Full wwPDB EM Validation Report ⓘ

Apr 24, 2025 – 01:37 PM EDT

PDB ID	:	9BM8 / pdb_00009bm8
EMDB ID	:	EMD-44691
Title	:	State-7c of motor domain from full-length human dynein-1 in 5 mM ATP
Authors	:	Chai, P.; Zhang, K.
Deposited on	:	2024-05-02
Resolution	:	3.22 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:

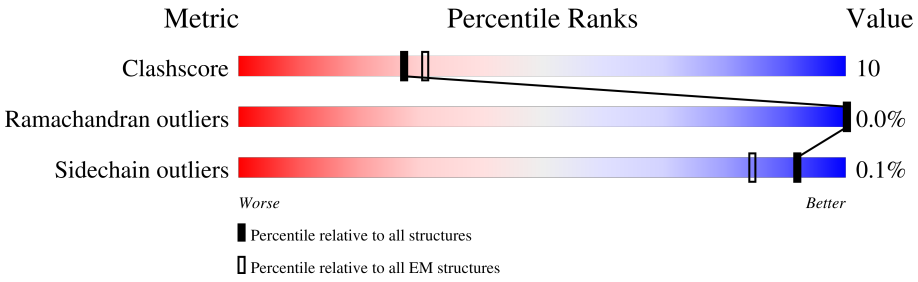
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.22 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	10% 49% 15% 36%

2 Entry composition

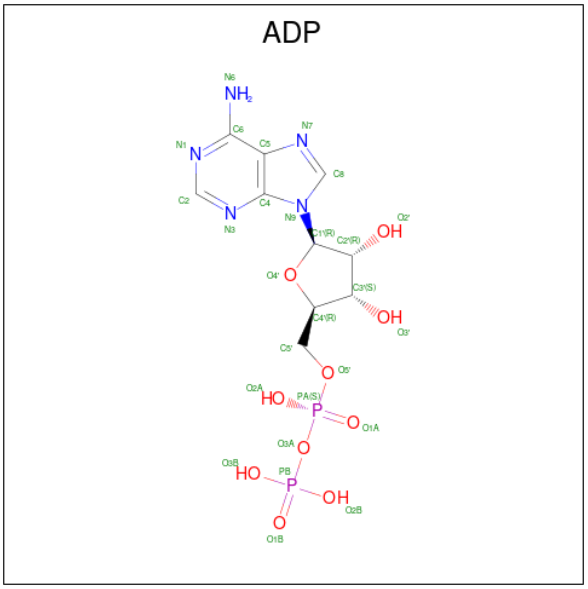
There are 3 unique types of molecules in this entry. The entry contains 24220 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

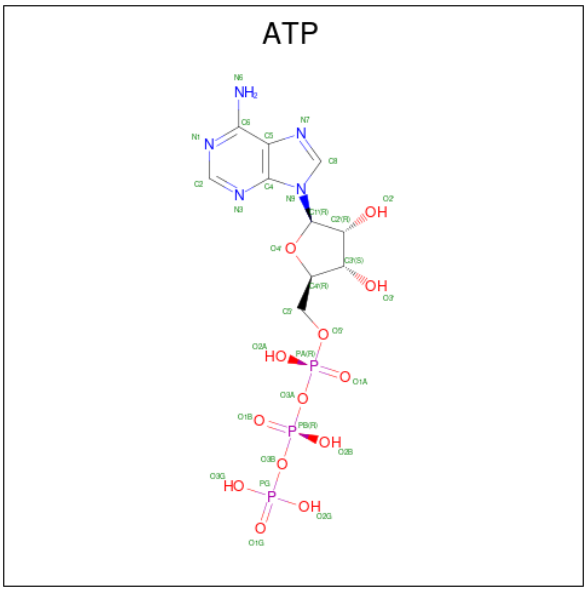
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2991	24104	15379	4162	4443	120	0	0

- 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

- 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).

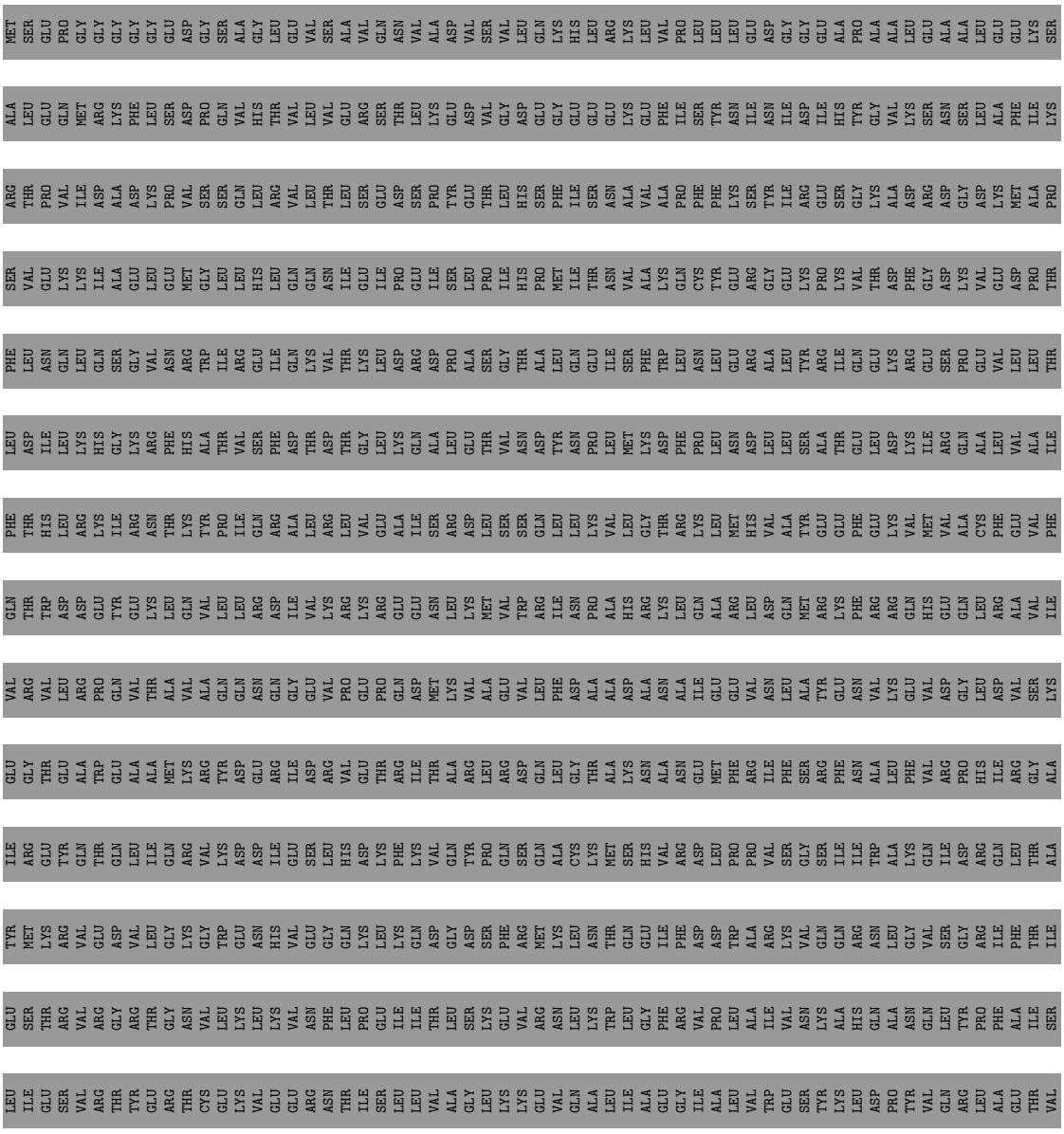


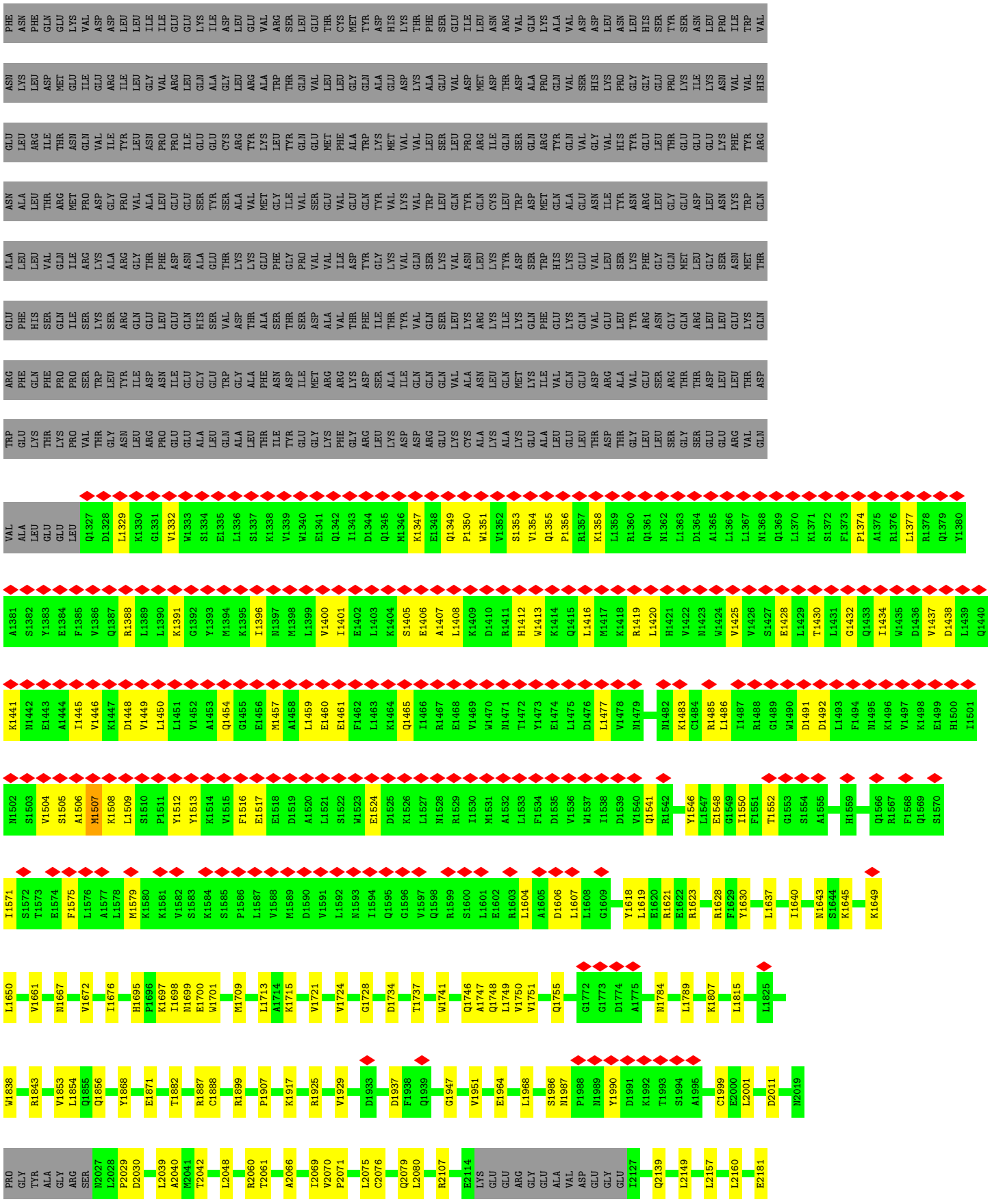
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

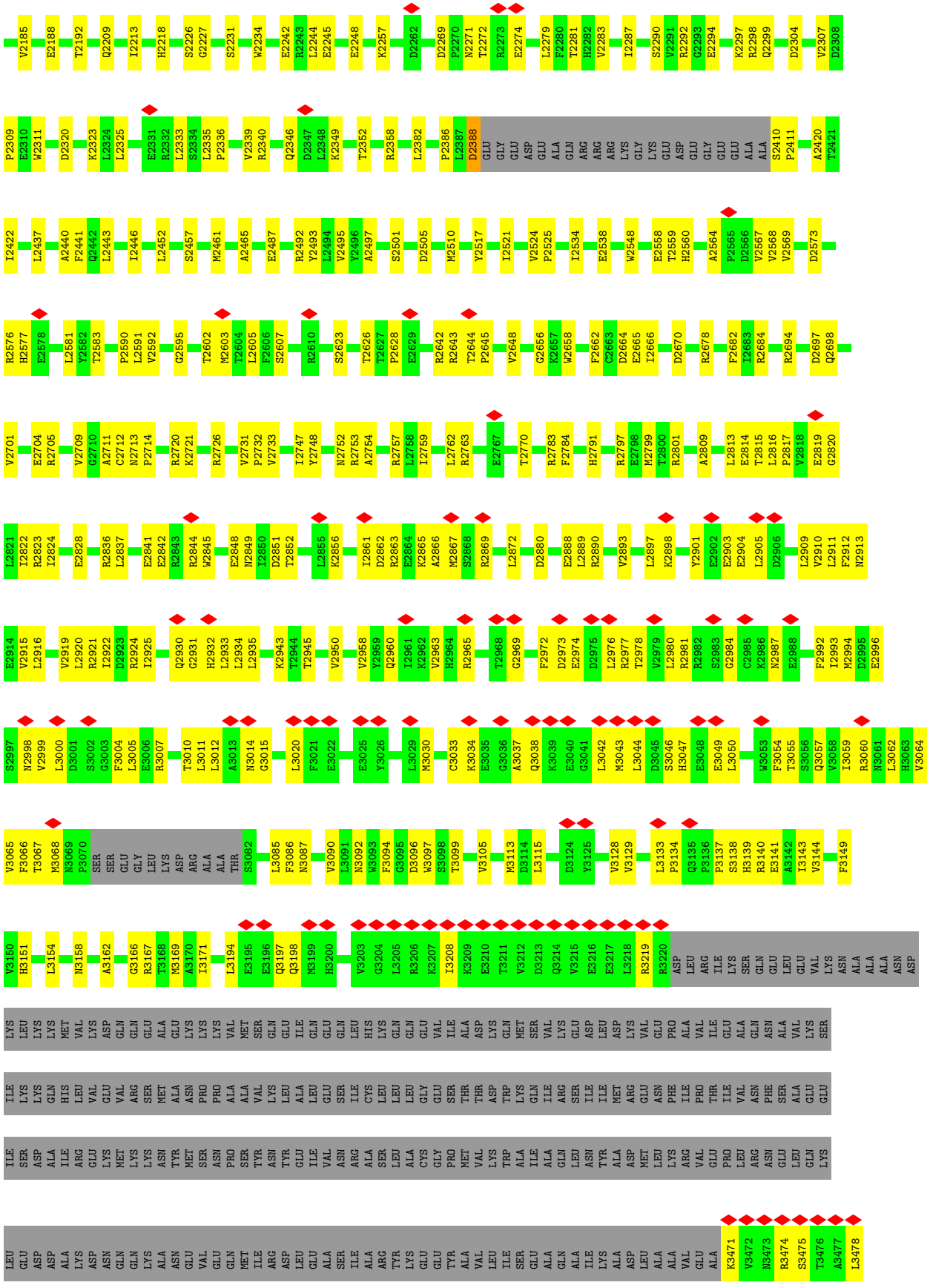
3 Residue-property plots (i)

