GLU:HA	1.98	0.46
1:A:3495:THR:HG23	1:A:3496:PHE:HD1	1.81	0.46
1:A:3974:TRP:NE1	1:A:3976:GLU:OE2	2.49	0.46
1:A:4281:GLU:N	1:A:4281:GLU:OE1	2.49	0.46
1:A:1640:ILE:HD11	1:A:1650:LEU:HG	1.97	0.45
1:A:2435:LYS:O	1:A:2438:GLU:HG2	2.16	0.45
1:A:2698:GLN:N	1:A:2698:GLN:OE1	2.48	0.45
1:A:2977:ARG:HG2	1:A:3021:PHE:CE1	2.51	0.45
1:A:1626:PHE:CZ	1:A:1702:LEU:HD12	2.52	0.45
1:A:3143:ILE:HD11	1:A:3183:TYR:OH	2.15	0.45
1:A:3512:ALA:O	1:A:3516:TYR:HB2	2.15	0.45
1:A:1628:ARG:HG3	1:A:1657:MET:HB2	1.97	0.45
1:A:2209:GLN:O	1:A:2213:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2252:HIS:NE2	1:A:2299:GLN:OE1	2.46	0.45
1:A:1717:LEU:O	1:A:1721:VAL:HG12	2.16	0.45
1:A:1968:LEU:O	1:A:1972:SER:OG	2.20	0.45
1:A:2635:PHE:HZ	1:A:2708:PHE:HZ	1.62	0.45
1:A:2076:CYS:HA	1:A:2080:LEU:HD23	1.97	0.45
1:A:3712:CYS:SG	1:A:3805:SER:HA	2.56	0.45
1:A:2030:ASP:OD1	1:A:2030:ASP:N	2.50	0.45
1:A:2648:VAL:HG12	1:A:2701:VAL:HG13	1.99	0.45
1:A:3790:VAL:HA	1:A:3794:VAL:HB	1.98	0.45
1:A:3856:LEU:O	1:A:3859:ILE:HG22	2.16	0.45
1:A:2892:TYR:OH	1:A:2896:ARG:NH1	2.49	0.45
1:A:3606:ASP:N	1:A:3606:ASP:OD1	2.50	0.45
1:A:4179:LEU:HD23	1:A:4179:LEU:HA	1.80	0.45
1:A:2553:PRO:HG2	1:A:2570:PRO:HG3	1.99	0.45
1:A:2584:TRP:CH2	1:A:2732:PRO:HB2	2.52	0.45
1:A:4171:LYS:HD3	1:A:4171:LYS:HA	1.73	0.45
1:A:1747:ALA:N	1:A:1807:LYS:HE3	2.32	0.45
1:A:1981:ALA:HB2	1:A:1999:CYS:HB3	1.99	0.45
1:A:2060:ARG:CZ	1:A:2060:ARG:HA	2.47	0.45
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.50	0.45
1:A:2718:PRO:HB2	1:A:3080:ALA:HA	1.98	0.45
1:A:2726:ARG:NE	3:A:4702:ATP:O1G	2.41	0.45
1:A:2948:ARG:HG3	1:A:2958:VAL:HG21	1.98	0.45
1:A:2536:ASP:O	1:A:2548:TRP:HD1	2.00	0.45
1:A:1809:GLU:O	1:A:1813:THR:HG22	2.17	0.44
1:A:3875:MET:HG2	1:A:3879:ASP:HB2	1.98	0.44
1:A:2387:LEU:HD11	1:A:2463:HIS:CG	2.52	0.44
1:A:3733:LYS:HA	1:A:3733:LYS:HD3	1.86	0.44
1:A:3966:PRO:HG3	1:A:3997:ARG:NH1	2.33	0.44
1:A:2287:ILE:HA	1:A:2294:GLU:HG3	1.99	0.44
1:A:2457:SER:HB2	1:A:2732:PRO:HB3	2.00	0.44
1:A:2951:ALA:O	1:A:2956:LEU:N	2.51	0.44
1:A:3066:PHE:CZ	1:A:3085:LEU:HD11	2.53	0.44
1:A:2935:LEU:O	1:A:3068:MET:N	2.40	0.44
1:A:3913:GLU:OE2	1:A:3913:GLU:N	2.51	0.44
1:A:1659:ALA:HB2	1:A:1926:PHE:HB2	1.99	0.44
1:A:2191:LEU:HD11	1:A:2232:MET:SD	2.57	0.44
1:A:2841:GLU:O	1:A:2844:ARG:HG2	2.17	0.44
1:A:3892:LEU:HD13	1:A:3983:ILE:HG21	2.00	0.44
1:A:4575:LEU:HB3	1:A:4635:PHE:HZ	1.82	0.44
1:A:1947:GLY:O	1:A:1951:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2111:ILE:HG21	1:A:2127:ILE:HG21	1.98	0.44
1:A:2583:THR:HG22	1:A:2584:TRP:HD1	1.82	0.44
1:A:4058:LEU:HA	1:A:4061:GLU:HG2	2.00	0.44
1:A:4297:PRO:HG3	1:A:4308:TRP:CD2	2.52	0.44
1:A:2810:LEU:HD11	1:A:2821:LEU:HD13	2.00	0.44
1:A:2823:ARG:HE	1:A:2871:ILE:HG12	1.82	0.44
1:A:2831:ARG:HD2	1:A:2921:ARG:HG2	2.00	0.44
1:A:3007:ARG:HG2	1:A:3007:ARG:HH11	1.83	0.44
1:A:3044:LEU:HD22	1:A:3049:GLU:HB2	1.99	0.44
1:A:3183:TYR:CE1	1:A:3508:LEU:HA	2.53	0.44
1:A:3582:ARG:HE	1:A:3582:ARG:HB3	1.62	0.44
1:A:2382:LEU:HD12	1:A:2463:HIS:CE1	2.52	0.44
1:A:2754:ALA:HA	1:A:2757:ARG:NH1	2.33	0.44
1:A:3151:HIS:ND1	1:A:3516:TYR:OH	2.32	0.44
1:A:4612:ASN:OD1	1:A:4614:THR:N	2.51	0.44
1:A:1665:ILE:N	1:A:1675:GLY:O	2.48	0.44
1:A:2075:LEU:HD22	1:A:4526:GLN:OE1	2.18	0.44
1:A:2319:LEU:HB2	1:A:2358:ARG:HG2	1.99	0.44
1:A:2602:THR:HG23	1:A:2662:PHE:CE1	2.52	0.44
1:A:3213:ASP:O	1:A:3216:GLU:HG2	2.18	0.44
1:A:4138:LEU:HD12	1:A:4138:LEU:HA	1.82	0.44
1:A:4190:ILE:HG13	1:A:4191:GLN:N	2.33	0.44
1:A:1928:LEU:HD23	1:A:1948:LEU:HD21	2.00	0.43
1:A:1959:GLU:OE1	1:A:2019:ASN:HB2	2.18	0.43
1:A:2791:HIS:HB3	1:A:3086:PHE:CE2	2.51	0.43
1:A:1910:THR:HG21	1:A:2041:MET:HB3	2.00	0.43
1:A:2203:TRP:CH2	1:A:2236:VAL:HG11	2.52	0.43
1:A:2304:ASP:OD1	1:A:2726:ARG:NH2	2.51	0.43
1:A:2912:PHE:CE1	1:A:2915:VAL:HG23	2.53	0.43
1:A:3113:MET:CE	1:A:3184:ALA:HA	2.48	0.43
1:A:2299:GLN:HB2	1:A:2339:VAL:HG22	2.00	0.43
1:A:3120:TYR:HD1	1:A:3139:HIS:HD2	1.66	0.43
1:A:3517:ALA:HA	1:A:3520:PHE:HD2	1.83	0.43
1:A:1864:ALA:HB1	1:A:1866:PHE:CE1	2.53	0.43
1:A:2480:PRO:HG2	1:A:2482:GLN:NE2	2.34	0.43
1:A:2275:TRP:CE2	1:A:2327:LEU:HD13	2.53	0.43
1:A:4338:ASP:OD1	1:A:4342:LYS:HE3	2.19	0.43
1:A:2895:ALA:O	1:A:2899:VAL:HG23	2.18	0.43
1:A:3009:ASN:HA	1:A:3012:LEU:HG	2.00	0.43
1:A:1698:ILE:HA	1:A:1701:TRP:NE1	2.34	0.43
1:A:2257:LYS:HA	1:A:2257:LYS:HD2	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3717:LEU:HD23	1:A:3717:LEU:HA	1.84	0.43
1:A:3808:CYS:SG	1:A:3836:TYR:HE2	2.42	0.43
1:A:4027:LEU:HB3	1:A:4058:LEU:HD12	2.00	0.43
1:A:1745:TYR:O	1:A:1807:LYS:HE2	2.19	0.43
1:A:2885:ASP:HB3	1:A:2888:GLU:HG3	2.01	0.43
1:A:3055:THR:O	1:A:3059:ILE:HG23	2.19	0.43
1:A:1640:ILE:HD12	1:A:1653:HIS:ND1	2.33	0.43
1:A:1736:ASN:O	1:A:1740:THR:HG23	2.18	0.43
1:A:2157:LEU:O	1:A:2161:LEU:HD23	2.19	0.43
1:A:2172:ARG:NH2	1:A:2205:GLU:OE1	2.51	0.43
1:A:2885:ASP:OD1	1:A:2886:GLN:N	2.51	0.43
1:A:1652:LYS:HG3	1:A:2330:GLY:HA2	2.01	0.43
1:A:2759:ILE:HG13	1:A:2759:ILE:O	2.19	0.43
1:A:2817:PRO:HB2	1:A:2819:GLU:OE1	2.19	0.43
1:A:3202:ASN:HA	1:A:3205:LEU:HD12	2.01	0.43
1:A:3620:ARG:NH1	1:A:3644:VAL:HG11	2.34	0.43
1:A:4102:ALA:O	1:A:4106:LEU:HD23	2.19	0.43
1:A:4489:LEU:HD11	1:A:4515:PHE:HE1	1.84	0.43
1:A:1789:LEU:HD11	1:A:1816:VAL:HG23	2.01	0.42
1:A:2594:CYS:HA	1:A:2712:CYS:O	2.19	0.42
1:A:2685:GLN:NE2	1:A:2692:PHE:HA	2.34	0.42
1:A:4277:SER:HA	1:A:4282:PHE:CG	2.54	0.42
1:A:1677:SER:OG	1:A:1678:SER:N	2.51	0.42
1:A:2452:LEU:HA	1:A:2452:LEU:HD12	1.64	0.42
1:A:2658:TRP:CE3	1:A:2705:ARG:HA	2.54	0.42
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	2.00	0.42
1:A:3783:LYS:O	1:A:3787:THR:HG23	2.19	0.42
1:A:4444:GLN:HB2	1:A:4449:ARG:NH2	2.34	0.42
1:A:2977:ARG:HG2	1:A:3021:PHE:HE1	1.84	0.42
1:A:3487:GLU:O	1:A:3491:LYS:HG2	2.19	0.42
1:A:4293:ASP:N	1:A:4293:ASP:OD1	2.51	0.42
1:A:1911:GLY:HA3	2:A:4701:ADP:C8	2.54	0.42