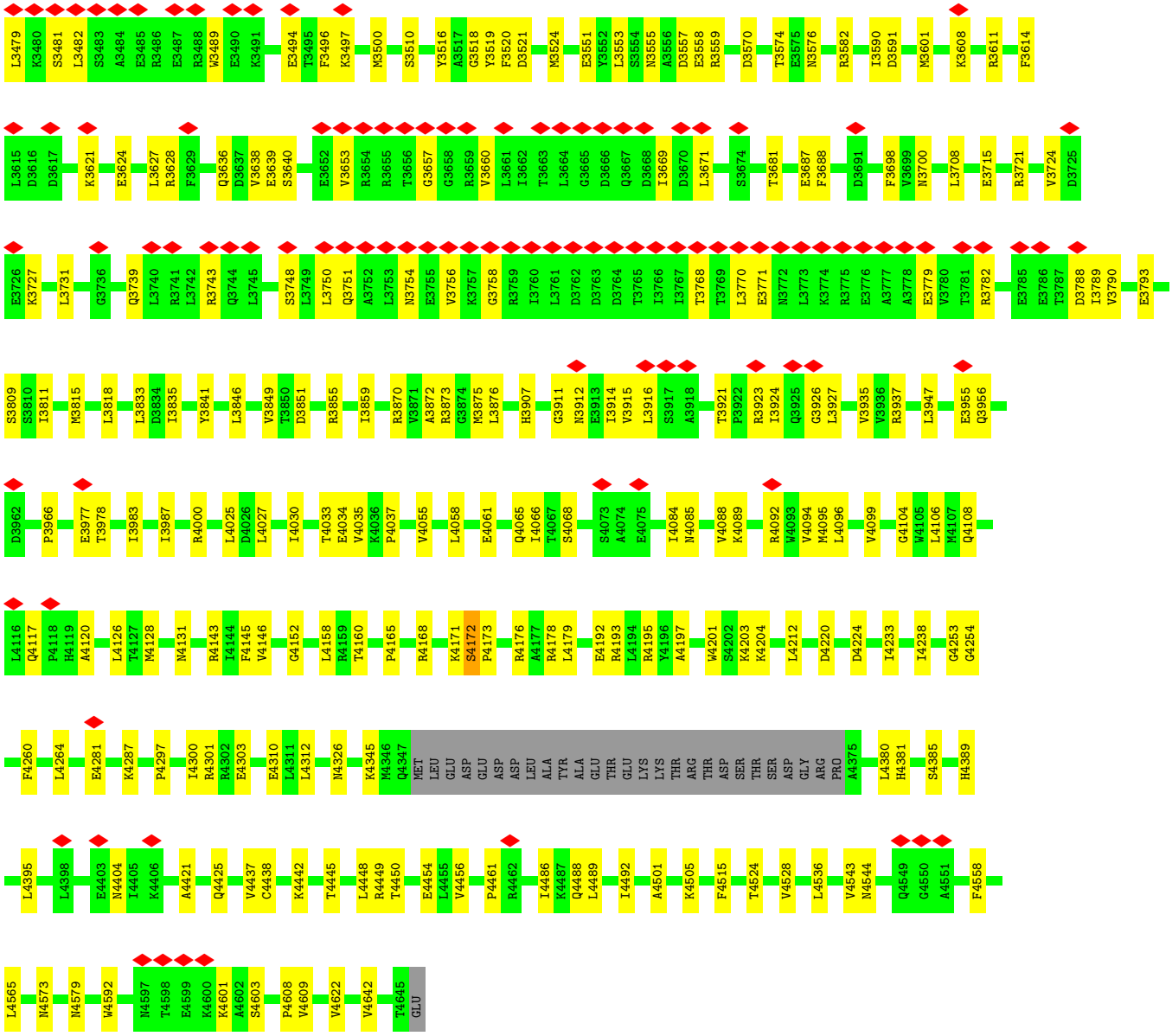
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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






V2185 E2188 T2192 Q2209 I2213 H2218 S2226 G2227 S2231 W2234 E2242 R2243 L2244 E2245 E2248 K2257 D2262 D2269 P2270 N2271 T2272 R2273 E2274 L2279 F2280 T2281 H2282 V2283 I2287 S2290 V2291 R2292 G2293 E2294 K2297 R2298 Q2299 D2304 V2307 D2308
P2309 E2310 W2311 D2320 K2323 L2324 L2325 E2331 R2332 L2333 S2334 L2335 P2336 V2339 R2340 Q2346 D2347 L2348 K2349 T2352 R2358 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 P2411 A2420 T2421
I2422 L2437 A2440 F2441 Q2442 L2443 I2446 L2452 S2457 M2461 A2465 E2487 R2492 Y2493 L2494 V2495 Y2496 A2497 S2501 D2505 M2510 Y2517 I2521 V2524 P2525 I2534 E2538 W2548 E2558 T2559 H2560 A2564 P2565 D2566 V2567 V2568 V2569 D2573
R2576 H2577 E2578 L2581 Y2582 T2583 P2590 L2591 V2592 G2595 T2602 M2603 T2604 L2605 F2606 S2607 R2610 S2623 T2626 T2627 P2628 E2629 R2642 R2643 T2644 P2645 V2648 G2656 K2657 W2658 F2662 C2663 D2664 E2665 I2666 D2670 R2678 F2682 I2683 R2684 R2694 D2697 Q2698
V2701 E2704 R2705 V2709 G2710 A2711 C2712 N2713 P2714 R2720 K2721 R2726 V2731 P2732 V2733 I2747 Y2748 N2752 R2753 A2754 R2757 L2758 I2759 L2762 R2763 E2767 T2770 R2783 F2784 H2791 R2797 E2798 M2799 T2800 R2801 A2809 L2813 E2814 T2815 L2816 P2817 V2818 E2819 G2820
L2821 I2822 R2823 I2824 E2828 R2836 L2837 E2841 E2842 R2843 R2844 W2845 E2848 N2849 I2850 D2851 T2852 L2855 K2856 I2861 D2862 R2863 E2864 K2865 A2866 M2867 S2868 R2869 L2872 D2880 E2888 L2889 R2890 V2893 L2897 K2898 Y2901 E2902 E2903 E2904 L2905 D2906 L2909 V2910 L2911 F2912 N2913
E2914 V2915 L2916 V2919 L2920 R2921 I2922 D2923 R2924 I2925 Q2930 G2931 H2932 L2933 L2934 L2935 K2943 T2944 T2945 V2950 V2958 Y2959 Q2960 I2961 K2962 V2963 H2964 R2965 T2968 G2969 F2972 D2973 E2974 D2975 L2976 R2977 T2978 V2979 L2980 R2981 R2982 S2983 G2984 C2985 K2986 N2987 E2988 F2992 I2993 M2994 D2995 E2996
S2997 N2998 V2999 L3000 D3001 S3002 G3003 F3004 L3005 E3006 R3007 T3010 L3011 L3012 A3013 N3014 G3015 L3020 F3021 E3022 E3025 Y3026 L3029 M3030 C3033 K3034 E3035 G3036 A3037 Q3038 K3039 E3040 G3041 L3042 M3043 L3044 D3045 S3046 H3047 E3048 E3049 L3050 W3053 F3054 T3055 S3056 Q3057 V3058 I3059 R3060 N3061 L3062 H3063 V3064
V3065 F3066 T3067 M3068 N3069 P3070 SER SER GLU GLY LEU LYS ASP ARG ALA ALA THR S3082 L3085 F3086 N3087 V3090 L3091 N3092 W3093 F3094 G3095 D3096 W3097 S3098 T3099 V3105 M3113 D3114 L3115 D3124 Y3125 V3128 V3129 L3133 P3134 Q3135 P3136 P3137 S3138 H3139 R3140 E3141 A3142 I3143 V3144 F3149
V3150 H3151 L3154 N3158 A3162 G3166 R3167 T3168 M3169 A3170 I3171 L3194 E3195 E3196 Q3197 Q3198 M3199 H3200 V3203 G3204 L3205 R3206 K3207 I3208 K3209 E3210 T3211 V3212 D3213 Q3214 V3215 E3216 E3217 L3218 R3219 R3220 ASP LEU ARG ILE LYS SER GLN GLU LEU GLU VAL LYS ASN ALA ALA ASN ASP
LYS LEU LYS LYS MET VAL LYS ASP GLN GLN GLU ALA GLU LYS LYS LYS PRO LYS VAL MET SER GLN GLU ILE GLU 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 ALA ILE GLU ALA GLN ASN ALA VAL LYS SER
ILE LYS LYS GLN HIS LEU VAL GLU VAL ARG SER MET ALA GLU LYS ASN PRO PRO ALA ALA VAL LYS LEU ALA LEU GLU GLN 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 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 ARG LEU ASN TYR ALA ASP MET LEU LYS ARG VAL ARG ASN GLU LEU GLN LYS
LEU GLU ASP ASP ALA LYS ASP ASN GLN GLN LYS ALA ASN GLU VAL GLU GLN MET ILE ARG ASP LEU GLU GLU ALA SER ILE ALA ARG TYR LYS GLU GLU TYR ALA VAL LEU ILE SER GLU ALA GLN ALA ILE LYS ALA ASP LEU ALA ALA VAL GLU K3471 V3472 N3473 R3474 S3475 T3476 A3477 L3478


L3479 K3480 S3481 L3482 S3483 A3484 E3485 R3486 E3487 R3488 W3489 E3490 K3491 E3494 T3495 F3496 K3497 M3500 S3510 Y3516 A3517 G3518 Y3519 F3520 D3521 M3524 E3551 Y3552 L3553 S3554 N3555 A3556 D3557 E3558 R3559 D3570 T3574 E3575 N3576 R3582 I3590 D3591 M3601 K3608 R3611 F3614
L3615 D3616 D3617 K3621 E3624 L3627 R3628 F3629 Q3636 D3637 V3638 E3639 S3640 E3652 V3653 R3654 R3655 T3656 G3657 G3658 R3659 V3660 L3661 I3662 T3663 L3664 G3665 D3666 Q3667 D3668 I3669 D3670 L3671 S3674 T3681 E3687 F3688 D3691 F3698 V3699 N3700 L3708 E3715 R3721 V3724 D3725
E3726 K3727 L3731 G3736 Q3739 L3740 R3741 L3742 R3743 Q3744 L3745 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 E3785 E3786 T3787 D3788 I3789 V3790 E3793
S3809 S3810 I3811 M3815 L3818 L3833 D3834 I3835 Y3841 L3846 V3849 T3850 D3851 R3855 I3859 R3870 V3871 A3872 R3873 G3874 M3875 L3876 H3907 G3911 N3912 E3913 I3914 V3915 L3916 S3917 A3918 T3921 P3922 R3923 I3924 Q3925 G3926 L3927 V3935 V3936 R3937 L3947 E3955 Q3956
D3962 P3966 E3977 T3978 I3983 I3987 R4000 L4025 D4026 L4027 I4030 T4033 E4034 V4035 K4036 P4037 V4055 L4058 E4061 Q4065 I4066 T4067 S4068 S4073 A4074 E4075 I4084 N4085 V4088 K4089 R4092 W4093 V4094 M4095 L4096 V4099 G4104 W4105 L4106 M4107 Q4108
L4116 Q4117 P4118 H4119 A4120 L4126 T4127 M4128 N4131 R4143 I4144 F4145 V4146 G4152 L4158 R4159 T4160 P4165 R4168 K4171 S4172 P4173 R4176 A4177 R4178 L4179 E4192 R4193 L4194 R4195 Y4196 A4197 W4201 S4202 K4203 K4204 L4212 D4220 D4224 I4233 I4238 G4253 G4254
F4260 L4264 E4281 K4287 P4297 I4300 R4301 R4302 E4303 E4310 L4311 L4312 N4326 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 PRO A4375 L4380 H4381 S4385 H4389
L4395 L4398 E4403 N4404 I4405 K4406 A4421 Q4425 V4437 C4438 K4442 T4445 L4448 R4449 T4450 E4454 L4455 V4456 P4461 R4462 I4486 K4487 Q4488 L4489 I4492 A4501 K4505 F4515 T4524 V4528 L4536 V4543 N4544 Q4549 G4550 A4551 F4558
L4565 N4573 N4579 W4592 N4597 T4598 E4599 K4600 K4601 A4602 S4603 P4608 V4609 V4622 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	66325	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.908	Depositor
Minimum map value	-0.483	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	332.80002, 332.80002, 332.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.26	0/24619	0.48	0/33363

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	24104	0	24208	463	0
2	A	54	0	24	0	0
3	A	62	0	24	2	0
All	All	24220	0	24256	463	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 10.