1:A:1939:GLN:O	1:A:1943:ARG:HG2	2.19	0.42
1:A:2377:ASN:OD1	3:A:4702:ATP:O2'	2.36	0.42
1:A:2490:ILE:HD13	1:A:2490:ILE:HA	1.88	0.42
1:A:2757:ARG:HA	1:A:2763:ARG:HH21	1.83	0.42
1:A:3733:LYS:C	1:A:3736:GLY:H	2.23	0.42
1:A:4277:SER:HA	1:A:4282:PHE:CD1	2.54	0.42
1:A:1697:LYS:O	1:A:1701:TRP:HD1	2.01	0.42
1:A:1884:LEU:HD21	1:A:2041:MET:SD	2.60	0.42
1:A:2275:TRP:HZ2	1:A:2281:THR:HG21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2657:LYS:O	1:A:2705:ARG:NH1	2.53	0.42
1:A:3126:MET:SD	1:A:3127:PRO:HD2	2.59	0.42
1:A:3945:LYS:HE3	1:A:3945:LYS:HB3	1.83	0.42
1:A:4075:GLU:OE1	1:A:4075:GLU:N	2.41	0.42
1:A:4466:HIS:CD2	1:A:4466:HIS:N	2.87	0.42
1:A:2697:ASP:OD1	1:A:2697:ASP:N	2.53	0.42
1:A:3186:LEU:HD23	1:A:3186:LEU:HA	1.90	0.42
1:A:1724:VAL:O	1:A:1728:GLY:N	2.53	0.42
1:A:2592:VAL:HG12	1:A:2710:GLY:HA3	2.02	0.42
1:A:2723:LEU:HD12	1:A:2723:LEU:H	1.83	0.42
1:A:2828:GLU:CD	1:A:2924:ARG:HH22	2.23	0.42
1:A:3029:LEU:HD23	1:A:3030:MET:SD	2.60	0.42
1:A:3971:PRO:HG2	1:A:3973:LEU:HD11	2.01	0.42
1:A:4050:ASP:N	1:A:4050:ASP:OD1	2.53	0.42
1:A:2029:PRO:HG2	1:A:2032:LEU:HD12	2.02	0.42
1:A:2137:LEU:HD12	1:A:2137:LEU:HA	1.91	0.42
1:A:3129:VAL:HG21	1:A:3149:PHE:HD2	1.84	0.42
1:A:3594:GLY:O	1:A:3597:THR:OG1	2.24	0.42
1:A:4319:SER:OG	1:A:4325:ASN:OD1	2.22	0.42
1:A:1749:LEU:HD23	1:A:1749:LEU:HA	1.84	0.42
1:A:1903:SER:N	1:A:2037:ARG:O	2.53	0.42
1:A:2922:ILE:HG22	1:A:2950:VAL:HG11	2.00	0.42
1:A:2933:LEU:HD21	1:A:2935:LEU:HG	2.02	0.42
1:A:3502:THR:HB	1:A:3544:ARG:HG2	2.02	0.42
1:A:3876:LEU:HD23	1:A:4146:VAL:HG11	2.02	0.42
1:A:4604:VAL:HA	1:A:4625:GLU:HA	2.01	0.42
1:A:2185:VAL:HG13	1:A:2239:LYS:HD2	2.02	0.42
1:A:2933:LEU:CD2	1:A:2935:LEU:HG	2.50	0.42
1:A:3034:LYS:HE3	1:A:3038:GLN:NE2	2.35	0.42
1:A:4612:ASN:OD1	1:A:4612:ASN:C	2.58	0.42
1:A:2329:ASN:OD1	1:A:2330:GLY:N	2.53	0.41
1:A:3591:ASP:HB3	1:A:3701:PHE:HB2	2.02	0.41
1:A:2074:LYS:HD2	1:A:2074:LYS:HA	1.64	0.41
1:A:3161:LEU:HB3	1:A:3168:THR:HG22	2.01	0.41
1:A:3589:ILE:HA	1:A:3699:VAL:HG23	2.01	0.41
1:A:4021:MET:HA	1:A:4021:MET:CE	2.50	0.41
1:A:2142:CYS:O	1:A:2146:VAL:HB	2.19	0.41
1:A:2230:LYS:H	1:A:2230:LYS:HG3	1.62	0.41
1:A:2273:ARG:HE	1:A:2329:ASN:HB2	1.86	0.41
1:A:2443:LEU:HD21	1:A:2510:MET:HG3	2.03	0.41
1:A:2558:GLU:H	1:A:2561:LYS:HZ3	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2996:GLU:HG2	1:A:2997:SER:N	2.36	0.41
1:A:3003:GLY:HA2	1:A:3006:GLU:HG3	2.02	0.41
1:A:3508:LEU:HD23	1:A:3536:LEU:HD11	2.01	0.41
1:A:3630:GLY:HA2	1:A:3675:PHE:HB2	2.03	0.41
1:A:4105:TRP:CH2	1:A:4109:LEU:HD22	2.55	0.41
1:A:1626:PHE:HD2	1:A:1629:PHE:CE1	2.37	0.41
1:A:1667:ASN:OD1	1:A:1667:ASN:N	2.53	0.41
1:A:1880:VAL:CG2	1:A:2049:ILE:HG12	2.47	0.41
1:A:2138:ILE:HD12	1:A:2168:VAL:HG22	2.01	0.41
1:A:4028:THR:HA	1:A:4058:LEU:HD11	2.02	0.41
1:A:4287:LYS:HE3	1:A:4291:HIS:HA	2.02	0.41
1:A:2313:GLU:HA	1:A:2316:ASN:HD22	1.85	0.41
1:A:3909:LEU:HD22	1:A:4344:LEU:HB2	2.02	0.41
1:A:3959:ILE:HD12	1:A:3959:ILE:H	1.84	0.41
1:A:4191:GLN:O	1:A:4194:LEU:HB2	2.21	0.41
1:A:1688:THR:OG1	1:A:1708:GLU:OE2	2.39	0.41
1:A:1722:THR:O	1:A:1725:GLU:HG3	2.20	0.41
1:A:1943:ARG:HA	1:A:1946:VAL:HG12	2.02	0.41
1:A:2665:GLU:HB3	1:A:2668:LEU:HB3	2.02	0.41
1:A:2673:LYS:H	1:A:2673:LYS:HG2	1.55	0.41
1:A:2726:ARG:HE	3:A:4702:ATP:PG	2.42	0.41
1:A:3546:ASP:OD1	1:A:3546:ASP:N	2.53	0.41
1:A:3715:GLU:OE1	1:A:3718:LYS:NZ	2.53	0.41
1:A:3854:GLN:O	1:A:3858:ILE:HG12	2.21	0.41
1:A:1652:LYS:HD2	1:A:1652:LYS:HA	1.78	0.41
1:A:2538:GLU:HB3	1:A:2548:TRP:NE1	2.36	0.41
1:A:2652:PRO:HD2	1:A:2705:ARG:CZ	2.51	0.41
1:A:2683:ILE:HG22	1:A:2727:PHE:HE1	1.86	0.41
1:A:3497:LYS:HD2	1:A:3497:LYS:HA	1.83	0.41
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	2.02	0.41
1:A:4578:SER:O	1:A:4638:ARG:NH2	2.54	0.41
1:A:2228:SER:C	1:A:2369:LEU:HD12	2.41	0.41
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.56	0.41
1:A:2258:ALA:HB1	1:A:2682:PHE:HD2	1.86	0.41
1:A:2612:LEU:CD2	1:A:2613:PRO:HD2	2.51	0.41
1:A:2818:VAL:O	1:A:2822:ILE:HG12	2.21	0.41
1:A:2873:TYR:O	1:A:2920:LEU:HD13	2.20	0.41
1:A:3509:LEU:HD23	1:A:3509:LEU:HA	1.87	0.41
1:A:3595:GLN:H	1:A:3595:GLN:HG3	1.71	0.41
1:A:3704:THR:HG22	1:A:3706:SER:H	1.86	0.41
1:A:3904:GLU:OE1	1:A:3904:GLU:N	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4069:ILE:O	1:A:4096:LEU:HA	2.20	0.41
1:A:2385:ILE:HA	1:A:2386:PRO:HD3	1.95	0.41
1:A:2507:ARG:O	1:A:2511:ARG:HG3	2.21	0.41
1:A:3171:ILE:HD13	1:A:3171:ILE:HA	1.87	0.41
1:A:2322:ASN:HB3	1:A:2324:LEU:HD23	2.03	0.40
1:A:2976:LEU:HD23	1:A:2976:LEU:HA	1.95	0.40
1:A:4202:SER:H	1:A:4202:SER:HG	1.68	0.40
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	2.04	0.40
1:A:2191:LEU:HA	1:A:2191:LEU:HD13	1.85	0.40
1:A:2238:LEU:HD12	1:A:2300:TRP:CE3	2.56	0.40
1:A:2259:ILE:HG12	1:A:2263:HIS:HB2	2.02	0.40
1:A:2369:LEU:HD21	3:A:4702:ATP:C5	2.56	0.40
1:A:2412:MET:O	1:A:2415:ILE:HG22	2.22	0.40
1:A:2453:ARG:NH2	1:A:2505:ASP:OD2	2.53	0.40
1:A:4581:ILE:HD12	1:A:4581:ILE:HA	1.88	0.40
1:A:1792:LEU:HD11	1:A:1811:LEU:HG	2.04	0.40
1:A:2113:ARG:HA	1:A:2113:ARG:NE	2.36	0.40
1:A:3164:ARG:HH21	1:A:4374:PRO:N	2.18	0.40
1:A:4517:PRO:HG2	1:A:4619:ILE:HD12	2.03	0.40
1:A:1797:LEU:HD12	1:A:1797:LEU:HA	1.84	0.40
1:A:2232:MET:O	1:A:2236:VAL:HG12	2.22	0.40
1:A:3703:VAL:HG21	1:A:3829:LEU:HD22	2.02	0.40
1:A:3931:GLN:O	1:A:3935:VAL:HG12	2.21	0.40
1:A:3938:LEU:HD11	1:A:3991:LEU:HB3	2.03	0.40
1:A:2093:LEU:HD12	1:A:2093:LEU:HA	1.97	0.40
1:A:2184:LYS:HB2	1:A:2184:LYS:HE3	1.97	0.40
1:A:2279:LEU:HD11	1:A:2693:TYR:CG	2.57	0.40
1:A:2285:ARG:NH2	1:A:2331:GLU:OE1	2.47	0.40
1:A:2718:PRO:CB	1:A:3080:ALA:HA	2.52	0.40
1:A:3167:ARG:NH2	1:A:3686:VAL:O	2.52	0.40
1:A:3984:GLY:O	1:A:3988:HIS:ND1	2.54	0.40
1:A:4035:VAL:HG23	1:A:4143:ARG:HD3	2.04	0.40
1:A:4071:ILE:HG23	1:A:4077:PHE:HE1	1.86	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%)	2343 (97%)	64 (3%)	40 65