All (463) 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:1448:ASP:OD1	1:A:3657:GLY:HA3	1.42	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1448:ASP:OD1	1:A:3657:GLY:CA	1.98	1.12
1:A:3151:HIS:HD1	1:A:3516:TYR:HH	1.18	0.90
1:A:1504:VAL:HA	1:A:1507:MET:SD	2.21	0.80
1:A:4068:SER:HA	1:A:4095:MET:HB3	1.66	0.78
1:A:3015:GLY:HA3	1:A:3059:ILE:HG22	1.68	0.76
1:A:3037:ALA:HB1	1:A:3042:LEU:HB2	1.69	0.74
1:A:2665:GLU:OE1	1:A:2720:ARG:NH1	2.21	0.73
1:A:3128:VAL:HG21	1:A:3149:PHE:HB2	1.71	0.72
1:A:4176:ARG:NH1	1:A:4220:ASP:OD1	2.23	0.71
1:A:2930:GLN:HE22	1:A:3090:VAL:HG23	1.56	0.71
1:A:2814:GLU:HG3	1:A:2815:THR:HG23	1.74	0.70
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	1.73	0.69
1:A:2922:ILE:HG12	1:A:2933:LEU:HD21	1.74	0.69
1:A:3519:TYR:HA	1:A:3700:ASN:HB2	1.73	0.69
1:A:2443:LEU:HD23	1:A:2510:MET:HB3	1.75	0.68
1:A:1504:VAL:HG11	1:A:1524:GLU:HB2	1.76	0.68
1:A:2888:GLU:OE1	1:A:2888:GLU:N	2.24	0.68
1:A:2965:ARG:NH2	1:A:3640:SER:O	2.28	0.67
1:A:2320:ASP:HB3	1:A:2358:ARG:HD3	1.75	0.67
1:A:2969:GLY:HA2	1:A:3004:PHE:HE1	1.60	0.66
1:A:2299:GLN:HB2	1:A:2339:VAL:HG22	1.78	0.66
1:A:2933:LEU:HB3	1:A:3065:VAL:HG12	1.78	0.65
1:A:3034:LYS:HD3	1:A:3044:LEU:HD13	1.78	0.65
1:A:3977:GLU:HG3	1:A:3978:THR:HG23	1.79	0.65
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.79	0.65
1:A:4176:ARG:NH2	1:A:4224:ASP:OD2	2.25	0.65
1:A:2801:ARG:NH2	1:A:3087:ASN:O	2.30	0.65
1:A:3727:LYS:HE2	1:A:3790:VAL:HG13	1.79	0.64
1:A:4437:VAL:HG21	1:A:4448:LEU:HD21	1.79	0.64
1:A:2670:ASP:HA	1:A:2721:LYS:HE3	1.80	0.64
1:A:2813:LEU:HD21	1:A:2816:LEU:HD13	1.78	0.64
1:A:2925:ILE:HG13	1:A:2933:LEU:HD13	1.78	0.64
1:A:3005:LEU:HD11	1:A:3085:LEU:HD22	1.78	0.64
1:A:2605:LEU:HD11	1:A:2709:VAL:HG11	1.79	0.64
1:A:1459:LEU:HB2	1:A:1516:PHE:CE2	2.33	0.64
1:A:3553:LEU:O	1:A:3582:ARG:NH1	2.31	0.64
1:A:1887:ARG:NH2	1:A:4253:GLY:O	2.32	0.63
1:A:3924:ILE:HG22	1:A:3927:LEU:HD23	1.80	0.63
1:A:1483:LYS:NZ	1:A:1548:GLU:OE2	2.30	0.63
1:A:2828:GLU:OE1	1:A:2924:ARG:NH2	2.27	0.63
1:A:2897:LEU:HD21	1:A:2909:LEU:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2925:ILE:HG21	1:A:2933:LEU:HB2	1.79	0.63
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.31	0.63
1:A:2643:ARG:O	1:A:2643:ARG:NH1	2.32	0.62
1:A:3167:ARG:HE	1:A:3167:ARG:HA	1.63	0.62
1:A:1448:ASP:HB2	1:A:3657:GLY:HA2	1.81	0.62
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.80	0.62
1:A:2495:VAL:HG21	1:A:2524:VAL:HG11	1.80	0.62
1:A:2346:GLN:HB2	1:A:2726:ARG:HD2	1.82	0.61
1:A:3043:MET:SD	1:A:3044:LEU:N	2.73	0.61
1:A:3924:ILE:HG23	1:A:3926:GLY:H	1.65	0.61
1:A:4172:SER:HB3	1:A:4173:PRO:HD2	1.82	0.61
1:A:2963:VAL:HG22	1:A:2998:ASN:HD22	1.65	0.61
1:A:2980:LEU:O	1:A:2984:GLY:N	2.30	0.61
1:A:2592:VAL:HB	1:A:2733:VAL:HG12	1.80	0.61
1:A:4281:GLU:OE2	1:A:4281:GLU:N	2.34	0.61
1:A:1509:LEU:O	1:A:3628:ARG:NH1	2.33	0.61
1:A:3551:GLU:OE1	1:A:3551:GLU:N	2.29	0.61
1:A:2783:ARG:HG2	1:A:2784:PHE:H	1.65	0.61
1:A:1408:LEU:HD13	1:A:1412:HIS:HB2	1.82	0.60
1:A:2965:ARG:HH22	1:A:3614:PHE:HB3	1.66	0.60
1:A:1619:LEU:HD22	1:A:1637:LEU:HD23	1.83	0.60
1:A:1420:LEU:HD13	1:A:1437:VAL:HG11	1.84	0.60
1:A:2605:LEU:HD23	1:A:2662:PHE:HE2	1.65	0.60
1:A:2963:VAL:HG21	1:A:2998:ASN:HA	1.83	0.60
1:A:4395:LEU:HD23	1:A:4486:ILE:HG23	1.83	0.60
1:A:3167:ARG:NH2	1:A:3687:GLU:OE1	2.35	0.60
1:A:1486:LEU:HD22	1:A:1541:GLN:HG3	1.83	0.60
1:A:1396:ILE:O	1:A:1400:VAL:HG23	2.02	0.60
1:A:1448:ASP:OD1	1:A:3657:GLY:HA2	1.96	0.60
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.82	0.59
1:A:4385:SER:O	1:A:4389:HIS:ND1	2.33	0.59
1:A:3835:ILE:HG12	1:A:3870:ARG:HD3	1.84	0.59
1:A:1728:GLY:O	1:A:1784:ASN:ND2	2.35	0.59
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.35	0.59
1:A:3158:ASN:ND2	1:A:3169:MET:O	2.35	0.59
1:A:4084:ILE:HG22	1:A:4094:VAL:HG11	1.84	0.59
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	1.84	0.59
1:A:2977:ARG:NH1	1:A:3020:LEU:O	2.36	0.59
1:A:2791:HIS:HD2	1:A:2836:ARG:HG2	1.67	0.58
1:A:2245:GLU:OE1	1:A:2298:ARG:NH2	2.31	0.58
1:A:2823:ARG:HD3	1:A:2865:LYS:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3044:LEU:HD12	1:A:3050:LEU:HD11	1.83	0.58
1:A:3046:SER:HB3	1:A:3049:GLU:HB2	1.85	0.58
1:A:2930:GLN:HG2	1:A:2931:GLY:H	1.68	0.58
1:A:2996:GLU:HB2	1:A:3068:MET:HG3	1.85	0.58
1:A:3134:PRO:HG2	1:A:3137:PRO:HA	1.86	0.58
1:A:2919:VAL:HG13	1:A:2950:VAL:HG22	1.85	0.58
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.69	0.58
1:A:1332:VAL:HB	1:A:1377:LEU:HD22	1.85	0.57
1:A:2642:ARG:NH2	1:A:2704:GLU:OE2	2.37	0.57
1:A:1506:ALA:HA	1:A:1509:LEU:HD12	1.86	0.57
1:A:2889:LEU:HD21	1:A:2920:LEU:HD21	1.86	0.57
1:A:2978:THR:O	1:A:2981:ARG:HG2	2.04	0.57
1:A:4033:THR:HG23	1:A:4034:GLU:HG3	1.86	0.57
1:A:2958:VAL:HG13	1:A:2993:ILE:HD12	1.86	0.57
1:A:2960:GLN:HG2	1:A:2993:ILE:HB	1.86	0.57
1:A:4601:LYS:HE2	1:A:4603:SER:HB3	1.86	0.57
1:A:2227:GLY:HA2	1:A:2452:LEU:HD12	1.85	0.57
1:A:4524:THR:HG23	1:A:4558:PHE:CD2	2.40	0.57
1:A:1699:ASN:OD1	1:A:1700:GLU:N	2.38	0.56
1:A:4233:ILE:HD11	1:A:4238:ILE:HD13	1.87	0.56
1:A:4037:PRO:HG3	1:A:4120:ALA:HA	1.86	0.56
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.87	0.56
1:A:3727:LYS:NZ	1:A:3793:GLU:OE1	2.39	0.56
1:A:3921:THR:OG1	1:A:3923:ARG:NE	2.39	0.56
1:A:1853:VAL:HG23	1:A:1854:LEU:HD12	1.88	0.56
1:A:1606:ASP:OD1	1:A:1607:LEU:N	2.39	0.56
1:A:3907:HIS:HA	1:A:3911:GLY:HA3	1.87	0.56
1:A:3628:ARG:HH12	1:A:3669:ILE:HG23	1.71	0.55
1:A:2325:LEU:HD23	1:A:2333:LEU:HD12	1.88	0.55
1:A:2192:THR:H	3:A:4702:ATP:HN61	1.54	0.55
1:A:2752:ASN:OD1	1:A:2770:THR:OG1	2.18	0.55
1:A:2922:ILE:HD11	1:A:2935:LEU:HD11	1.87	0.55
1:A:3115:LEU:HD23	1:A:3143:ILE:HG13	1.88	0.55
1:A:4099:VAL:HG22	1:A:4128:MET:HB3	1.87	0.55
1:A:2149:LEU:HD11	1:A:2157:LEU:HD22	1.89	0.55
1:A:3621:LYS:HA	1:A:3624:GLU:OE2	2.07	0.55
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.89	0.55
1:A:3194:LEU:HD22	1:A:3500:MET:SD	2.47	0.54
1:A:4543:VAL:HG21	1:A:4622:VAL:HG12	1.88	0.54
1:A:3000:LEU:H	1:A:3004:PHE:HD2	1.53	0.54
1:A:3779:GLU:OE2	1:A:3782:ARG:NH1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1640:ILE:HG23	1:A:1650:LEU:HD21	1.88	0.54
1:A:2866:ALA:O	1:A:2869:ARG:NH2	2.41	0.54
1:A:2872:LEU:HD13	1:A:2920:LEU:HD11	1.89	0.54
1:A:1509:LEU:HD22	1:A:3624:GLU:HG3	1.89	0.54
1:A:2492:ARG:HH12	1:A:2525:PRO:HB2	1.73	0.54
1:A:2581:LEU:HG	1:A:2591:LEU:HD11	1.90	0.54
1:A:1329:LEU:HD12	1:A:1329:LEU:H	1.73	0.54
1:A:2994:MET:HB3	1:A:3066:PHE:HD1	1.73	0.54
1:A:1461:GLU:O	1:A:1465:GLN:HG3	2.08	0.54
1:A:2040:ALA:N	1:A:4254:GLY:O	2.41	0.54
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.91	0.53
1:A:1448:ASP:CB	1:A:3657:GLY:HA2	2.38	0.53
1:A:4505:LYS:HG2	1:A:4558:PHE:CE1	2.43	0.53
1:A:2819:GLU:HB3	1:A:2865:LYS:HD2	1.90	0.53
1:A:4192:GLU:OE1	1:A:4195:ARG:NE	2.32	0.53
1:A:3154:LEU:HG	1:A:3516:TYR:CD1	2.43	0.53
1:A:4201:TRP:O	1:A:4203:LYS:N	2.41	0.53
1:A:1349:GLN:NE2	1:A:1353:SER:O	2.42	0.53
1:A:3113:MET:O	1:A:3140:ARG:NH2	2.42	0.53
1:A:2841:GLU:OE2	1:A:2844:ARG:NH1	2.41	0.53
1:A:3133:LEU:HB3	1:A:3134:PRO:HD3	1.90	0.53
1:A:3011:LEU:O	1:A:3015:GLY:N	2.41	0.52
1:A:1505:SER:O	1:A:1509:LEU:HG	2.08	0.52
1:A:2248:GLU:HB3	1:A:2297:LYS:HG2	1.91	0.52
1:A:4065:GLN:HE21	1:A:4092:ARG:HD3	1.74	0.52
1:A:1407:ALA:HA	1:A:1457:MET:SD	2.50	0.52
1:A:3639:GLU:OE2	1:A:3681:THR:OG1	2.27	0.52
1:A:2851:ASP:OD1	1:A:2852:THR:N	2.43	0.52
1:A:1513:TYR:CZ	1:A:1517:GLU:HG2	2.45	0.52
1:A:2281:THR:HG22	1:A:2325:LEU:HD21	1.92	0.52
1:A:2573:ASP:O	1:A:2577:HIS:ND1	2.43	0.52
1:A:2845:TRP:O	1:A:2849:ASN:ND2	2.41	0.52
1:A:1709:MET:O	1:A:1713:LEU:HD23	2.10	0.52
1:A:1937:ASP:OD1	1:A:1937:ASP:N	2.42	0.52
1:A:2558:GLU:HG3	1:A:2560:HIS:H	1.74	0.52
1:A:2992:PHE:HD2	1:A:3064:VAL:HG23	1.75	0.52
1:A:4178:ARG:NH2	1:A:4297:PRO:O	2.43	0.52
1:A:2242:GLU:HG3	1:A:2248:GLU:HA	1.90	0.51
1:A:3591:ASP:N	1:A:3591:ASP:OD1	2.42	0.51
1:A:1882:THR:HG22	1:A:2048:LEU:HD23	1.91	0.51
1:A:3739:GLN:N	1:A:3739:GLN:OE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3653:VAL:HG13	1:A:3660:VAL:HG23	1.93	0.51
1:A:3873:ARG:HD2	1:A:4025:LEU:HD13	1.93	0.51
1:A:2662:PHE:CZ	1:A:2664:ASP:HB3	2.46	0.51
1:A:3557:ASP:OD1	1:A:3558:GLU:N	2.44	0.51
1:A:1374:PRO:HD2	1:A:1377:LEU:HD12	1.93	0.51
1:A:3208:ILE:HD12	1:A:3489:TRP:CH2	2.47	0.50
1:A:3033:CYS:SG	1:A:3054:PHE:HB2	2.51	0.50
1:A:4489:LEU:HD11	1:A:4515:PHE:HE2	1.77	0.50
1:A:4524:THR:HG22	1:A:4592:TRP:CD1	2.46	0.50
1:A:1907:PRO:HD2	1:A:2042:THR:HA	1.93	0.50
1:A:1438:ASP:HB3	1:A:1441:LYS:HB3	1.94	0.50
1:A:2382:LEU:HD23	1:A:2420:ALA:HB2	1.94	0.50
1:A:1947:GLY:O	1:A:1951:VAL:HG12	2.12	0.50
1:A:3057:GLN:OE1	1:A:3060:ARG:NH2	2.44	0.50
1:A:3519:TYR:HB2	1:A:3698:PHE:HB3	1.94	0.50
1:A:1454:GLN:HA	1:A:1457:MET:HE2	1.94	0.50
1:A:1548:GLU:O	1:A:1552:THR:OG1	2.22	0.50
1:A:1747:ALA:HB2	1:A:1807:LYS:HG2	1.92	0.50
1:A:2935:LEU:O	1:A:3067:THR:HA	2.12	0.50
1:A:4088:VAL:HG21	1:A:4117:GLN:OE1	2.12	0.50
1:A:4300:ILE:HG23	1:A:4301:ARG:HG3	1.94	0.50
1:A:1751:VAL:O	1:A:1755:GLN:HG3	2.11	0.50
1:A:2446:ILE:HD11	1:A:2714:PRO:HG3	1.93	0.50
1:A:3494:GLU:HA	1:A:3497:LYS:HE3	1.93	0.50
1:A:3955:GLU:HG2	1:A:3956:GLN:OE1	2.12	0.50
1:A:2279:LEU:HA	1:A:2698:GLN:HG2	1.94	0.49
1:A:2934:LEU:HD12	1:A:3066:PHE:O	2.12	0.49
1:A:3162:ALA:HA	1:A:3166:GLY:HA2	1.93	0.49
1:A:3715:GLU:OE2	1:A:3841:TYR:OH	2.25	0.49
1:A:4565:LEU:HD13	1:A:4642:VAL:HG22	1.94	0.49
1:A:2898:LYS:HA	1:A:2901:TYR:CE1	2.47	0.49
1:A:2987:ASN:OD1	1:A:3057:GLN:NE2	2.45	0.49
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.46	0.49
1:A:1460:GLU:HB2	1:A:1516:PHE:CE1	2.47	0.49
1:A:2440:ALA:HA	1:A:2443:LEU:HD13	1.95	0.49
1:A:2694:ARG:NH2	1:A:2697:ASP:OD2	2.42	0.49
1:A:3921:THR:HG1	1:A:3923:ARG:HE	1.60	0.49
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.93	0.48
1:A:3721:ARG:HE	1:A:3724:VAL:HG21	1.78	0.48
1:A:4099:VAL:HG23	1:A:4106:LEU:HD11	1.95	0.48
1:A:1416:LEU:HG	1:A:1449:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2283:VAL:O	1:A:2287:ILE:HG13	2.13	0.48
1:A:3115:LEU:H	1:A:3140:ARG:HH21	1.59	0.48
1:A:2863:ARG:HG3	1:A:2867:MET:HB2	1.95	0.48
1:A:1509:LEU:HB3	1:A:3628:ARG:NH2	2.28	0.48
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.96	0.48
1:A:2753:ARG:O	1:A:2757:ARG:HG3	2.14	0.48
1:A:2461:MET:HG2	1:A:2583:THR:HG21	1.95	0.48
1:A:2852:THR:O	1:A:2856:LYS:HG2	2.13	0.48
1:A:2656:GLY:H	1:A:2705:ARG:HH11	1.62	0.48
1:A:2932:HIS:HB2	1:A:3012:LEU:HG	1.95	0.48
1:A:4168:ARG:NH2	1:A:4220:ASP:OD2	2.46	0.48
1:A:1507:MET:O	1:A:1513:TYR:HB2	2.14	0.48
1:A:1698:ILE:HD12	1:A:1701:TRP:NE1	2.28	0.48
1:A:2568:VAL:HG22	1:A:2603:MET:SD	2.54	0.48
1:A:3030:MET:SD	1:A:3047:HIS:HB3	2.54	0.48
1:A:3055:THR:O	1:A:3059:ILE:HG23	2.13	0.48
1:A:2999:VAL:HG13	1:A:3004:PHE:HB2	1.95	0.48
1:A:3611:ARG:NH2	1:A:3636:GLN:OE1	2.46	0.48
1:A:2602:THR:HG23	1:A:2662:PHE:CZ	2.49	0.47
1:A:2694:ARG:NE	1:A:2697:ASP:OD1	2.44	0.47
1:A:3037:ALA:O	1:A:3042:LEU:N	2.45	0.47
1:A:4380:LEU:HD21	1:A:4456:VAL:HG12	1.97	0.47
1:A:2921:ARG:O	1:A:2925:ILE:HG12	2.15	0.47
1:A:1350:PRO:HA	1:A:1430:THR:HA	1.97	0.47
1:A:2386:PRO:C	1:A:2388:ASP:H	2.18	0.47
1:A:2648:VAL:HB	1:A:2701:VAL:HG12	1.96	0.47
1:A:4165:PRO:HD2	1:A:4168:ARG:HD3	1.97	0.47
1:A:4287:LYS:O	1:A:4287:LYS:HD3	2.14	0.47
1:A:1408:LEU:HB3	1:A:1413:TRP:CD1	2.49	0.47
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.97	0.47
1:A:2290:SER:HA	1:A:2294:GLU:OE2	2.14	0.47
1:A:2623:SER:N	1:A:2626:THR:OG1	2.47	0.47
1:A:2809:ALA:HB1	1:A:2824:ILE:HD13	1.96	0.47
1:A:2931:GLY:O	1:A:3064:VAL:HG12	2.14	0.47
1:A:2992:PHE:HB3	1:A:3064:VAL:HG23	1.95	0.47
1:A:3601:MET:CE	1:A:3611:ARG:HG2	2.44	0.47
1:A:3846:LEU:HD11	1:A:3859:ILE:HG13	1.96	0.47
1:A:3478:LEU:O	1:A:3482:LEU:HD23	2.15	0.47
1:A:2292:ARG:HB3	1:A:2292:ARG:NH1	2.30	0.47
1:A:3914:ILE:O	1:A:3937:ARG:NE	2.48	0.47
1:A:1713:LEU:CD1	1:A:1749:LEU:HD21	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4197:ALA:HB2	1:A:4204:LYS:HE3	1.96	0.47
1:A:4437:VAL:HG21	1:A:4448:LEU:CD2	2.45	0.47
1:A:1509:LEU:HD13	1:A:3624:GLU:HG3	1.96	0.46
1:A:2912:PHE:CE1	1:A:2915:VAL:HG23	2.50	0.46
1:A:2628:PRO:HB3	1:A:2682:PHE:CD2	2.50	0.46
1:A:3876:LEU:HD23	1:A:4146:VAL:HG11	1.97	0.46
1:A:4193:ARG:NH2	1:A:4264:LEU:HD11	2.30	0.46
1:A:1571:ILE:HG23	1:A:1604:LEU:HD22	1.97	0.46
1:A:2658:TRP:CE3	1:A:2705:ARG:HA	2.50	0.46
1:A:3756:VAL:HG23	1:A:3758:GLY:H	1.79	0.46
1:A:3608:LYS:HE3	1:A:3608:LYS:HB2	1.65	0.46
1:A:1667:ASN:HB2	1:A:1672:VAL:HG22	1.96	0.46
1:A:1968:LEU:HD21	1:A:2029:PRO:HG3	1.98	0.46
1:A:2837:LEU:HD23	1:A:2842:GLU:CB	2.45	0.46
1:A:3731:LEU:HD11	1:A:3790:VAL:HG12	1.98	0.46
1:A:4055:VAL:HA	1:A:4058:LEU:HG	1.98	0.46
1:A:4104:GLY:O	1:A:4108:GLN:HG2	2.15	0.46
1:A:2218:HIS:HA	1:A:2340:ARG:HD2	1.98	0.46
1:A:2757:ARG:HG2	1:A:2763:ARG:HE	1.80	0.46
1:A:2335:LEU:HD12	1:A:2336:PRO:HD2	1.98	0.46
1:A:4096:LEU:HB2	1:A:4126:LEU:HD23	1.98	0.46
1:A:1351:TRP:CE3	1:A:1434:ILE:HD12	2.51	0.46
1:A:1917:LYS:HD2	1:A:1929:VAL:HG21	1.97	0.46
1:A:2079:GLN:HB2	1:A:2160:LEU:HD11	1.98	0.46
1:A:2890:ARG:NH1	1:A:2911:LEU:O	2.49	0.46
1:A:2837:LEU:HD23	1:A:2842:GLU:HB3	1.98	0.46
1:A:1695:HIS:HB3	1:A:1700:GLU:HG3	1.97	0.45
1:A:3471:LYS:HB3	1:A:3474:ARG:HD3	1.98	0.45
1:A:3751:GLN:HA	1:A:3754:ASN:HD21	1.81	0.45
1:A:3956:GLN:OE1	1:A:3956:GLN:N	2.49	0.45
1:A:4035:VAL:HG22	1:A:4143:ARG:HG3	1.99	0.45
1:A:4152:GLY:N	1:A:4192:GLU:OE2	2.37	0.45
1:A:4454:GLU:OE2	1:A:4461:PRO:HA	2.15	0.45
1:A:1899:ARG:HG3	1:A:1986:SER:HB3	1.99	0.45
1:A:2974:GLU:OE1	1:A:2977:ARG:NH2	2.42	0.45
1:A:4058:LEU:HA	1:A:4061:GLU:HG2	1.98	0.45
1:A:2070:VAL:HB	1:A:2071:PRO:HD3	1.97	0.45
1:A:2534:ILE:HD12	1:A:2534:ILE:H	1.81	0.45
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.98	0.45
1:A:2304:ASP:OD1	1:A:2684:ARG:NH1	2.39	0.45
1:A:2880:ASP:OD1	1:A:2880:ASP:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3748:SER:O	1:A:3751:GLN:HG2	2.16	0.45
1:A:3788:ASP:OD1	1:A:3789:ILE:N	2.49	0.45
1:A:2973:ASP:HB3	1:A:3020:LEU:HD22	1.98	0.45
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.52	0.45
1:A:3768:THR:O	1:A:3771:GLU:HG3	2.17	0.45
1:A:1741:TRP:CH2	1:A:1750:VAL:HG13	2.52	0.45
1:A:2271:ASN:OD1	1:A:2272:THR:N	2.50	0.45
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	1.99	0.45
1:A:2569:VAL:HB	1:A:2747:ILE:HG13	1.98	0.45
1:A:2932:HIS:ND1	1:A:3012:LEU:HD11	2.32	0.45
1:A:2759:ILE:HD12	1:A:2762:LEU:HD12	1.99	0.45
1:A:2903:GLU:O	1:A:2904:GLU:HB2	2.16	0.45
1:A:2665:GLU:N	1:A:2711:ALA:O	2.50	0.44
1:A:2889:LEU:O	1:A:2893:VAL:HG12	2.16	0.44
1:A:1618:TYR:O	1:A:1621:ARG:HG2	2.18	0.44
1:A:1697:LYS:HB3	1:A:1700:GLU:HG2	1.99	0.44
1:A:2623:SER:N	1:A:2626:THR:HG1	2.14	0.44
1:A:2748:TYR:CD2	1:A:2799:MET:HE2	2.52	0.44
1:A:2890:ARG:NH2	1:A:2913:ASN:OD1	2.51	0.44
1:A:4301:ARG:NH1	1:A:4303:GLU:OE1	2.50	0.44
1:A:1789:LEU:HG	1:A:1815:LEU:HB3	2.00	0.44
1:A:2457:SER:HB3	1:A:2732:PRO:HB3	1.99	0.44
1:A:3198:GLN:HG3	1:A:3496:PHE:HD2	1.82	0.44
1:A:3811:ILE:O	1:A:3815:MET:HG3	2.18	0.44
1:A:3935:VAL:HG13	1:A:3947:LEU:HD23	1.99	0.44
1:A:1491:ASP:OD1	1:A:1492:ASP:N	2.50	0.44
1:A:2963:VAL:CG2	1:A:2998:ASN:HD22	2.31	0.44
1:A:1425:VAL:HB	1:A:1428:GLU:HB2	1.98	0.44
1:A:1546:TYR:CZ	1:A:1550:ILE:HD11	2.53	0.44
1:A:2497:ALA:O	1:A:2501:SER:OG	2.27	0.44
1:A:2844:ARG:O	1:A:2848:GLU:HG2	2.18	0.44
1:A:2905:LEU:HD21	1:A:2945:THR:HG23	1.99	0.44
1:A:4158:LEU:HD21	1:A:4310:GLU:HG3	2.00	0.44
1:A:1748:GLN:NE2	1:A:1868:TYR:OH	2.34	0.44
1:A:2797:ARG:O	1:A:2801:ARG:HG3	2.17	0.44
1:A:2862:ASP:OD1	1:A:2862:ASP:N	2.51	0.44
1:A:3034:LYS:O	1:A:3038:GLN:HG2	2.17	0.44
1:A:4027:LEU:H	1:A:4027:LEU:HD23	1.83	0.44
1:A:4404:ASN:ND2	1:A:4501:ALA:HB3	2.32	0.44
1:A:1987:ASN:HB2	1:A:1990:TYR:HB3	1.98	0.44
1:A:2257:LYS:O	1:A:2678:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2678:ARG:NH1	1:A:2678:ARG:HB2	2.32	0.44
1:A:3614:PHE:HE2	1:A:3638:VAL:HG23	1.83	0.44
1:A:1446:VAL:O	1:A:1450:LEU:HG	2.18	0.43
1:A:3555:ASN:HA	1:A:3559:ARG:HH21	1.82	0.43
1:A:1643:ASN:HD22	1:A:1649:LYS:HG3	1.83	0.43
1:A:2935:LEU:HD21	1:A:3092:ASN:HD22	1.83	0.43
1:A:3576:ASN:ND2	1:A:3700:ASN:O	2.49	0.43
1:A:4445:THR:O	1:A:4449:ARG:HG3	2.19	0.43
1:A:1350:PRO:O	1:A:1354:VAL:HG23	2.18	0.43
1:A:1355:GLN:HG3	1:A:1358:LYS:H	1.82	0.43
1:A:1477:LEU:HB3	1:A:1485:ARG:HB3	2.00	0.43
1:A:1628:ARG:NH1	1:A:1871:GLU:OE2	2.52	0.43
1:A:2915:VAL:O	1:A:2919:VAL:HG23	2.18	0.43
1:A:2943:LYS:NZ	1:A:3067:THR:HB	2.34	0.43
1:A:3849:VAL:HG12	1:A:3855:ARG:HG2	2.00	0.43
1:A:4066:ILE:HG21	1:A:4095:MET:HB2	1.99	0.43
1:A:1661:VAL:HG22	1:A:1676:ILE:HD12	1.99	0.43
1:A:2349:LYS:HB2	1:A:2349:LYS:HE2	1.67	0.43
1:A:2564:ALA:HB3	1:A:2567:VAL:HB	2.00	0.43
1:A:2605:LEU:HD23	1:A:2662:PHE:CE2	2.51	0.43
1:A:3140:ARG:O	1:A:3144:VAL:HG23	2.18	0.43
1:A:2642:ARG:HG2	1:A:2645:PRO:HD3	2.00	0.43
1:A:3099:THR:HG22	1:A:3129:VAL:HG22	2.00	0.43
1:A:1459:LEU:HD11	1:A:1512:TYR:HB2	1.99	0.43
1:A:3005:LEU:C	1:A:3007:ARG:H	2.22	0.43
1:A:1623:ARG:HB3	1:A:1630:TYR:CZ	2.54	0.43
1:A:2075:LEU:HD11	1:A:4536:LEU:HD22	2.01	0.43
1:A:3208:ILE:HD12	1:A:3489:TRP:HH2	1.82	0.43
1:A:3983:ILE:O	1:A:3987:ILE:HG12	2.19	0.43
1:A:4544:ASN:HA	1:A:4573:ASN:HD21	1.84	0.43
1:A:1459:LEU:CD1	1:A:1512:TYR:HB2	2.49	0.43
1:A:1715:LYS:HD3	1:A:1715:LYS:HA	1.84	0.43
1:A:1728:GLY:HA2	1:A:1784:ASN:HD21	1.84	0.43
1:A:2568:VAL:HG21	1:A:2607:SER:HB3	2.01	0.43
1:A:2992:PHE:CD2	1:A:3064:VAL:HG23	2.53	0.43
1:A:1419:ARG:HD2	1:A:1445:ILE:HG12	2.01	0.43
1:A:1964:GLU:CD	1:A:1964:GLU:H	2.22	0.43
1:A:2932:HIS:HE2	1:A:3066:PHE:HB3	1.84	0.43
1:A:2943:LYS:HG2	1:A:3094:PHE:CD2	2.54	0.43
1:A:3743:ARG:HD2	1:A:3743:ARG:HA	1.79	0.43
1:A:2628:PRO:HG2	1:A:2678:ARG:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4488:GLN:O	1:A:4492:ILE:HG12	2.18	0.42
1:A:2185:VAL:HA	1:A:2188:GLU:HG2	2.01	0.42
1:A:3169:MET:HG2	1:A:3519:TYR:CE2	2.54	0.42
1:A:3475:SER:O	1:A:3479:LEU:HD23	2.19	0.42
1:A:3851:ASP:O	1:A:3855:ARG:HG3	2.19	0.42
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	2.00	0.42
1:A:4172:SER:HB3	1:A:4173:PRO:CD	2.48	0.42
1:A:2559:THR:HG22	1:A:2754:ALA:O	2.19	0.42
1:A:2209:GLN:O	1:A:2213:ILE:HD12	2.19	0.42
1:A:3197:GLN:HB3	1:A:3496:PHE:HE2	1.84	0.42
1:A:1698:ILE:HD12	1:A:1701:TRP:HE1	1.83	0.42
1:A:2820:GLY:O	1:A:2824:ILE:HG13	2.20	0.42
1:A:2893:VAL:HG11	1:A:2916:LEU:HD13	2.00	0.42
1:A:3138:SER:OG	1:A:3139:HIS:N	2.53	0.42
1:A:3751:GLN:HA	1:A:3754:ASN:ND2	2.34	0.42
1:A:4179:LEU:HD23	1:A:4179:LEU:HA	1.89	0.42
1:A:2422:ILE:HD13	1:A:2487:GLU:HA	2.00	0.42
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.19	0.42
1:A:2666:ILE:HG22	1:A:2712:CYS:HB3	2.02	0.42
1:A:3627:LEU:O	1:A:3627:LEU:HD23	2.20	0.42
1:A:3916:LEU:HD23	1:A:3916:LEU:HA	1.94	0.42
1:A:4085:ASN:O	1:A:4089:LYS:HG2	2.20	0.42
1:A:4260:PHE:CE2	1:A:4608:PRO:HB3	2.54	0.42
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	2.01	0.42
1:A:1925:ARG:HE	1:A:2011:ASP:HB3	1.85	0.42
1:A:1999:CYS:SG	1:A:2001:LEU:HD23	2.59	0.42
1:A:2437:LEU:HG	1:A:2441:PHE:CE2	2.54	0.42
1:A:4421:ALA:O	1:A:4425:GLN:HG2	2.20	0.42
1:A:2856:LYS:HA	1:A:2856:LYS:HD3	1.82	0.42
1:A:3219:ARG:NH2	1:A:3479:LEU:HD21	2.34	0.42
1:A:4442:LYS:HE3	1:A:4442:LYS:HB2	1.87	0.42
1:A:1419:ARG:HG2	1:A:1445:ILE:HD13	2.00	0.42
1:A:2517:TYR:CE2	1:A:2521:ILE:HD13	2.55	0.42
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.55	0.42
1:A:3638:VAL:HG13	1:A:3688:PHE:HE1	1.85	0.42
1:A:4345:LYS:HB2	1:A:4345:LYS:HE3	1.79	0.42
1:A:1388:ARG:HA	1:A:1391:LYS:HE2	2.02	0.41
1:A:2548:TRP:CE2	1:A:2576:ARG:HG2	2.54	0.41
1:A:3010:THR:O	1:A:3014:ASN:HB2	2.20	0.41
1:A:4312:LEU:HD23	1:A:4312:LEU:HA	1.90	0.41
1:A:4524:THR:HG23	1:A:4558:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2713:ASN:OD1	1:A:2720:ARG:NH2	2.53	0.41
1:A:2791:HIS:HB3	1:A:3086:PHE:CD1	2.56	0.41
1:A:2980:LEU:HD23	1:A:3062:LEU:HD13	2.02	0.41
1:A:3660:VAL:HG22	1:A:3671:LEU:HB3	2.02	0.41
1:A:1645:LYS:HA	1:A:1645:LYS:HD3	1.70	0.41
1:A:1888:CYS:HA	1:A:2039:LEU:HD21	2.01	0.41
1:A:2076:CYS:O	1:A:2080:LEU:HB2	2.20	0.41
1:A:2307:VAL:HA	1:A:2311:TRP:HE1	1.85	0.41
1:A:2932:HIS:CD2	1:A:2933:LEU:N	2.88	0.41
1:A:3521:ASP:OD1	1:A:3521:ASP:N	2.52	0.41
1:A:3601:MET:HE1	1:A:3611:ARG:HG2	2.02	0.41
1:A:2030:ASP:OD2	1:A:4131:ASN:ND2	2.45	0.41
1:A:2309:PRO:HG3	1:A:2352:THR:HG23	2.02	0.41
1:A:1356:PRO:HB3	1:A:1401:ILE:HG12	2.01	0.41
1:A:1575:PHE:O	1:A:1579:MET:HG2	2.20	0.41
1:A:1698:ILE:HA	1:A:1701:TRP:CD1	2.55	0.41
1:A:1838:TRP:CZ2	1:A:1843:ARG:HG2	2.55	0.41
1:A:2910:VAL:HG11	1:A:3105:VAL:HG22	2.03	0.41
1:A:3570:ASP:O	1:A:3574:THR:HG23	2.21	0.41
1:A:3590:ILE:HA	1:A:3681:THR:HG22	2.03	0.41
1:A:1508:LYS:NZ	1:A:1524:GLU:HG2	2.35	0.41
1:A:2410:SER:N	1:A:2411:PRO:HD2	2.36	0.41
1:A:3815:MET:O	1:A:3818:LEU:HB2	2.21	0.41
1:A:3873:ARG:HD3	1:A:3873:ARG:HA	1.91	0.41
1:A:1405:SER:OG	1:A:1406:GLU:N	2.54	0.41
1:A:2822:ILE:HD13	1:A:2861:ILE:HD13	2.03	0.41
1:A:3915:VAL:HG13	1:A:3915:VAL:O	2.21	0.41
1:A:4450:THR:O	1:A:4454:GLU:HG3	2.21	0.41
1:A:1734:ASP:HB3	1:A:1737:THR:HG22	2.02	0.41
1:A:2060:ARG:HG3	1:A:2061:THR:HG23	2.03	0.41
1:A:3481:SER:HB2	1:A:3770:LEU:HD13	2.02	0.41
1:A:1746:GLN:HB2	1:A:1749:LEU:HD23	2.02	0.41
1:A:2226:SER:OG	3:A:4702:ATP:O2G	2.28	0.41
1:A:3158:ASN:ND2	1:A:3171:ILE:HG12	2.36	0.41
1:A:4171:LYS:HG2	1:A:4172:SER:N	2.36	0.40
1:A:1853:VAL:HA	1:A:1856:GLN:HG3	2.03	0.40
1:A:2269:ASP:HB2	1:A:2274:GLU:H	1.86	0.40
1:A:2783:ARG:HG2	1:A:2784:PHE:N	2.34	0.40
1:A:3518:GLY:O	1:A:3519:TYR:HB3	2.22	0.40
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.56	0.40
1:A:2595:GLY:O	1:A:2714:PRO:HD3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3750:LEU:O	1:A:3754:ASN:ND2	2.54	0.40
1:A:3833:LEU:HD23	1:A:3833:LEU:HA	1.89	0.40
1:A:2323:LYS:HB3	1:A:2335:LEU:HB3	2.03	0.40
1:A:2972:PHE:CE2	1:A:2976:LEU:HD11	2.56	0.40
1:A:3138:SER:HB3	1:A:3141:GLU:OE1	2.21	0.40
1:A:3872:ALA:HA	1:A:3875:MET:HB3	2.02	0.40
1:A:3912:ASN:O	1:A:3937:ARG:HD2	2.22	0.40
1:A:1347:LYS:HE3	1:A:1432:GLY:HA2	2.03	0.40
1:A:2231:SER:HA	1:A:2234:TRP:NE1	2.36	0.40
1:A:2505:ASP:HB3	1:A:2733:VAL:HG23	2.03	0.40
1:A:2644:THR:OG1	1:A:2645:PRO:HD3	2.21	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	2977/4646 (64%)	2896 (97%)	80 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4172	SER