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1695	HIS
1	A	1727	PHE
1	A	1729	LYS
1	A	1759	SER
1	A	1837	GLU
1	A	1866	PHE
1	A	1867	ASN
1	A	1926	PHE
1	A	1941	MET
1	A	1960	PHE
1	A	1962	ARG
1	A	2030	ASP
1	A	2045	ASP

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Mol	Chain	Res	Type
1	A	2232	MET
1	A	2263	HIS
1	A	2273	ARG
1	A	2347	ASP
1	A	2357	SER
1	A	2388	ASP
1	A	2481	MET
1	A	2606	PHE
1	A	2612	LEU
1	A	2614	ASP
1	A	2615	MET
1	A	2664	ASP
1	A	2670	ASP
1	A	2688	GLU
1	A	2692	PHE
1	A	2863	ARG
1	A	2867	MET
1	A	2881	TYR
1	A	2926	PHE
1	A	2947	SER
1	A	2992	PHE
1	A	3007	ARG
1	A	3086	PHE
1	A	3094	PHE
1	A	3107	LYS
1	A	3146	SER
1	A	3176	TYR
1	A	3191	ARG
1	A	3474	ARG
1	A	3488	ARG
1	A	3499	GLN
1	A	3524	MET
1	A	3619	PHE
1	A	3712	CYS
1	A	3747	LYS
1	A	3817	SER
1	A	3819	LYS
1	A	3875	MET
1	A	3902	ASP
1	A	3999	ASP
1	A	4029	HIS
1	A	4106	LEU

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Mol	Chain	Res	Type
1	A	4171	LYS
1	A	4217	ASP
1	A	4289	ASP
1	A	4321	LEU
1	A	4447	TYR
1	A	4451	LEU
1	A	4453	ASN
1	A	4462	ARG
1	A	4463	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2271	ASN
1	A	2707	GLN
1	A	2730	HIS
1	A	2857	HIS
1	A	3602	ASN
1	A	3650	ASN
1	A	4526	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	$\#\|Z\| > 2$
3	ATP	A	4702	-	28,33,33	0.67	0	34,52,52	0.60	1 (2%)
2	ADP	A	4703	-	24,29,29	0.92	1 (4%)	29,45,45	1.17	2 (6%)
2	ADP	A	4704	-	24,29,29	0.86	0	29,45,45	1.21	2 (6%)
2	ADP	A	4701	-	24,29,29	0.84	0	29,45,45	1.29	2 (6%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4703	ADP	PA-O3A	2.12	1.61	1.59

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4701	ADP	N3-C2-N1	-3.78	123.54	128.67
2	A	4703	ADP	N3-C2-N1	-3.74	123.60	128.67
2	A	4704	ADP	N3-C2-N1	-3.69	123.66	128.67
2	A	4703	ADP	C4-C5-N7	-2.62	106.57	109.34
2	A	4704	ADP	C4-C5-N7	-2.55	106.64	109.34
3	A	4702	ATP	C5-C6-N6	2.34	123.87	120.31
2	A	4701	ADP	C4-C5-N7	-2.29	106.91	109.34

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4703	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	O4'-C4'-C5'-O5'
2	A	4704	ADP	C3'-C4'-C5'-O5'
2	A	4703	ADP	O4'-C4'-C5'-O5'
2	A	4703	ADP	C3'-C4'-C5'-O5'
2	A	4704	ADP	PA-O3A-PB-O1B
2	A	4701	ADP	C5'-O5'-PA-O1A
2	A	4704	ADP	C5'-O5'-PA-O1A
2	A	4703	ADP	PB-O3A-PA-O2A
2	A	4703	ADP	PB-O3A-PA-O1A

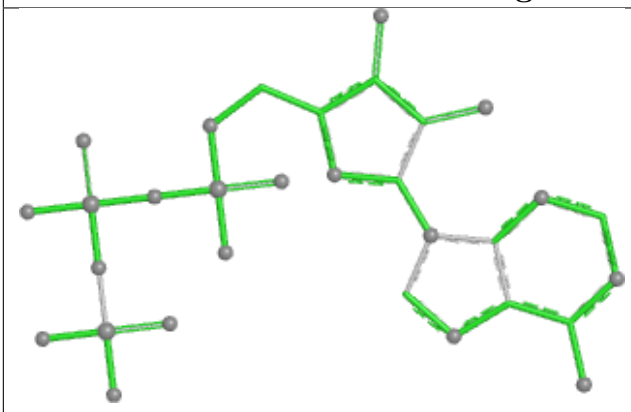
There are no ring outliers.

3 monomers are involved in 15 short contacts:

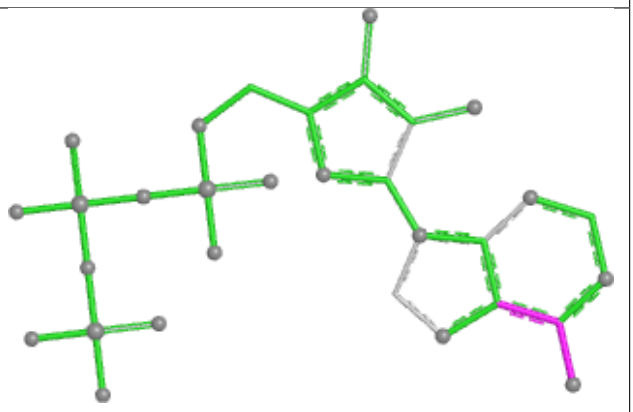
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4702	ATP	7	0
2	A	4703	ADP	2	0
2	A	4701	ADP	6	0

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.

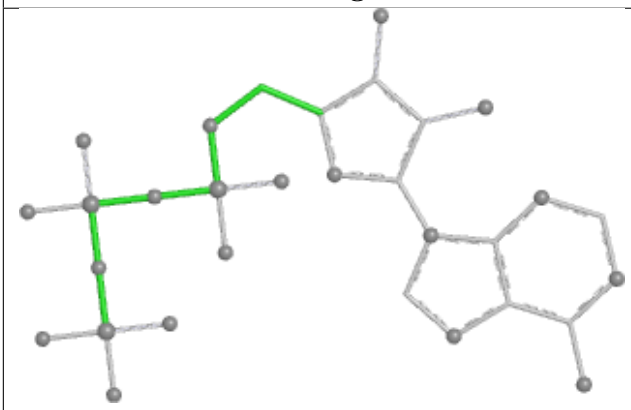
Ligand ATP A 4702



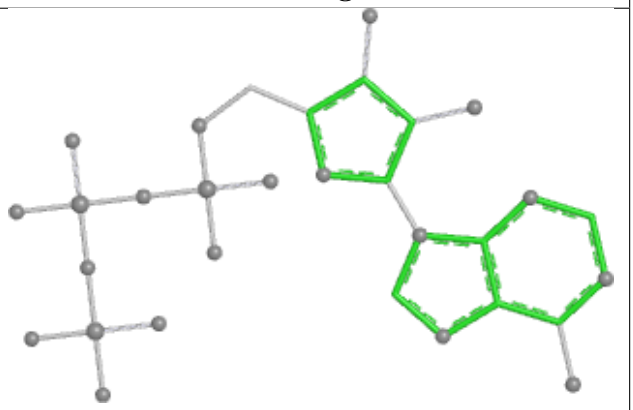
Bond lengths



Bond angles

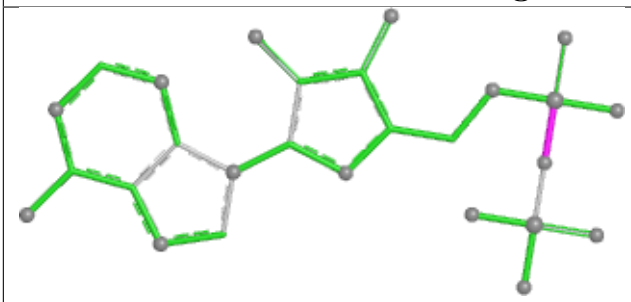


Torsions

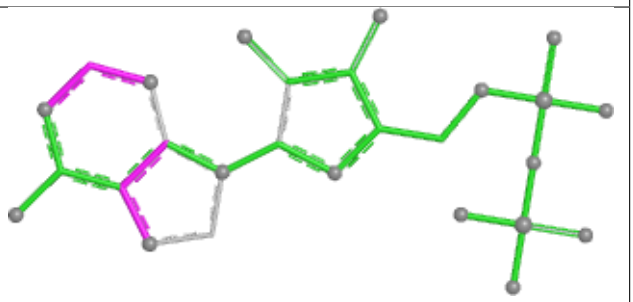


Rings

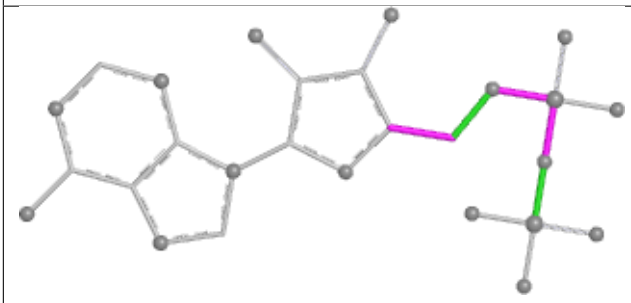
Ligand ADP A 4703



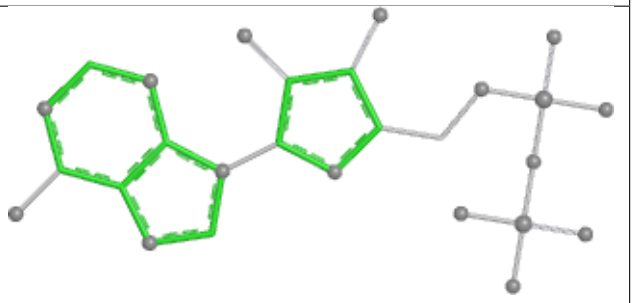
Bond lengths



Bond angles

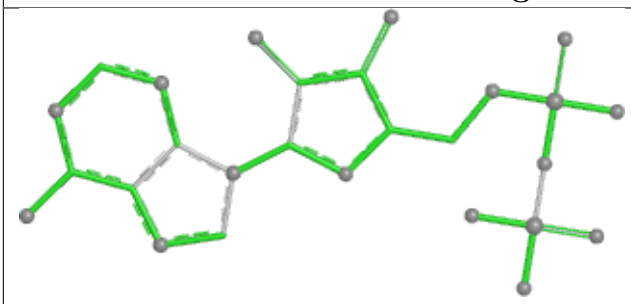


Torsions

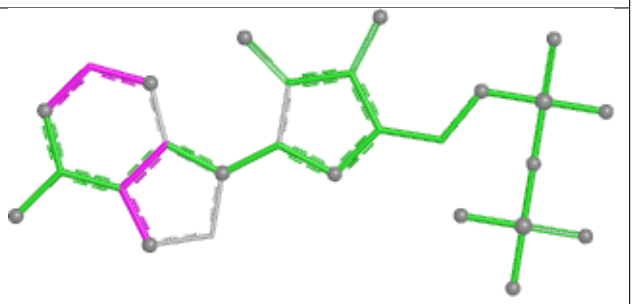


Rings

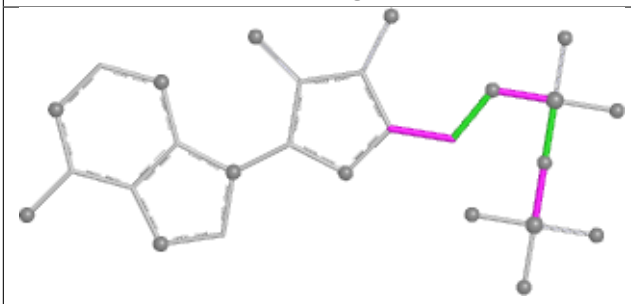
Ligand ADP A 4704



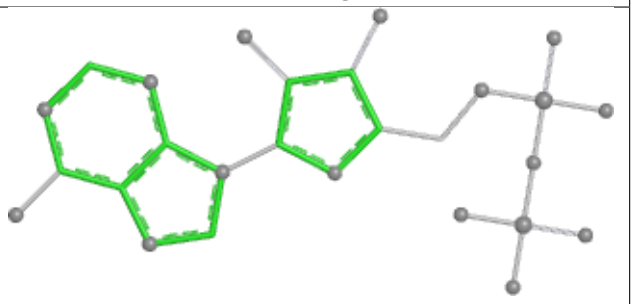
Bond lengths



Bond angles

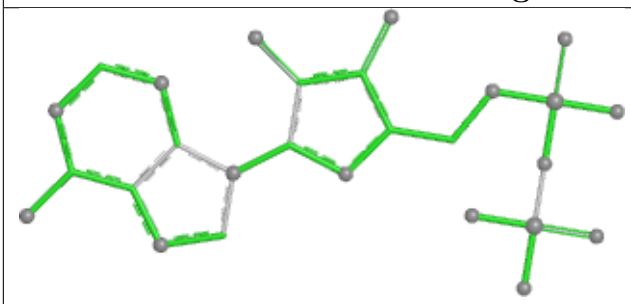


Torsions

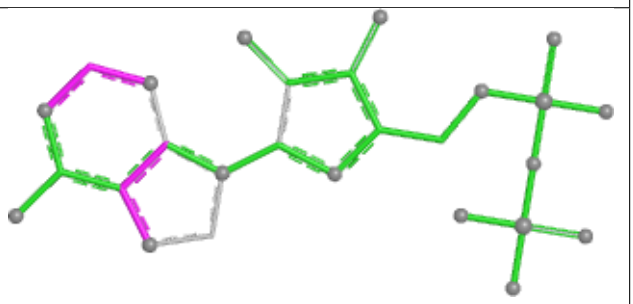


Rings

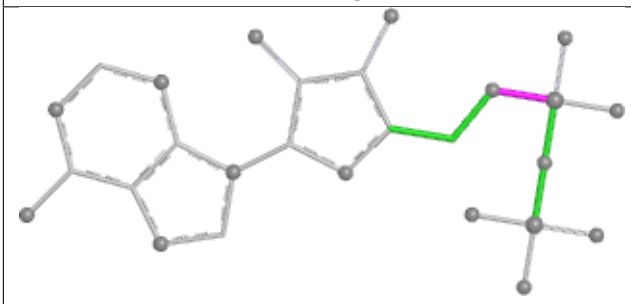
Ligand ADP A 4701



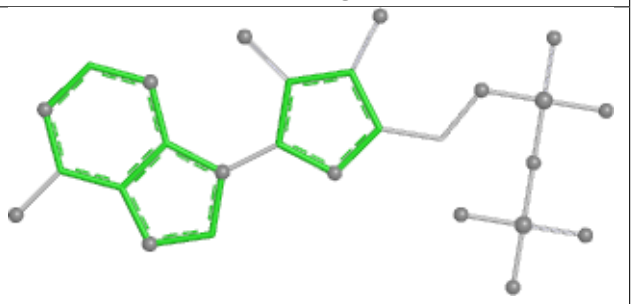
Bond lengths



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.

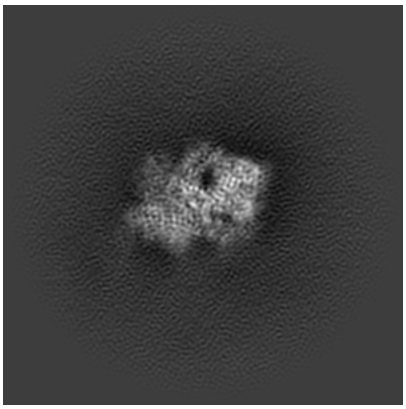
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44705. These allow visual inspection of the internal detail of the map and identification of artifacts.