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	2666/4125 (65%)	2664 (100%)	2 (0%)	92 97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1507	MET
1	A	2388	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1755	GLN
1	A	1784	ASN
1	A	2212	GLN
1	A	2588	HIS
1	A	2834	GLN
1	A	2930	GLN
1	A	3155	HIS
1	A	3602	ASN
1	A	4065	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	4703	-	28,33,33	0.65	0	34,52,52	0.61	1 (2%)
2	ADP	A	4701	-	24,29,29	0.87	0	29,45,45	1.25	2 (6%)
3	ATP	A	4702	-	28,33,33	0.68	0	34,52,52	0.59	1 (2%)
2	ADP	A	4704	-	24,29,29	0.88	0	29,45,45	1.28	3 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	4703	-	-	1/18/38/38	0/3/3/3
2	ADP	A	4701	-	-	3/12/32/32	0/3/3/3
3	ATP	A	4702	-	-	8/18/38/38	0/3/3/3
2	ADP	A	4704	-	-	5/12/32/32	0/3/3/3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4704	ADP	N3-C2-N1	-3.84	123.46	128.67
2	A	4701	ADP	N3-C2-N1	-3.69	123.67	128.67
2	A	4704	ADP	C4-C5-N7	-2.57	106.62	109.34
2	A	4701	ADP	C4-C5-N7	-2.56	106.64	109.34
3	A	4702	ATP	C5-C6-N6	2.30	123.82	120.31
3	A	4703	ATP	C5-C6-N6	2.29	123.81	120.31
2	A	4704	ADP	O4'-C1'-N9	2.09	111.52	108.75

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4701	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	A	4704	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A
3	A	4702	ATP	PB-O3B-PG-O3G
3	A	4702	ATP	C5'-O5'-PA-O1A
3	A	4702	ATP	C5'-O5'-PA-O2A
3	A	4702	ATP	C5'-O5'-PA-O3A
2	A	4704	ADP	O4'-C4'-C5'-O5'
2	A	4704	ADP	C3'-C4'-C5'-O5'
2	A	4701	ADP	C5'-O5'-PA-O1A
3	A	4702	ATP	PB-O3B-PG-O2G
3	A	4703	ATP	O4'-C4'-C5'-O5'
3	A	4702	ATP	PA-O3A-PB-O1B
3	A	4702	ATP	O4'-C4'-C5'-O5'
3	A	4702	ATP	PA-O3A-PB-O2B

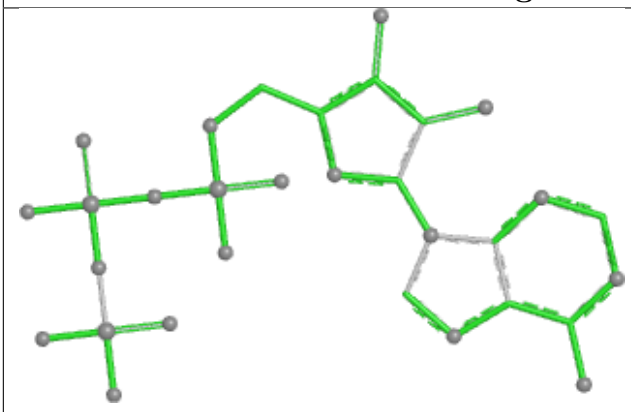
There are no ring outliers.

1 monomer is involved in 2 short contacts:

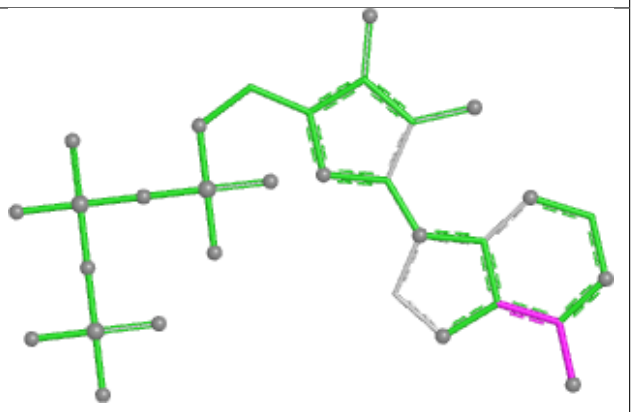
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4702	ATP	2	0

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.