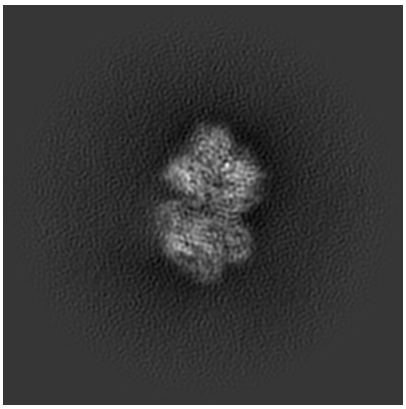
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

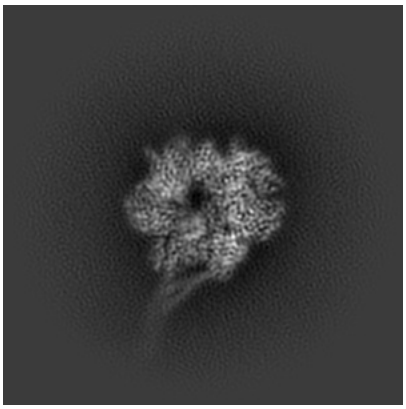
6.1.1 Primary map



X

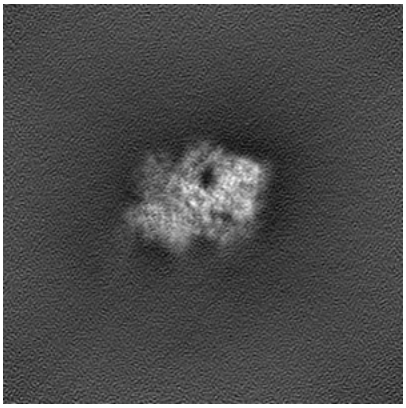


Y

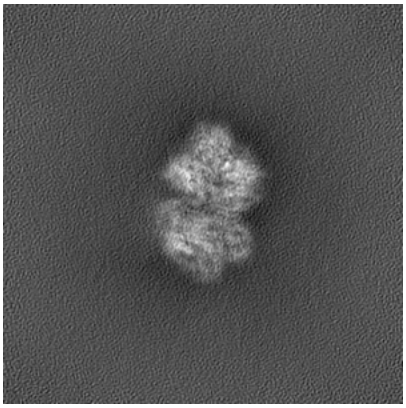


Z

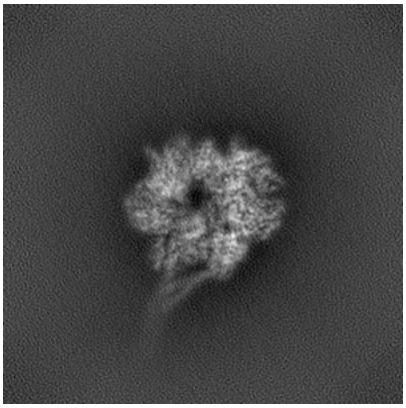
6.1.2 Raw map



X



Y

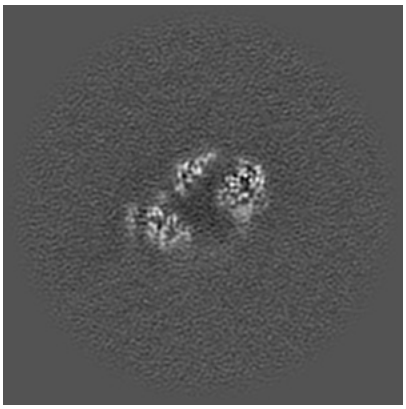


Z

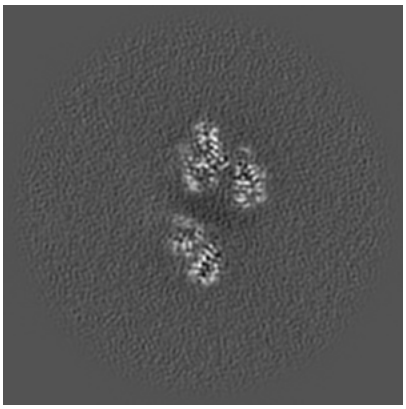
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

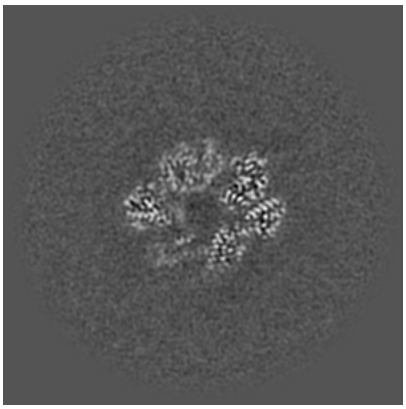
6.2.1 Primary map



X Index: 128



Y Index: 128

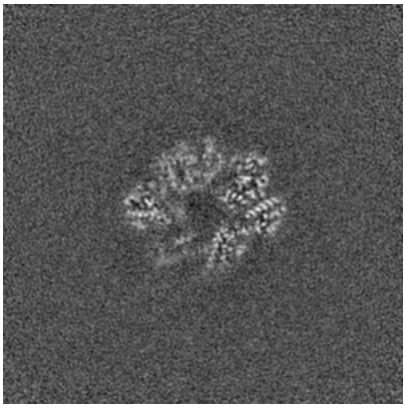


Z Index: 128

6.2.2 Raw map

X Index: 128

Y Index: 128

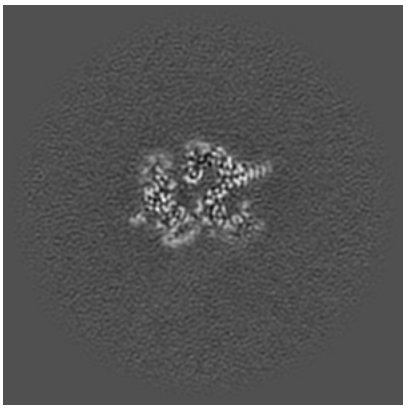


Z Index: 128

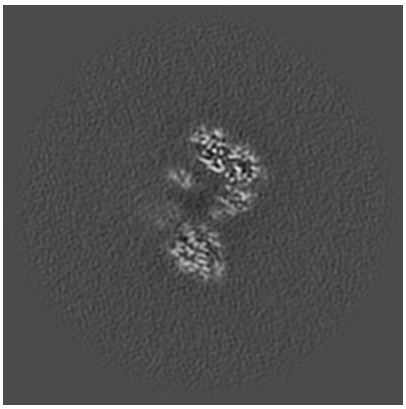
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

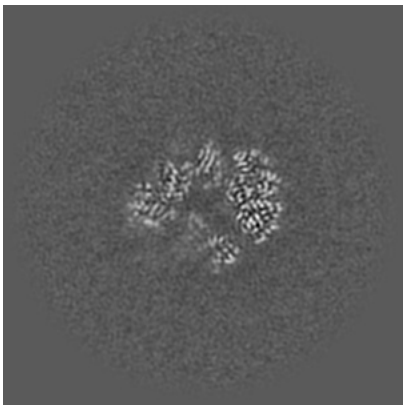
6.3.1 Primary map



X Index: 146

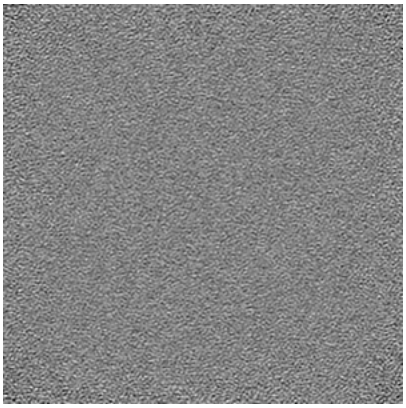


Y Index: 120

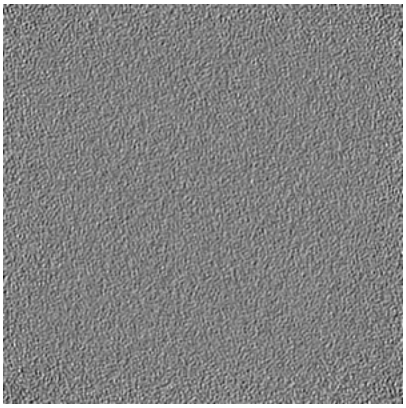


Z Index: 135

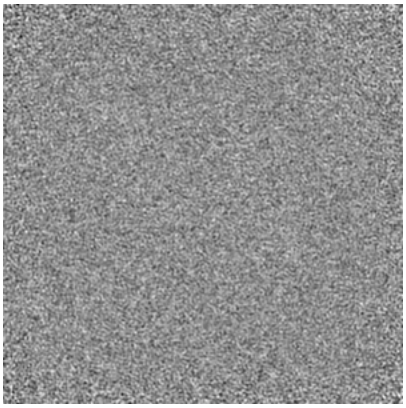
6.3.2 Raw map



X Index: 0



Y Index: 0

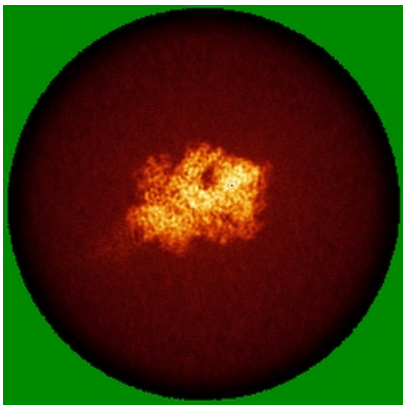


Z Index: 0

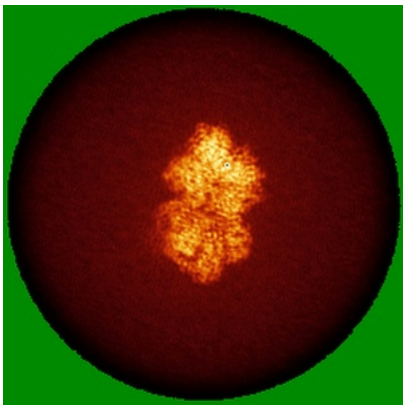
The images above show the largest variance slices of the map in three orthogonal directions.