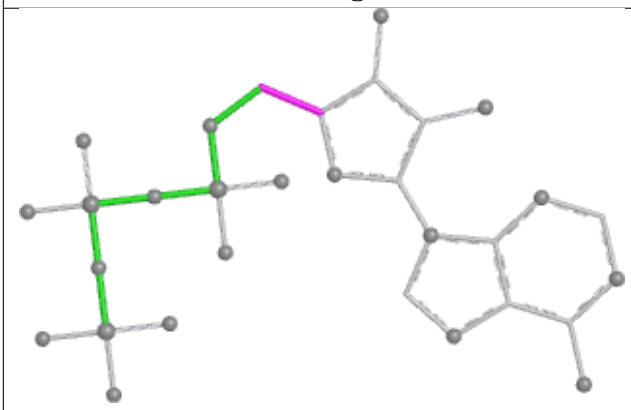
Ligand ATP A 4703



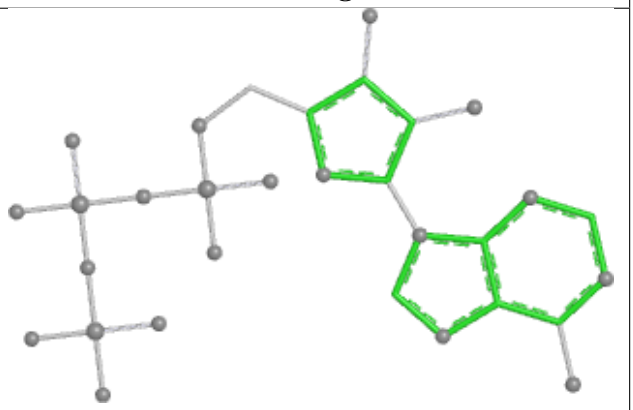
Bond lengths



Bond angles

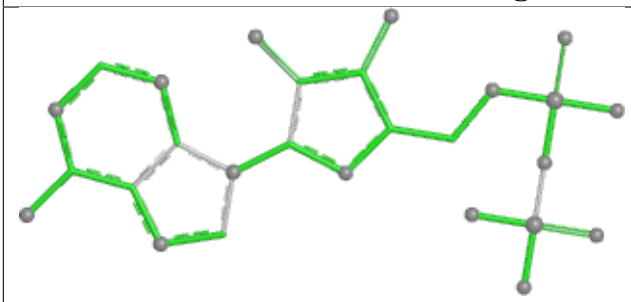


Torsions

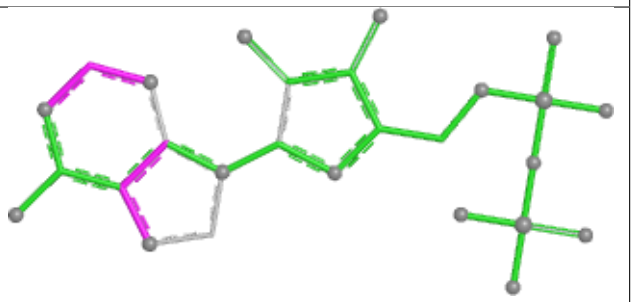


Rings

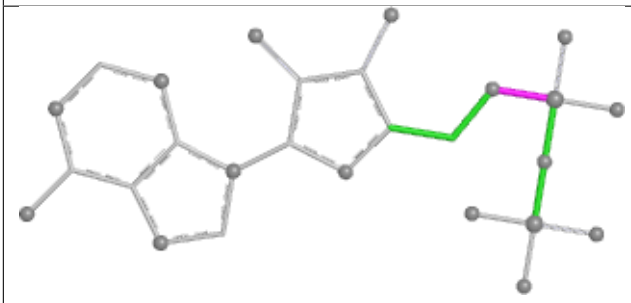
Ligand ADP A 4701



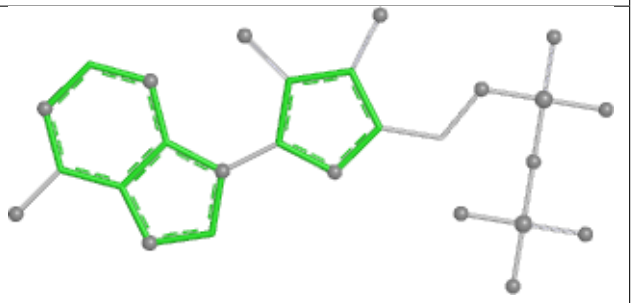
Bond lengths



Bond angles

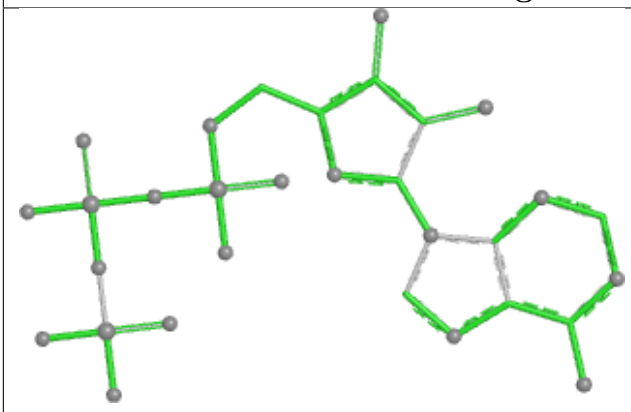


Torsions

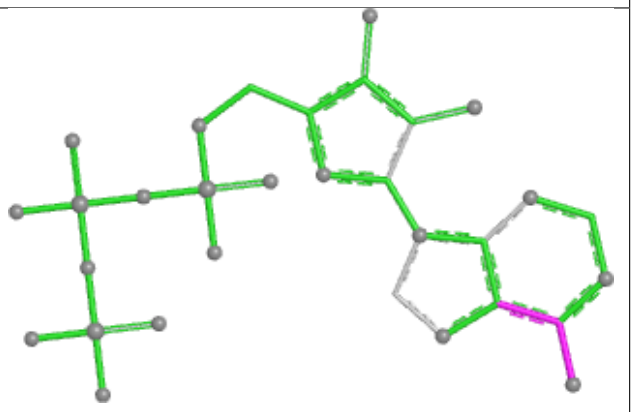


Rings

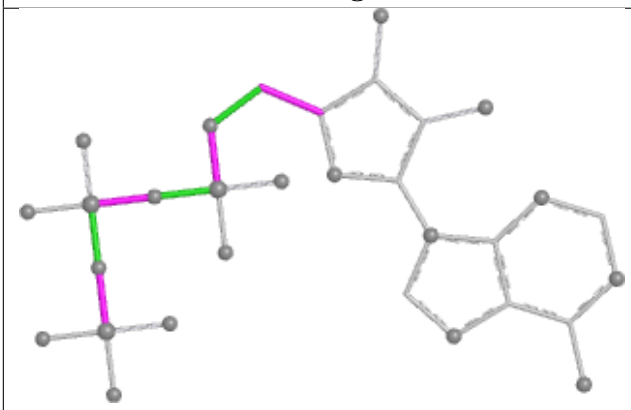
Ligand ATP A 4702



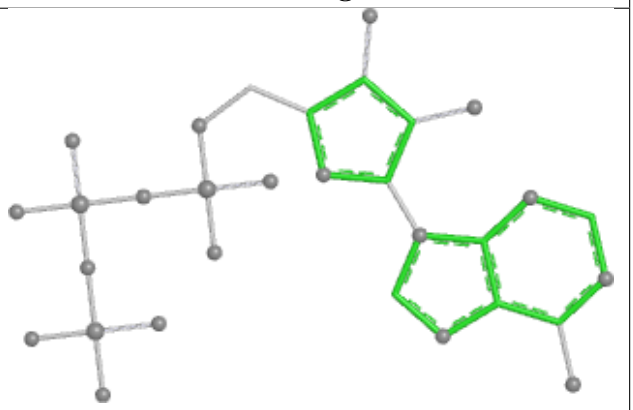
Bond lengths



Bond angles

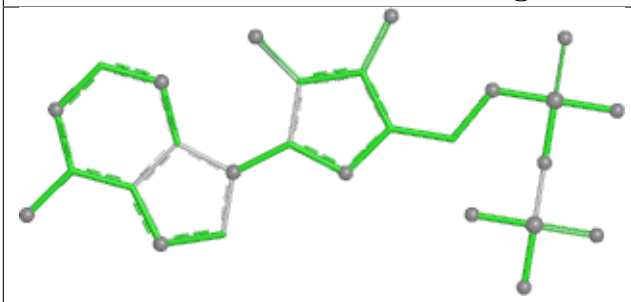


Torsions

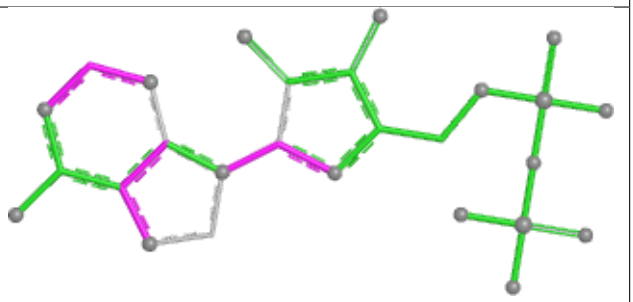


Rings

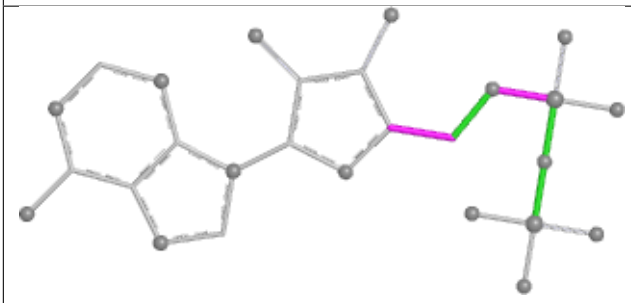
Ligand ADP A 4704



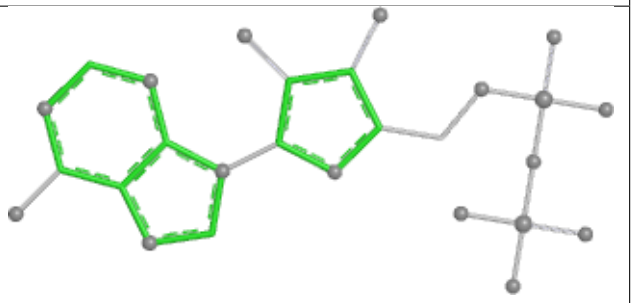
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

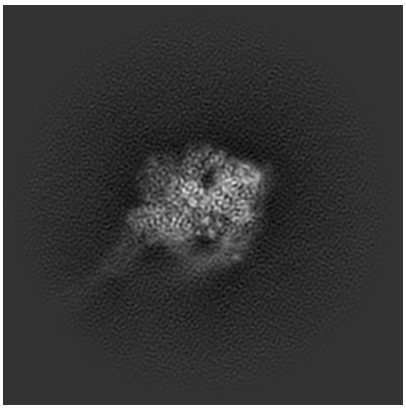
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44691. These allow visual inspection of the internal detail of the map and identification of artifacts.

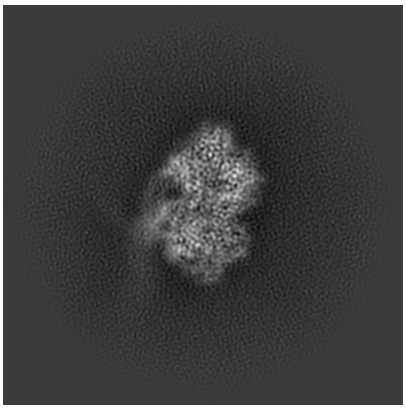
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

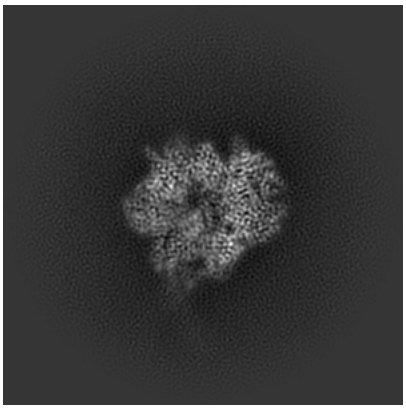
6.1.1 Primary map



X

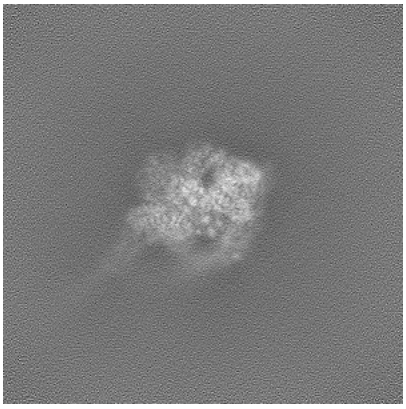


Y

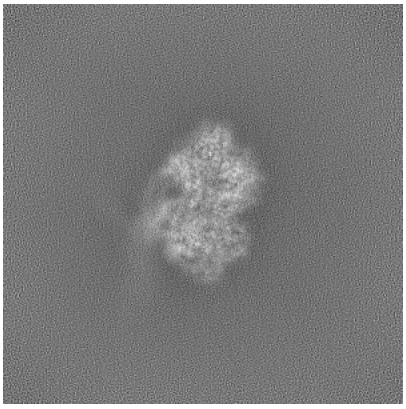


Z

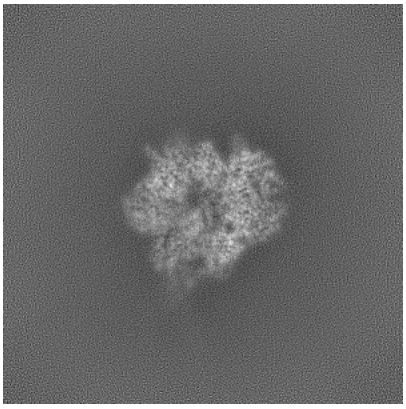
6.1.2 Raw map



X



Y

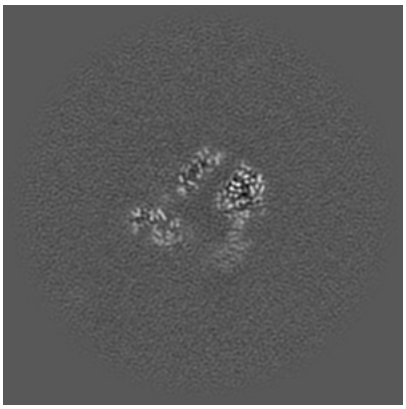


Z

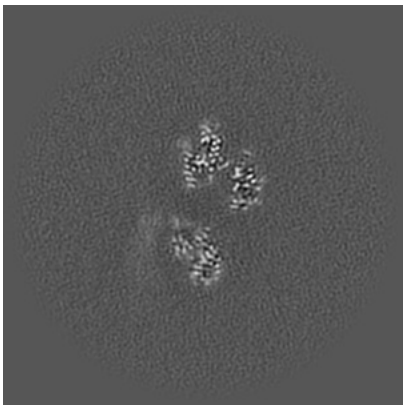
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

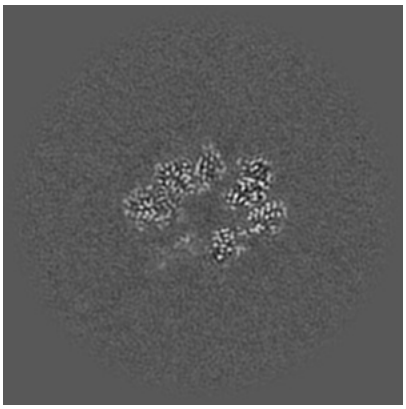
6.2.1 Primary map



X Index: 200

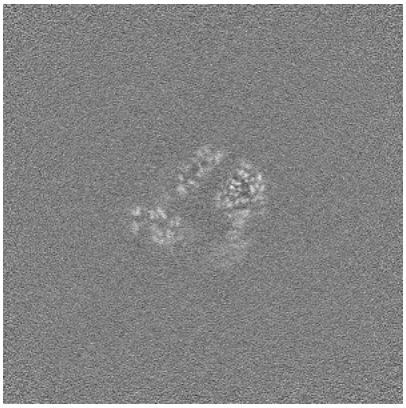


Y Index: 200

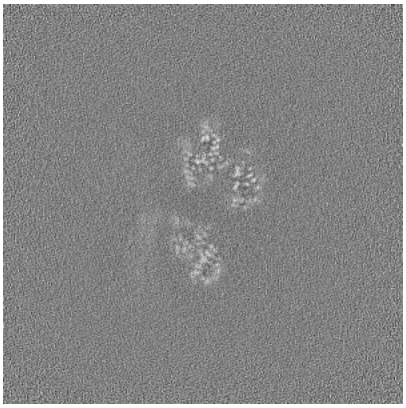


Z Index: 200

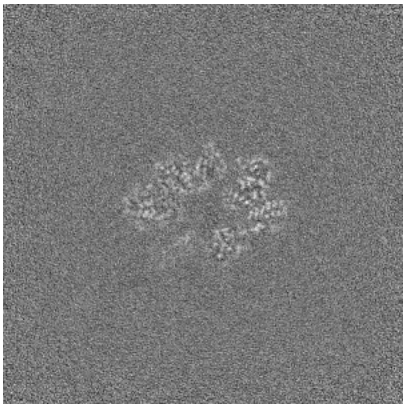
6.2.2 Raw map



X Index: 200



Y Index: 200

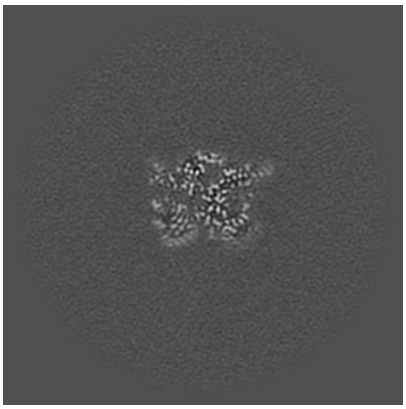


Z Index: 200

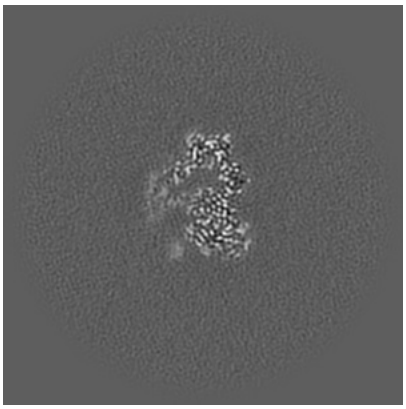
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

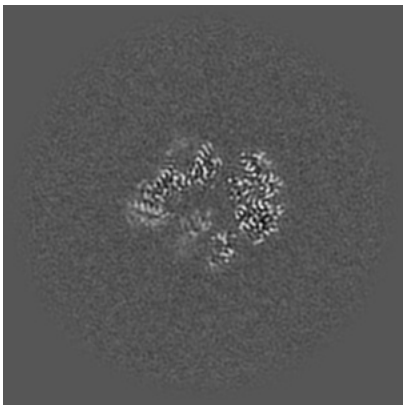
6.3.1 Primary map



X Index: 235

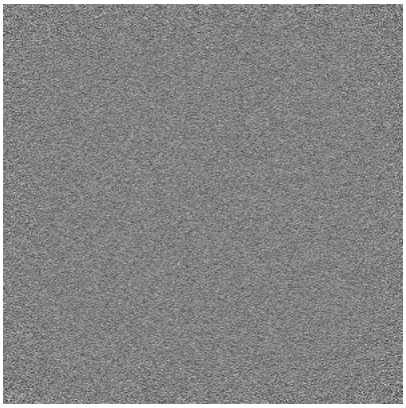


Y Index: 230

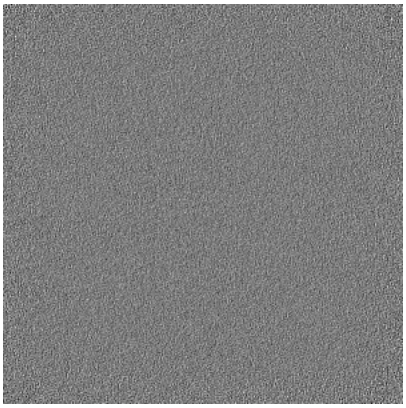


Z Index: 214

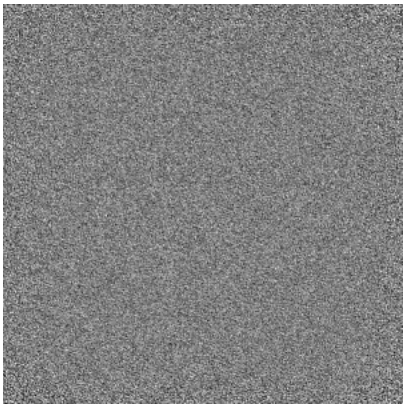
6.3.2 Raw map



X Index: 0



Y Index: 0

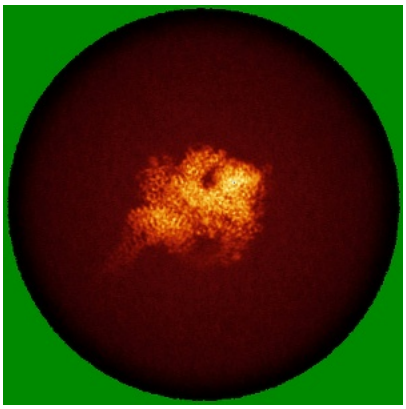


Z Index: 0

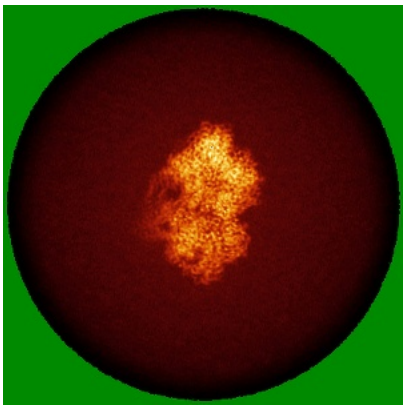
The images above show the largest variance slices of the map in three orthogonal directions.

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

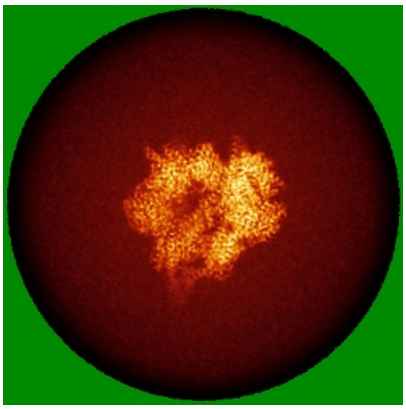
6.4.1 Primary map



X

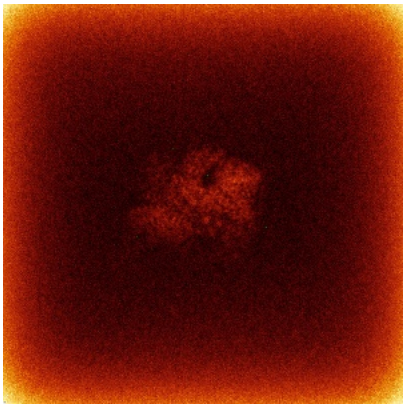


Y

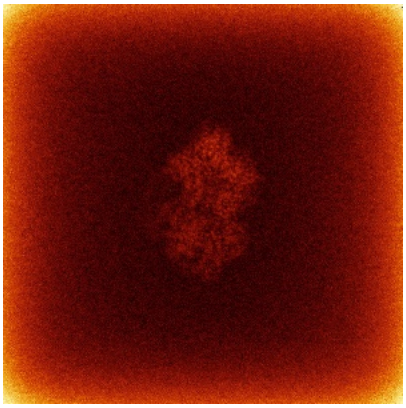


Z

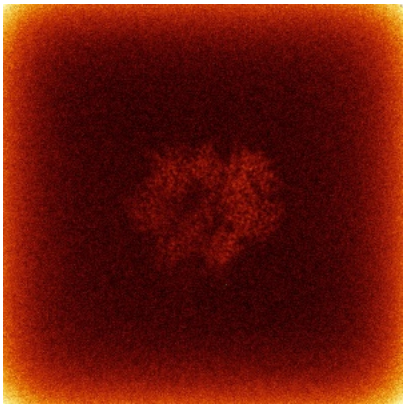
6.4.2 Raw map



X



Y

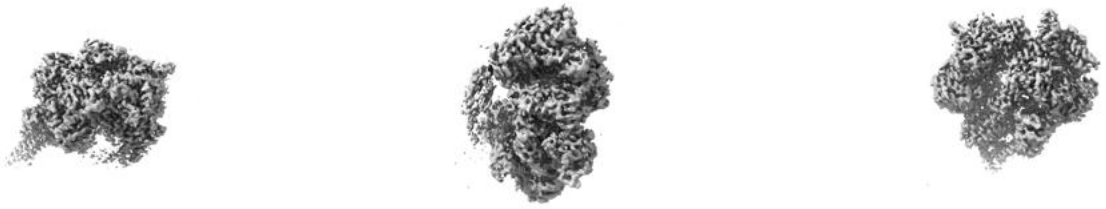


Z

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 0.12. 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.

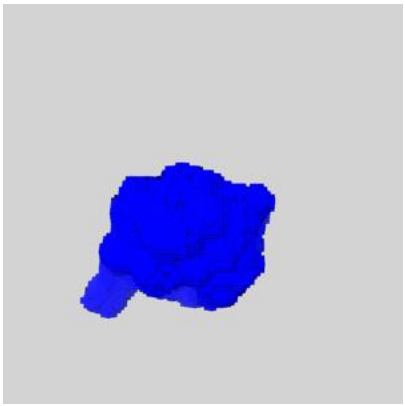
6.6 Mask visualisation

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

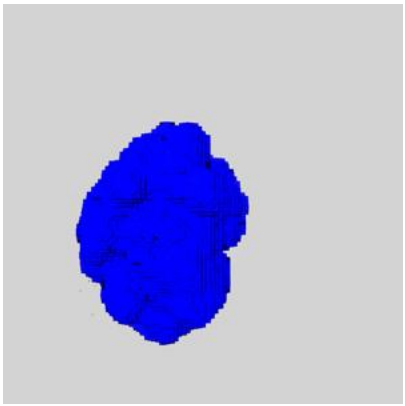
A mask typically either:

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

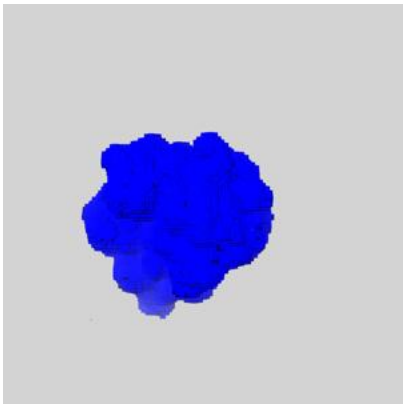
6.6.1 emd_44691_msk_1.map



X



Y

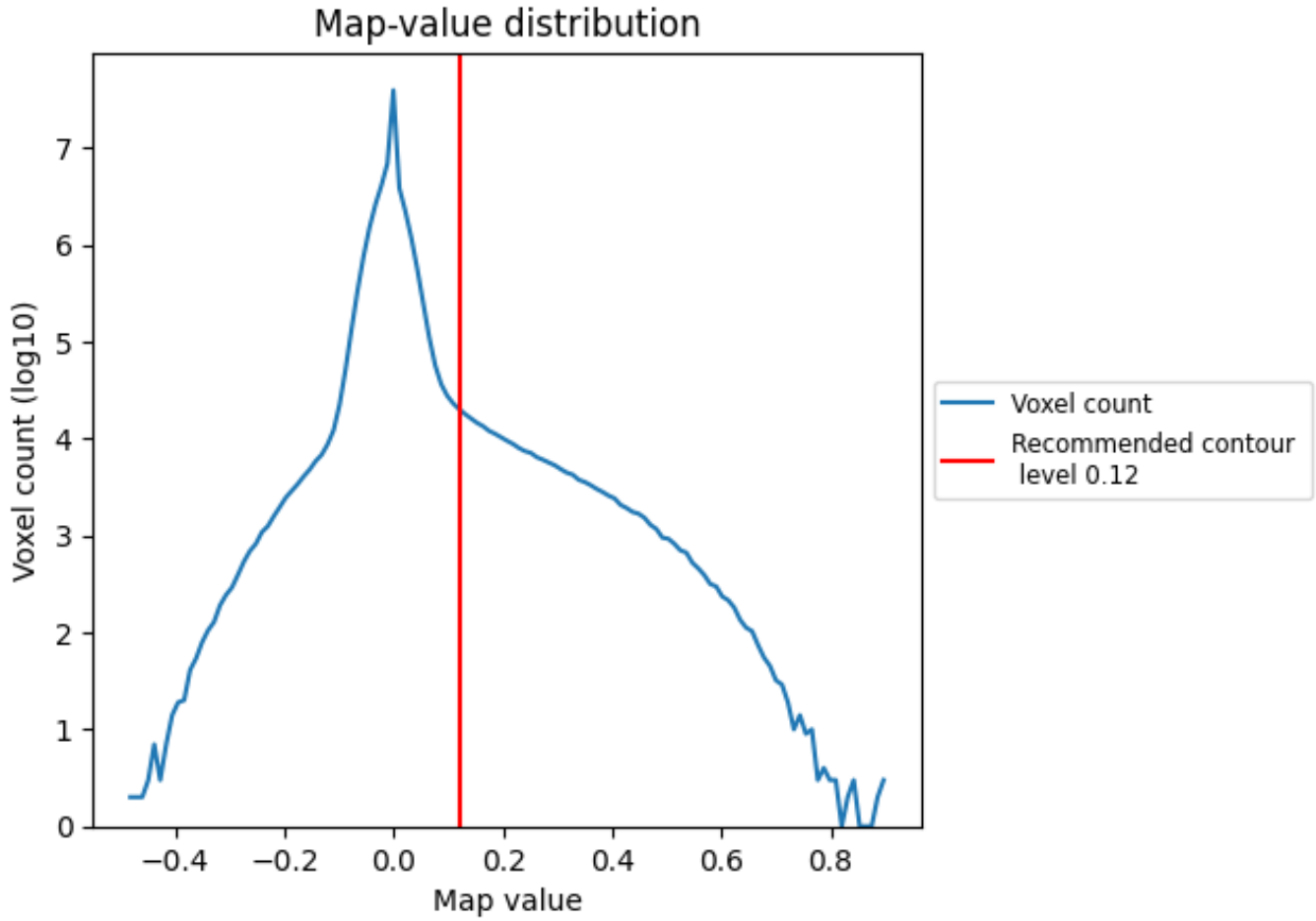


Z

7 Map analysis

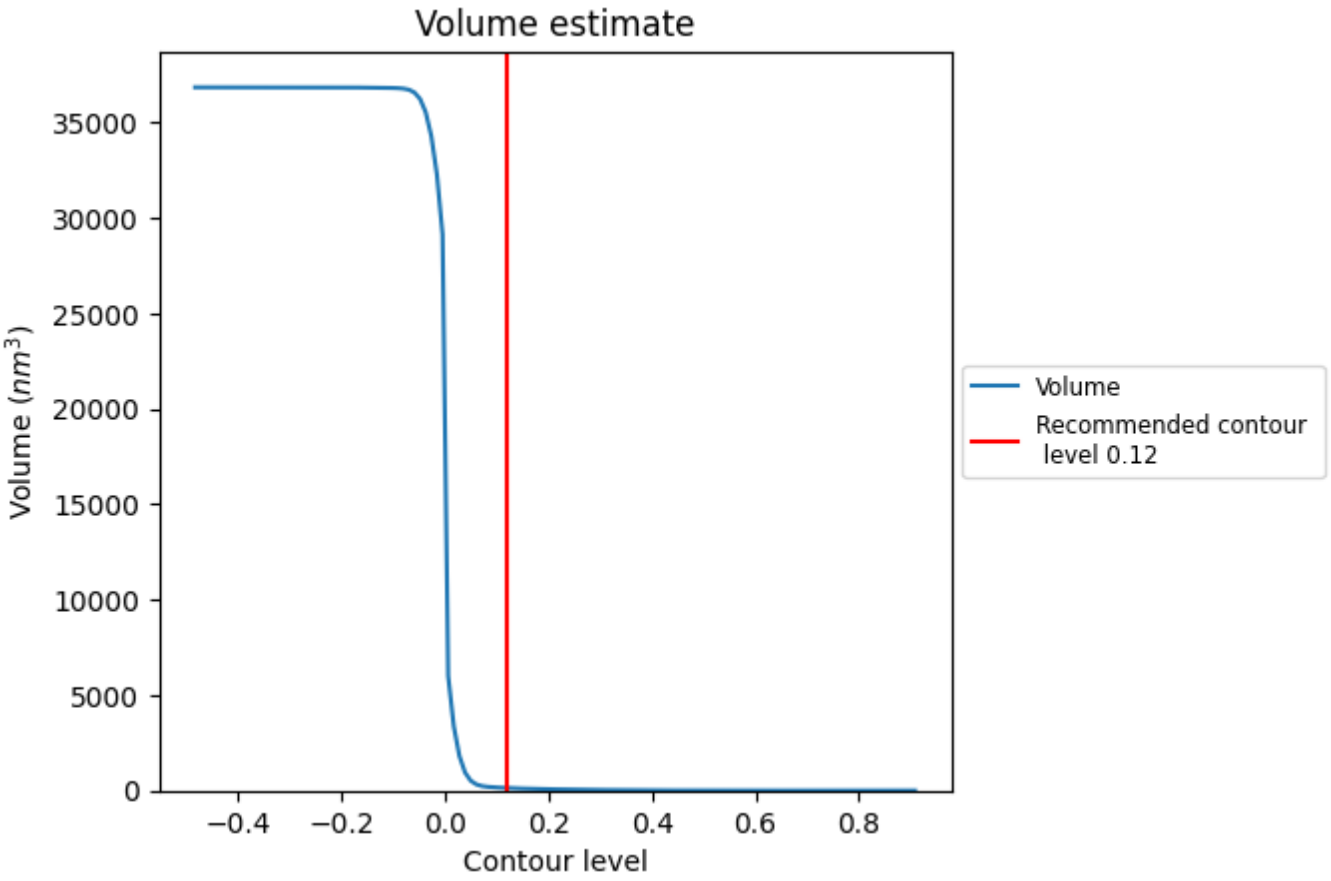
This section contains the results of statistical analysis of the map.

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.