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

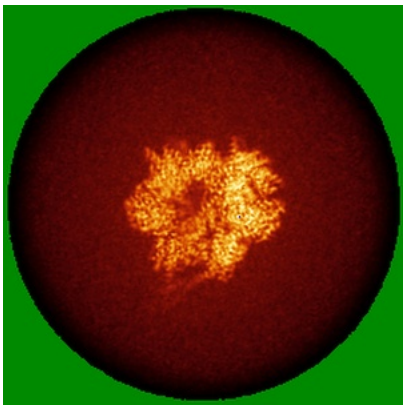
6.4.1 Primary map



X

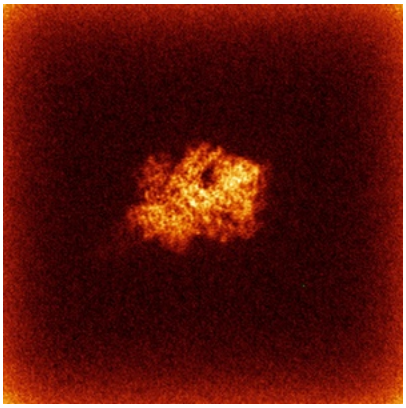


Y

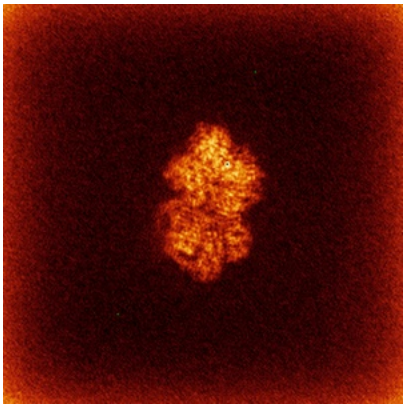


Z

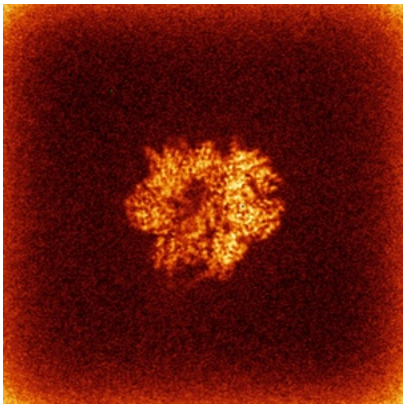
6.4.2 Raw map



X



Y

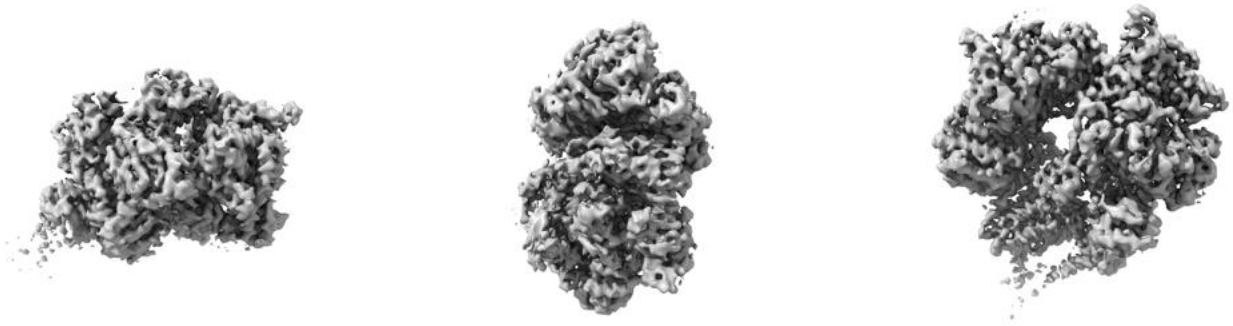


Z

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.

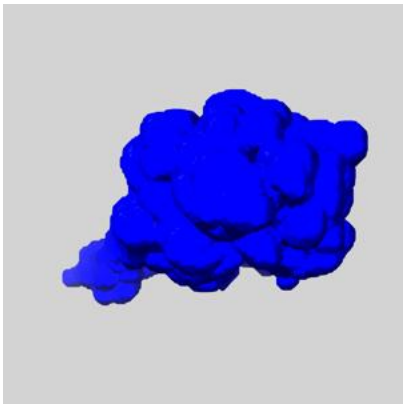
6.6 Mask visualisation (i)

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

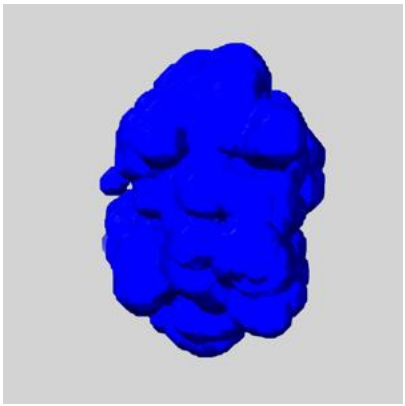
A mask typically either:

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

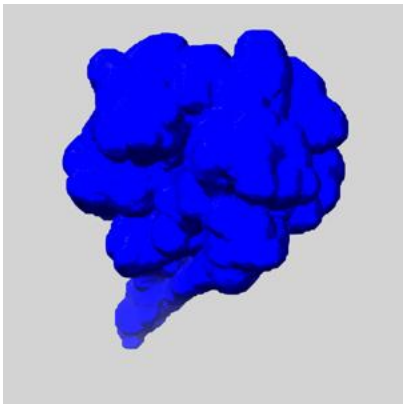
6.6.1 emd_44705_msk_1.map (i)



X



Y

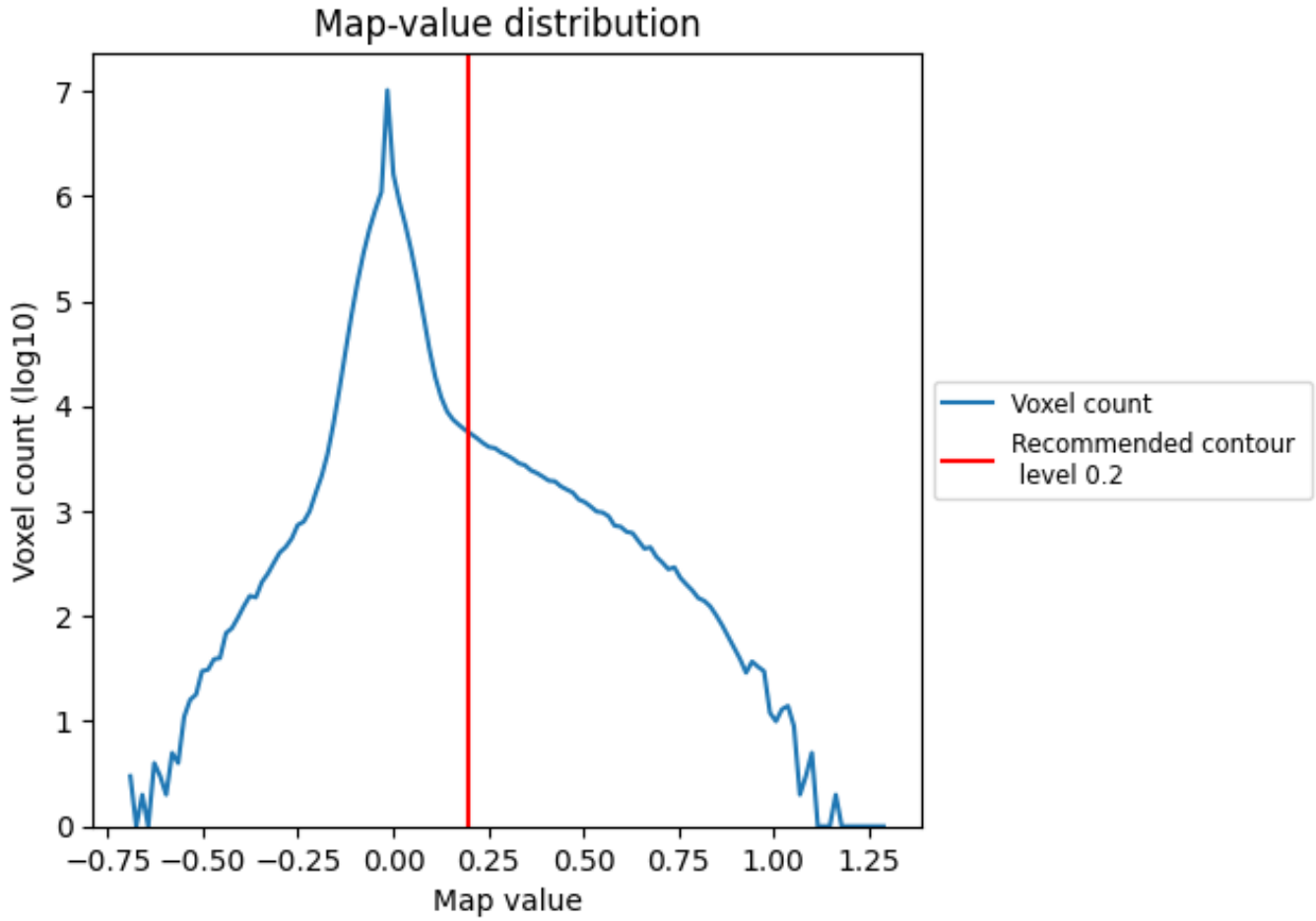


Z

7 Map analysis

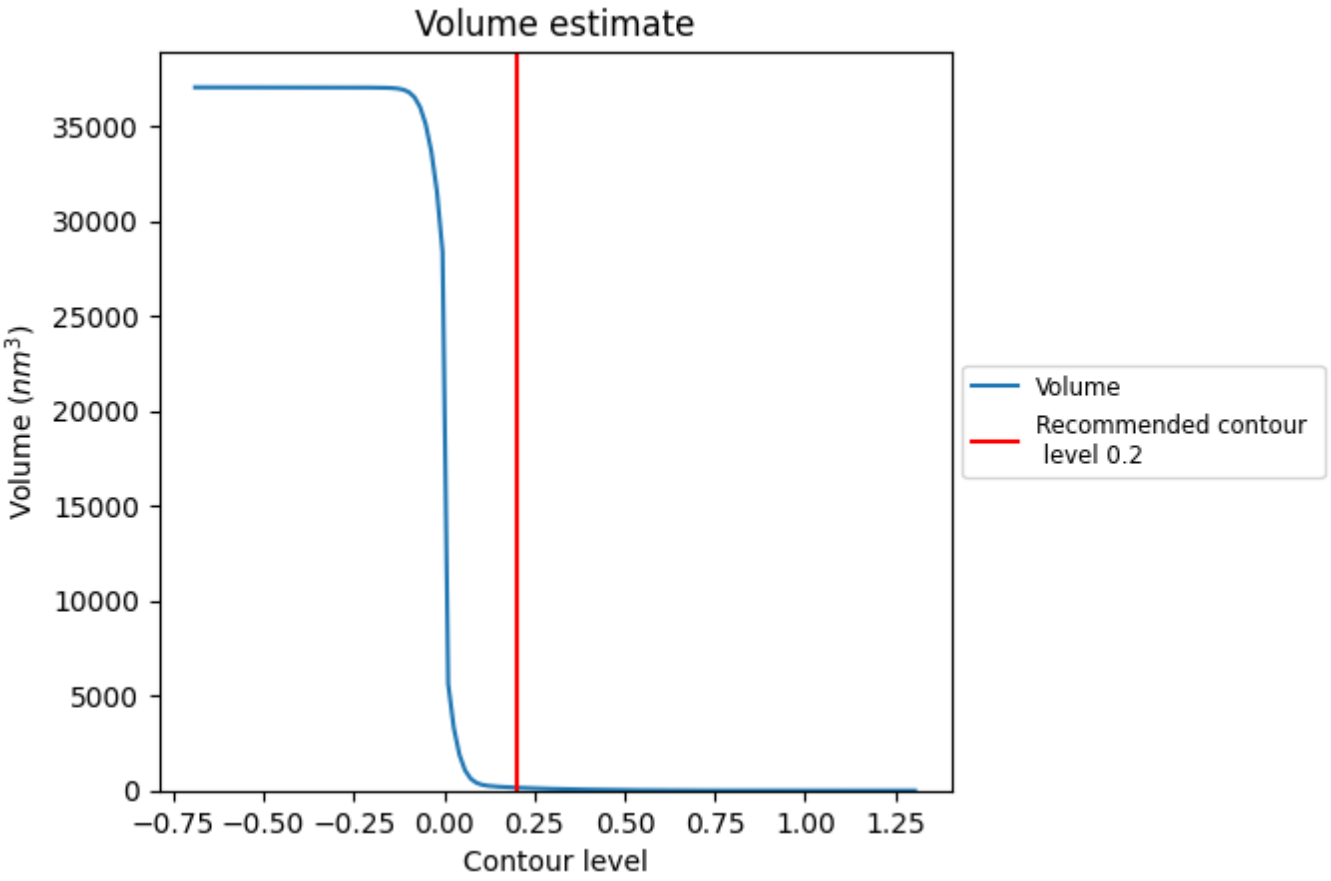
This section contains the results of statistical analysis of the map.

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.

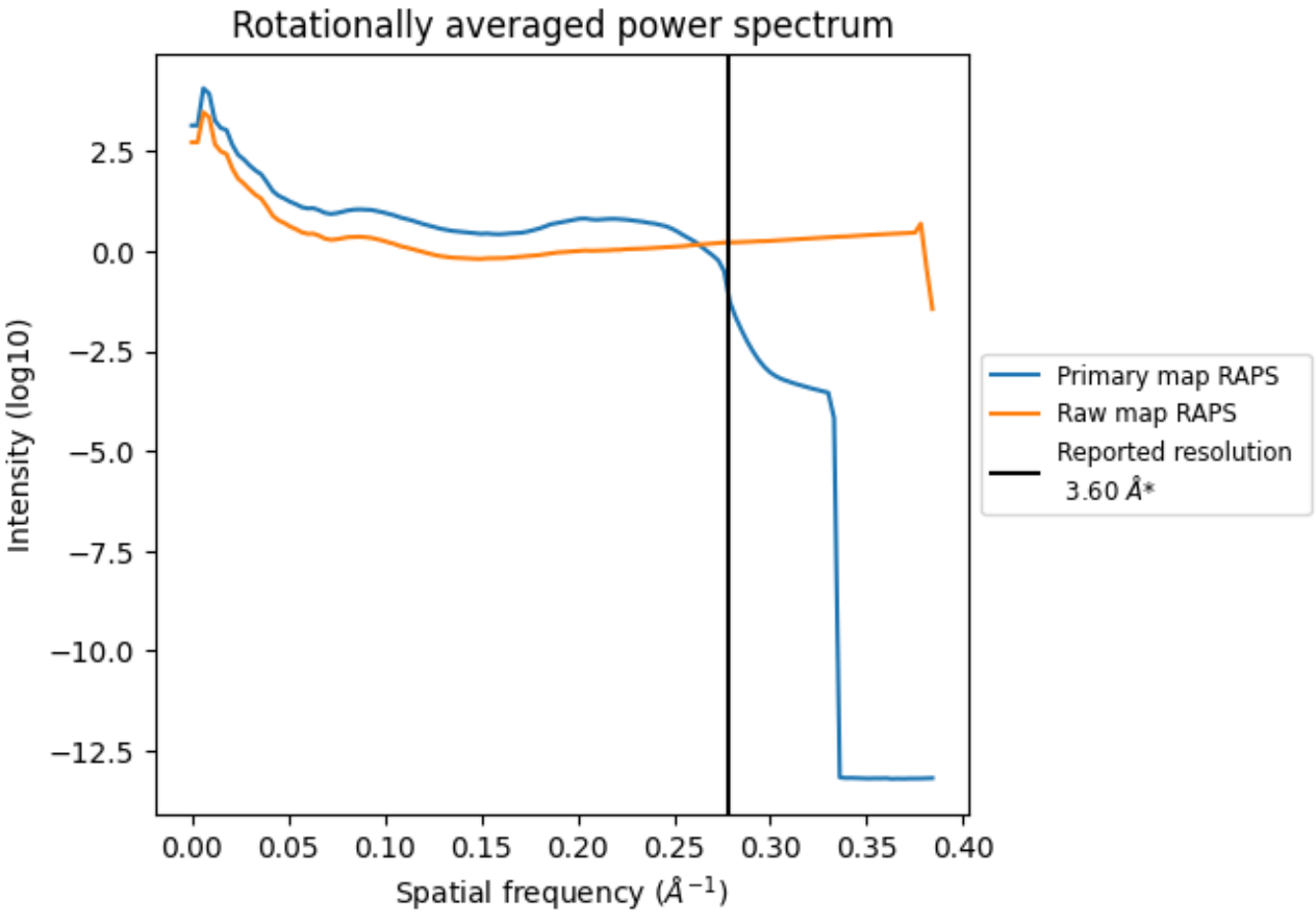
7.2 Volume estimate



The volume at the recommended contour level is 154 nm^3; this corresponds to an approximate mass of 139 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)

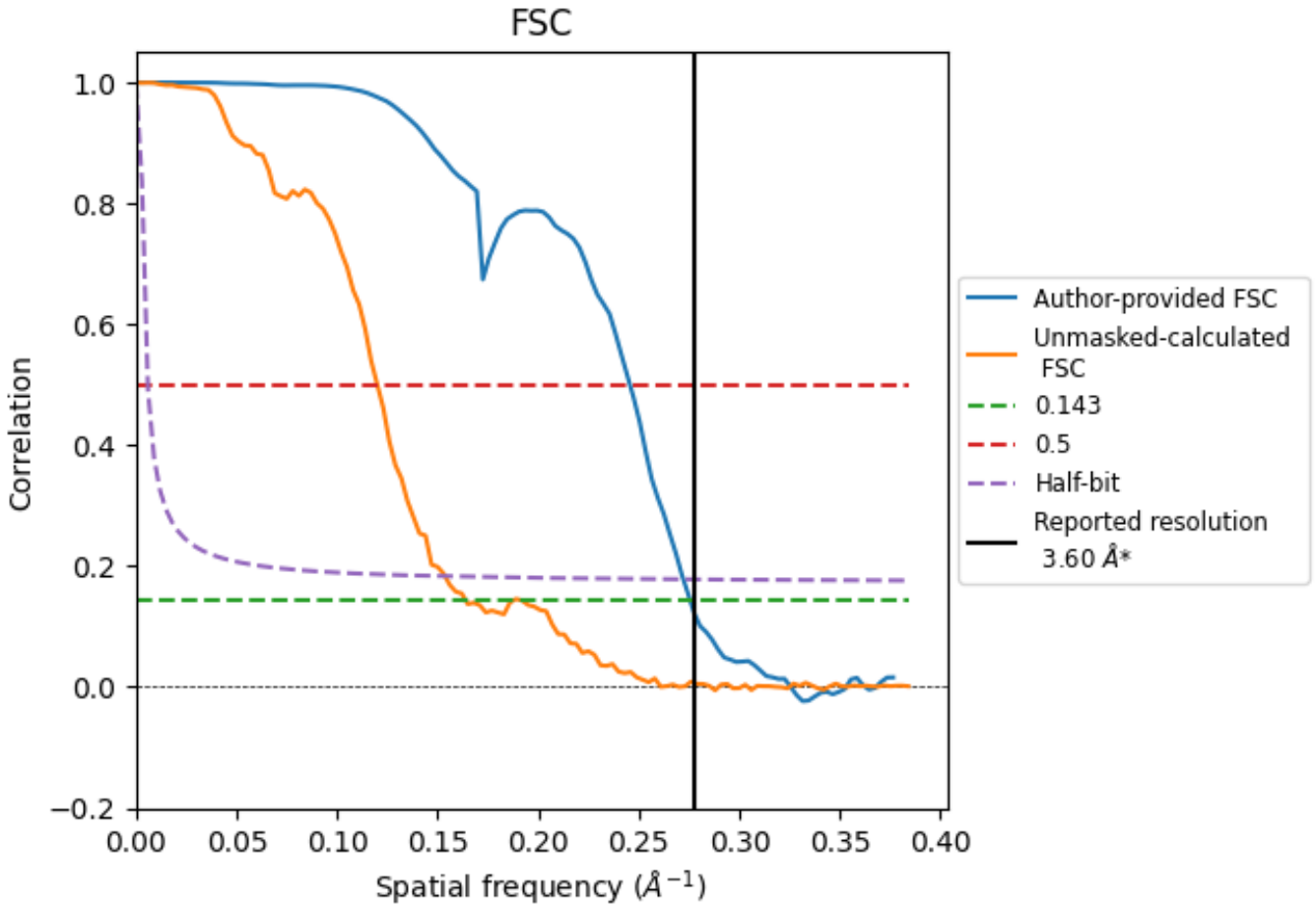


*Reported resolution corresponds to spatial frequency of 0.278 $Å^{-1}$

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

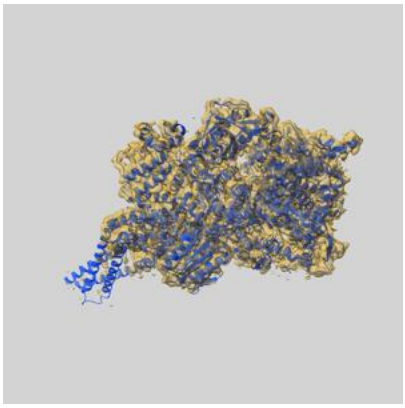
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.63	4.07	3.67
Unmasked-calculated*	6.10	8.33	6.51