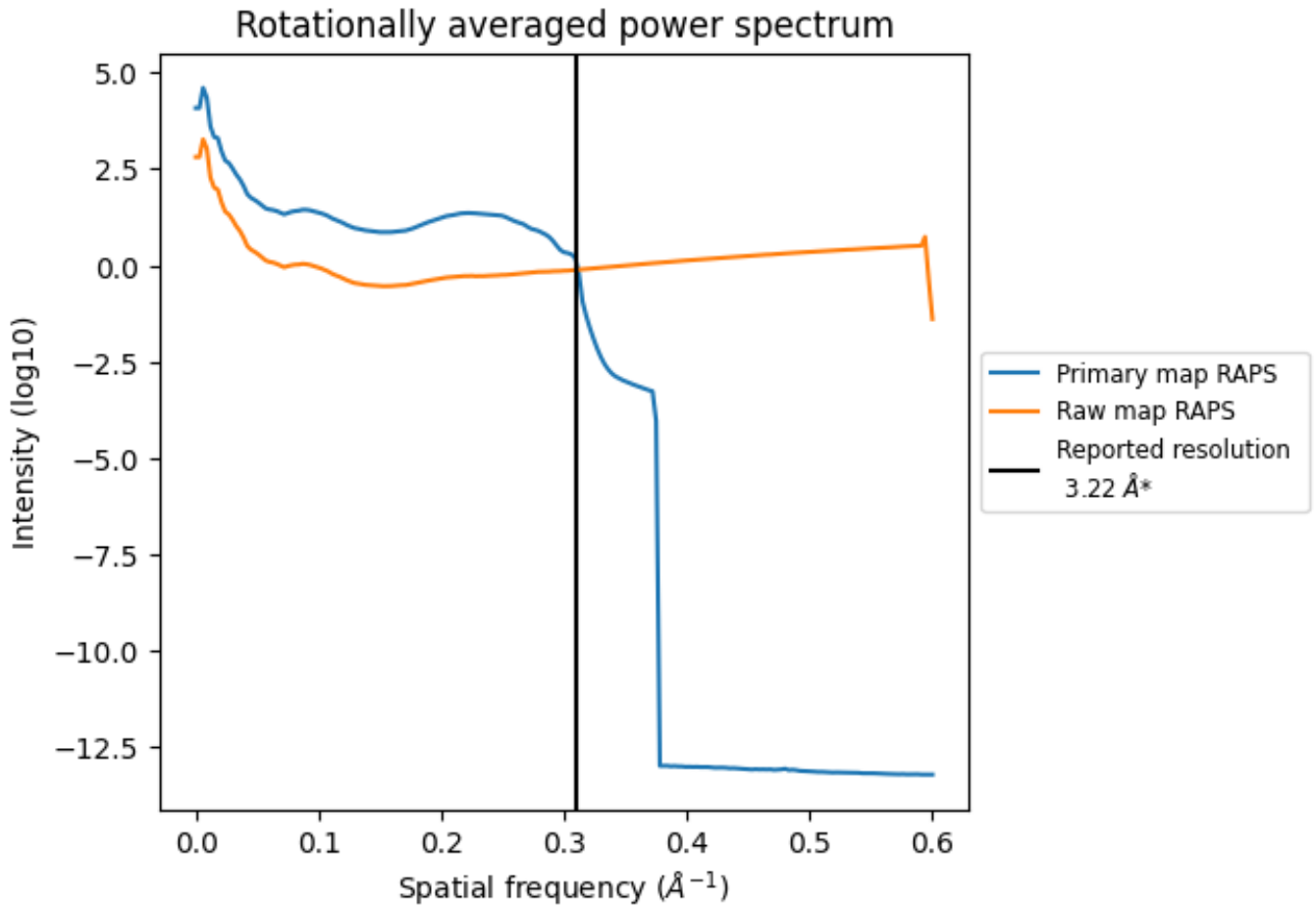
7.2 Volume estimate



The volume at the recommended contour level is 134 nm^3; this corresponds to an approximate mass of 121 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)

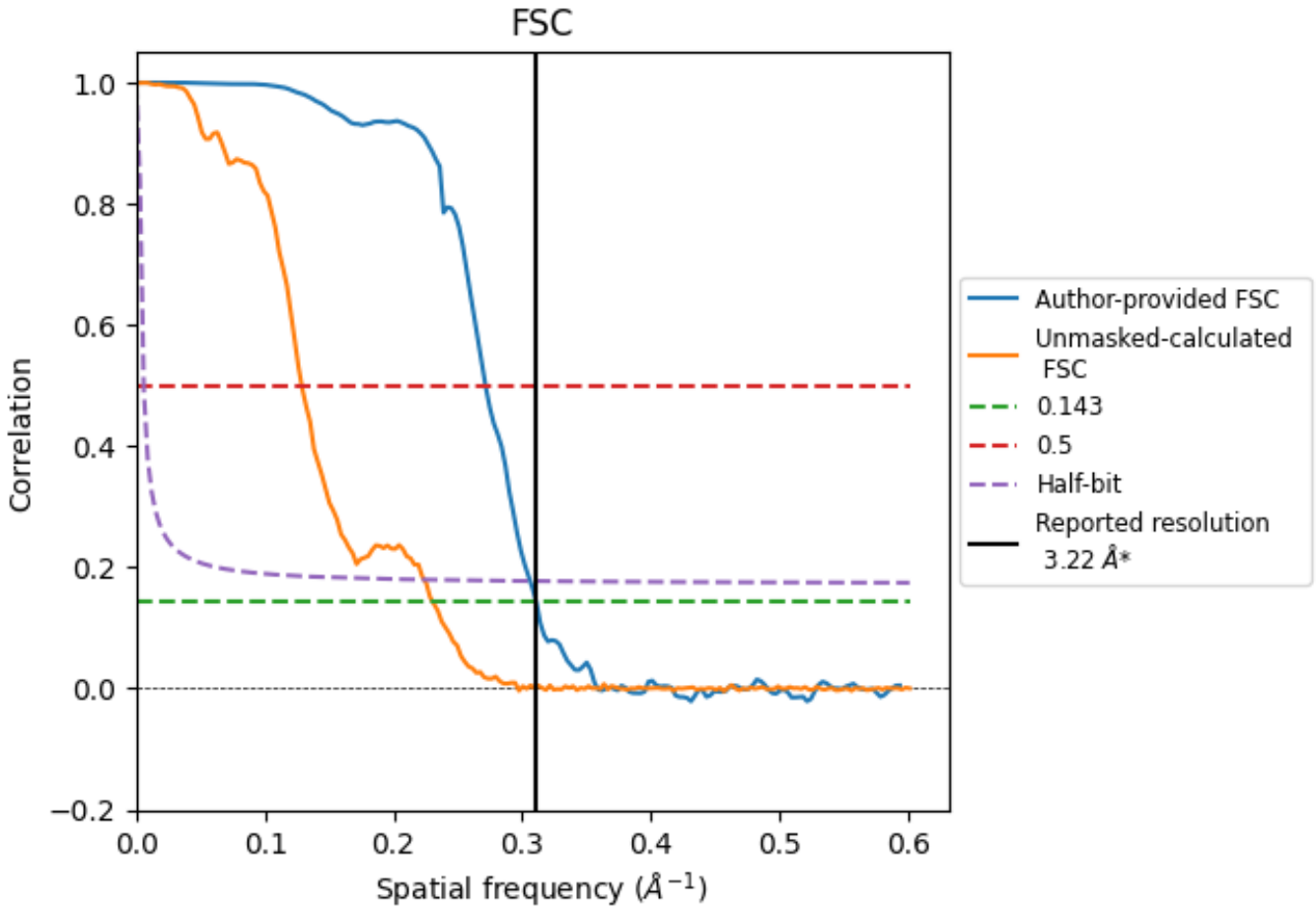


*Reported resolution corresponds to spatial frequency of 0.311 $Å^{-1}$

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 0.311 Å^{-1}

8.2 Resolution estimates (i)

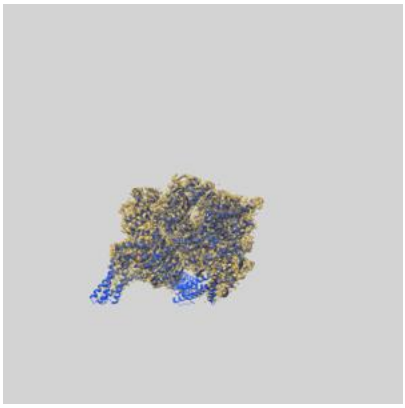
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.22	-	-
Author-provided FSC curve	3.22	3.68	3.27
Unmasked-calculated*	4.34	7.77	4.47

*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 4.34 differs from the reported value 3.22 by more than 10 %

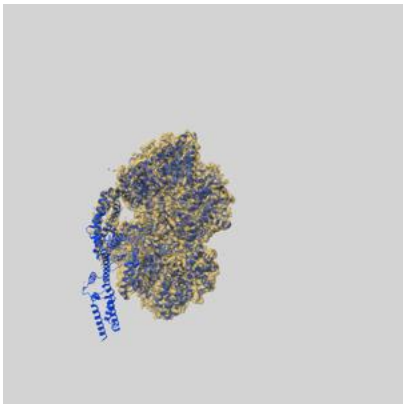
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44691 and PDB model 9BM8. Per-residue inclusion information can be found in section 3 on page 5.

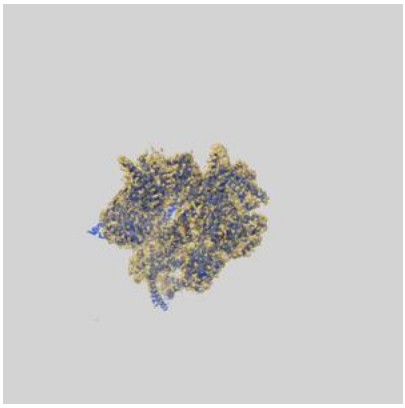
9.1 Map-model overlay



X



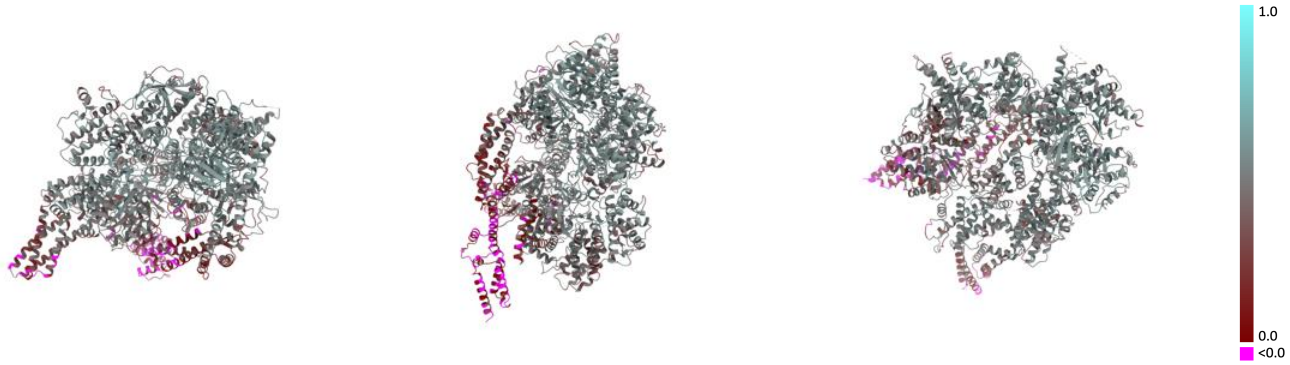
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

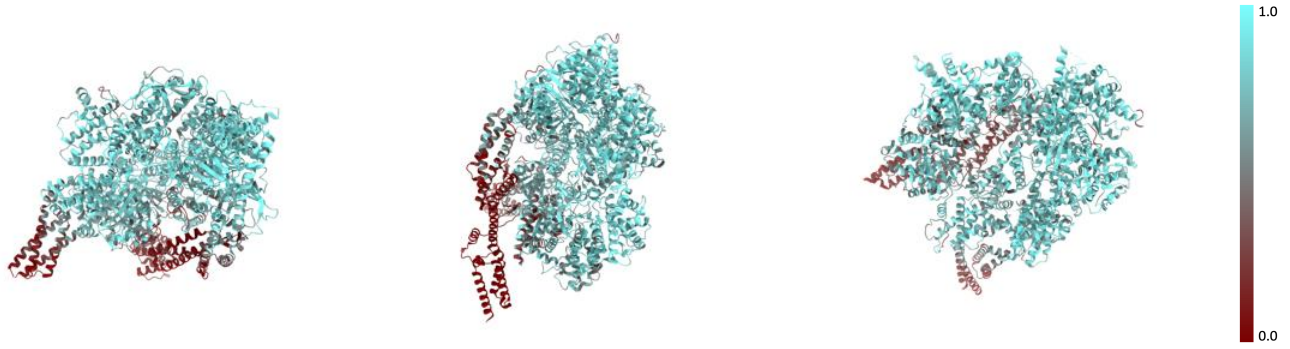
9.2 Q-score mapped to coordinate model (i)



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.

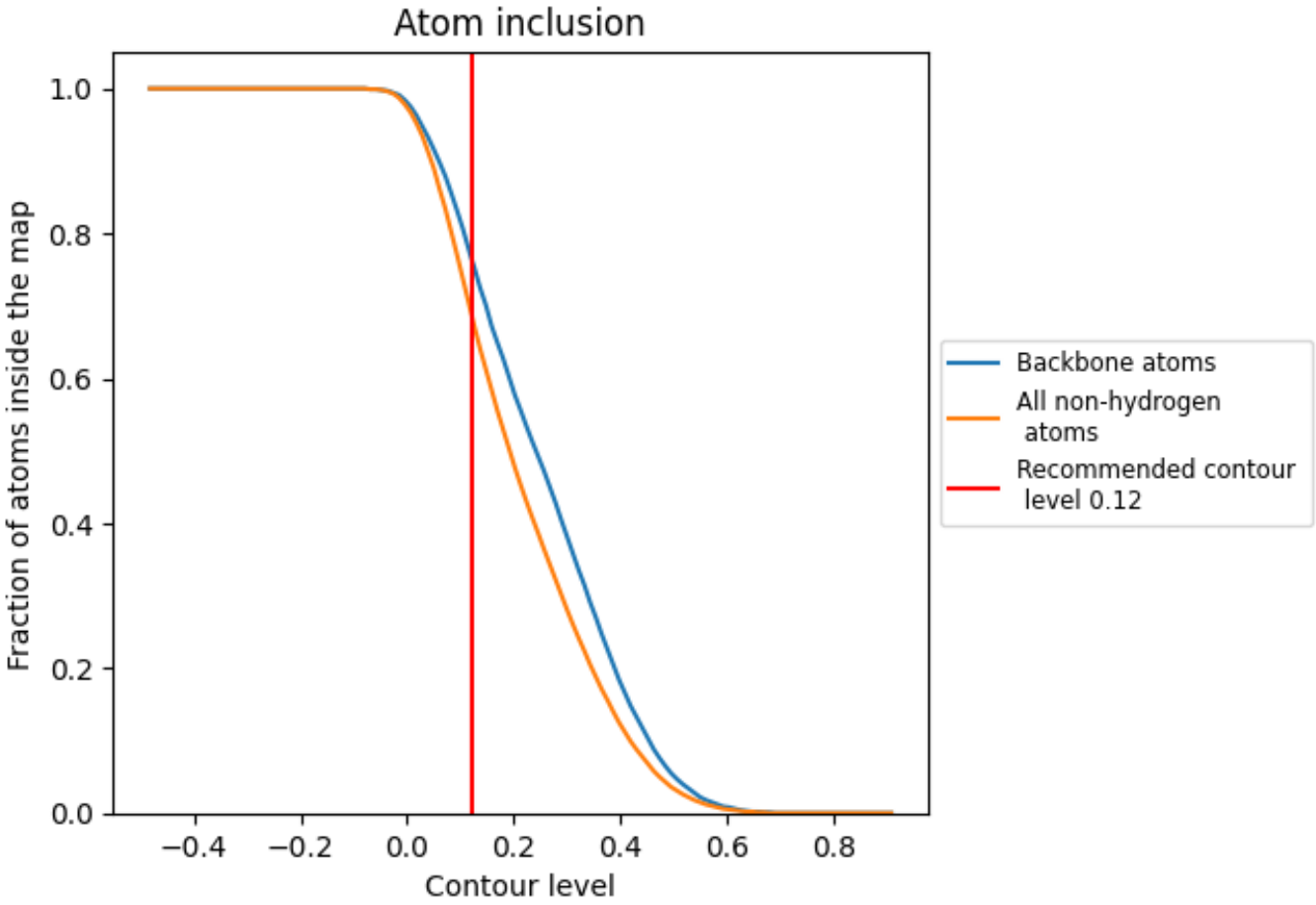
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6890	0.4340
A	0.6890	0.4340