*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 6.10 differs from the reported value 3.6 by more than 10 %

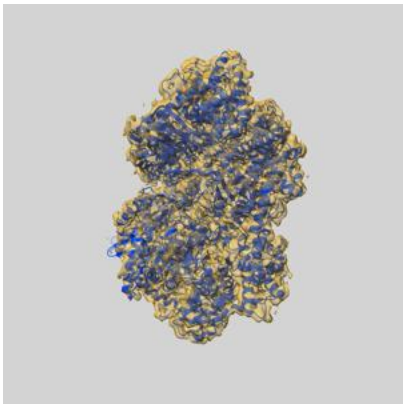
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44705 and PDB model 9BMO. Per-residue inclusion information can be found in section 3 on page 5.

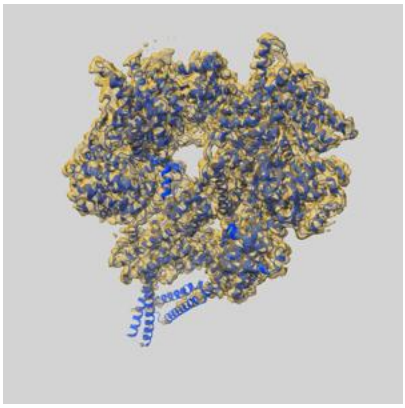
9.1 Map-model overlay



X



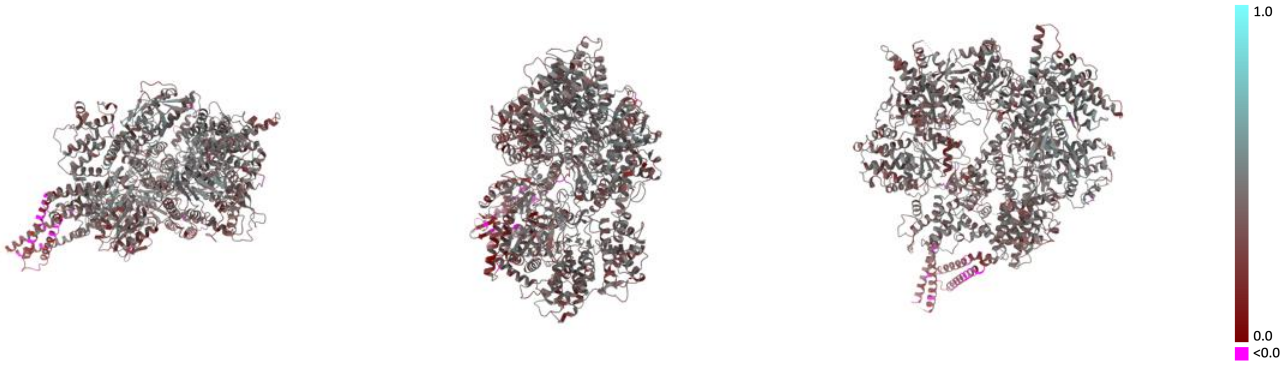
Y



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.

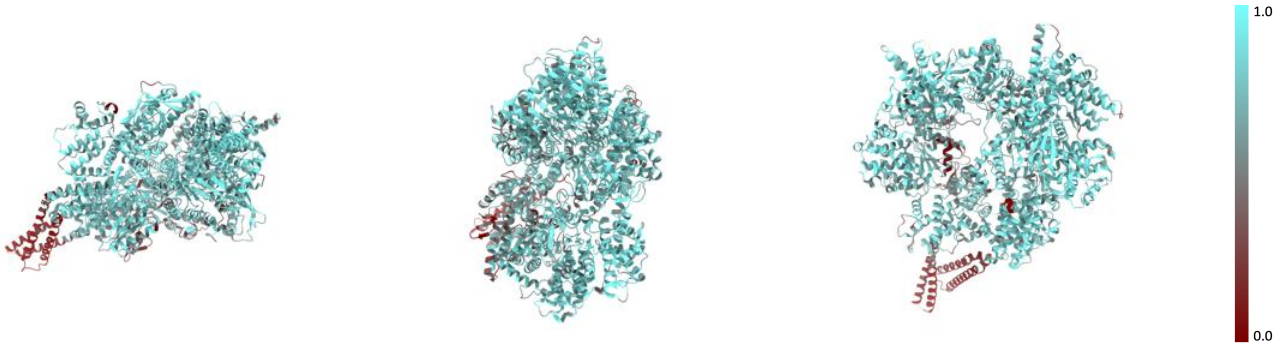
9.2 Q-score mapped to coordinate model (i)



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.

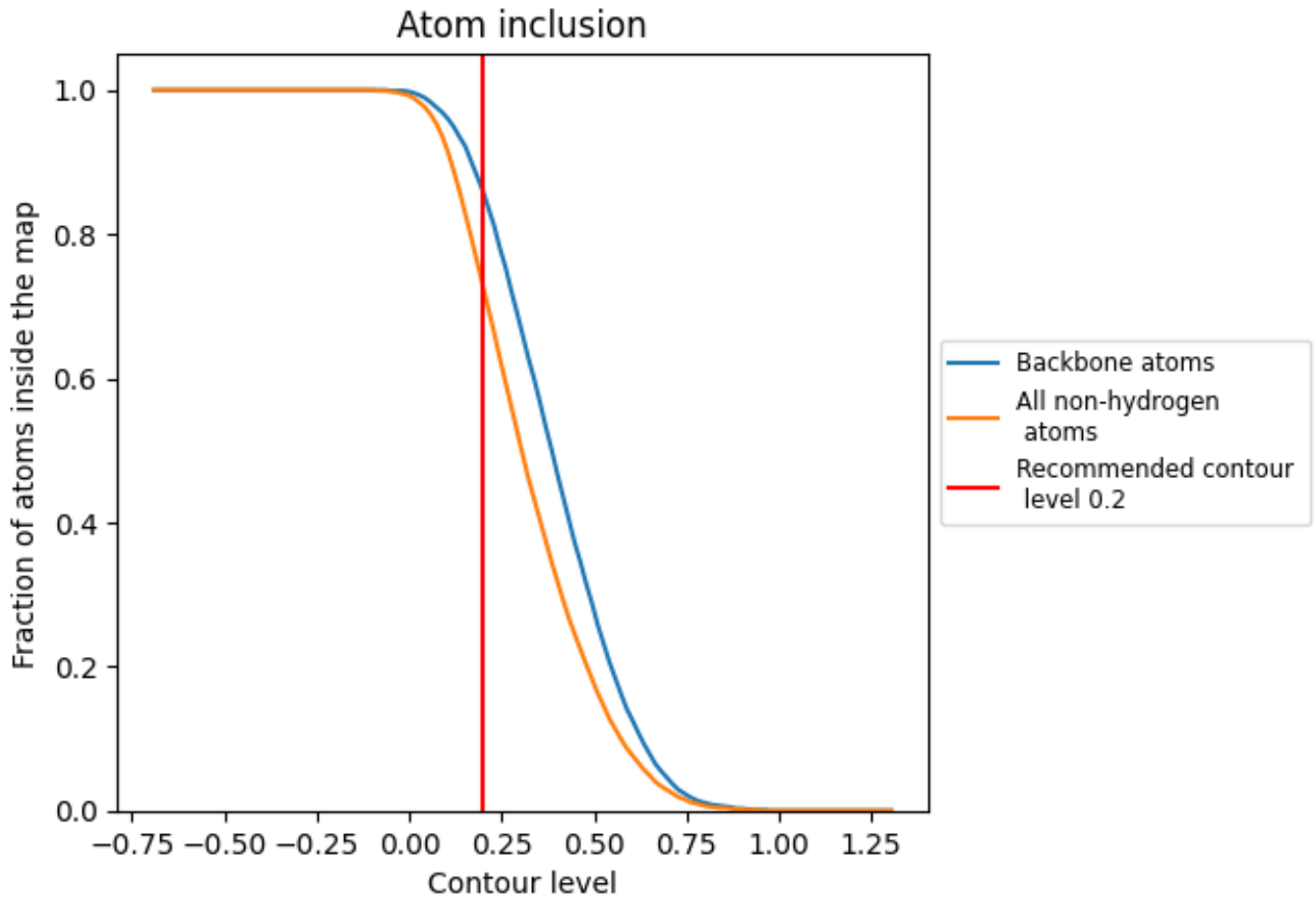
9.3 Atom inclusion mapped to coordinate model (i)



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, 86% of all backbone atoms, 73% 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	0.7280	0.3970
A	0.7280	0.3970